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TECHNICAL SUPPORT DOCUMENT FOR SECTION 194.24:

EVALUATION OF THE COMPLIANCE RECERTIFICATION ACTINIDE SOURCE TERM AND CULEBRA DOLOMITE DISTRIBUTION COEFFICIENT VALUES

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ACRONYM LIST

AMWTF	Advanced Mixed Waste Treatment Facility
Brine A	Simulated Salado brine formulation
CAPMIC	Maximum actinide concentrations associated with mobile microbes
CAPHUM	Maximum actinide concentrations associated with mobile humic colloids
CCA	Compliance Certification Application
CPR	Cellulosics, plastics, and rubber
CRA	Compliance Recertification Application
DOE	Department of Energy
DOR	Direct oxide reduction
EDTA	Ethylenediaminetetraacetic acid
EEG	Environmental Evaluation Group
ERDA-6	Simulated Castile brine formulation
FMT	Fracture Matrix Transport
FMT_021120.CHEMDAT	Thermodynamic database used in the CRA PA
FMT_040628.CHEMDAT	Thermodynamic database used after the CRA PA
FMT_970407.CHEMDAT	Thermodynamic database used in the PAVT
GWB	Generic Weep Brine simulated Salado brine formulation
ISA	Isosaccharinic acid
K_d	Distribution coefficient
LANL	Los Alamos National Laboratory
m	molal, moles/kg solution
M	molar, moles/liter
PA	Performance assessment
PABC	Performance Assessment Baseline Calculations
PAVT	Performance Assessment Verification Testing
PHUMCIM	Proportionality constant for concentration of actinides associated with mobile humic colloids in Castile brine
PHUMSIM	Proportionality constant for concentration of actinides associated with mobile humic colloids in Salado brine
PROPMIC	Proportionality constant for concentration of actinides associated with mobile microbes
PVC	Polyvinylchloride
RPB	Revised Parameter Baseline
SEM	Scanning electron microscope
SNL	Sandia National Laboratories
STTP	Actinide Source-Term Waste Test Program
TDOP	Ten-drum overpack

ACRONYM LIST (continued)

TRU	Transuranic waste
US DOE	U.S. Department of Energy
US EPA	U.S. Environmental Protection Agency
WIPP	Waste Isolation Pilot Plant
XRD	X-ray diffraction

EXECUTIVE SUMMARY AND REPORT OUTLINE

The U.S. Department of Energy (DOE) operates the Waste Isolation Pilot Plant (WIPP) for the disposal of transuranic (TRU) defense-related waste. DOE submitted the first Compliance Recertification Application (CRA) to the U.S. Environmental Protection Agency (the Agency) in March 2004 (US DOE 2004b). This report summarizes the Agency's review of chemistry-related issues important to actinide source term modeling and actinide transport in the Culebra for the WIPP CRA. The principal documents included in this review were, CRA Appendix PA Attachment SOTERM and the references cited by this attachment, portions of CRA Appendix BARRIERS and its supporting references, and portions of CRA Appendix TRU WASTE and its supporting references (US DOE 2004b). Additional information has been obtained from the U.S. Department of Energy's (DOE's) responses to requests for additional information and from reports describing previous reviews of chemistry-related issues carried out by the Agency and its contractors since the CCA. As a result of this review EPA directed DOE to change many parameters related to chemistry (EPA 2005b, see Docket A-98-49 Item II-B2-25). DOE implemented these changes in a new performance assessment, called the Performance Assessment Baseline Calculation or PABC. EPA reviewed these changes (EPA 2006, see Docket A-98-49 Item II-B1-16) and found that DOE adequately implemented then in the PABC.

Section 1.0 provides a brief introduction to the WIPP and the CRA. Summaries of the issues reviewed in the report and the resulting conclusions are also provided.

In Section 2.0, the Fracture Matrix Transport (FMT) geochemical modeling code and its associated database were reviewed for changes since the Compliance Certification Application (CCA) and Performance Assessment Verification Testing (PAVT). No revisions were made to the FMT code or conceptual models for the CRA performance assessment (PA). However, revisions were made to the FMT database since the PAVT. These changes included the addition of new aqueous actinide species to the database and revisions to existing species data because of the availability of new experimental data. The Agency reviewed these changes and found that they are technically adequate and appropriately documented.

In actinide solubility calculations for the CRA PA and PABC, DOE used the GWB Salado brine chemistry formulation instead of the Brine A formulation used in the CCA PA and PAVT (Section 3.0). The most significant differences between the brine formulations are the lower magnesium concentration and higher sulfate concentration in GWB relative to Brine A. Comparison of geochemical modeling results using the two brine formulations indicates that GWB brines had slightly lower predicted +III actinide solubilities and higher +V actinide solubilities compared to Brine A. The formulation of GWB appears to have been adequately documented by Snider (2003d). Because GWB is reported to more closely match the composition of Salado intergranular brines, use of this brine in place of Brine A for the CRA PA and PABC actinide solubility calculations is appropriate.

Section 4.0 addresses the effects of microbial activity on repository chemistry, including microbial gas generation, the production of organic compounds that form aqueous actinide complexes, and the mobilization of radionuclides by colloidal microbes. New data have become available since the CCA regarding microbial degradation rates, reaction pathways, and degradation products. Available data from the microbial degradation experiments indicate that the assumed probability of significant microbial degradation of cellulosics, plastics, and rubber (CPR) may have been too low in the CCA PA, PAVT, and CRA PA. The experimental results indicate that microbial degradation of CPR is highly likely under many conditions, and the probability of microbial degradation used in PA should be 1, this change was included in the PABC. The microbial gas generation rates used in BRAGFLO for both the CCA PA and the CRA PA appear to provide appropriate upper bounds. However, these relatively high rates were based on initial data from the microbial degradation experiments, and combined with a higher probability of microbial degradation of CPR, may overestimate gas generation rates. Use of initially rapid rates followed by much slower degradation rates is likely to provide a more accurate representation of microbial degradation of CPR in the WIPP repository, this changes was also included in the PABC.

Because of the presence of sulfate in brines, in the Salado Formation anhydrite interbeds, and dispersed in Salado Formation halite, sufficient sulfate may be available for all CPR in the repository to degrade via denitrification or sulfate reduction. Therefore, for the purposes of calculating the amounts of MgO backfill, DOE should assume that all carbon in CPR could potentially be converted to carbon dioxide. Data from the microbial degradation experiments indicate that ligands such as acetate and lactate may form during microbial degradation of cellulosic materials and persist in solution. However calculations carried out to test the sensitivity of actinide solubilities to ligands concentrations indicate that microbially produced acetate and lactate are unlikely to significantly affect actinide solubilities in the repository.

Section 5.0 provides a review of data regarding the efficacy of the MgO backfill for controlling pH and carbon dioxide concentrations in the repository to maintain relatively low actinide solubilities in WIPP brines. Section 5.0 also provides a review of calculations of the MgO quantities required to maintain the appropriate chemical conditions in the repository. The MgO hydration and carbonation reactions used in the CRA actinide solubility calculations are consistent with data developed since the CCA. MgO will react to form brucite [$Mg(OH)_2(s)$] and possibly $Mg_2Cl(OH)_3 \bullet 4H_2O$. MgO and brucite will react with carbon dioxide to produce hydroxymagnesite$_{5424}$ [$Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O(s)$], and DOE appropriately used hydromagnesite$_{5424}$ as the magnesium-carbonate phase most likely to form in the repository and control carbon dioxide fugacities.

However, for the CRA PA, DOE assumed that methanogenesis will be the dominant reaction for microbial degradation of CPR, which cannot be proven because of the presence of abundant sulfate in the brine, halites, and Salado interbeds. DOE removed the methanogenesis assumption from the PABC. DOE also did not adequately account for the effects of heterogeneous waste loading on the MgO safety factor, made a mistaken assumption that ten drum overpacks (TDOPs) occupy the space of three 55-gallon drum seven packs instead of two, and omitted external packaging materials such as shrink wrap and support sheets from the CPR inventory used for the safety factor calculations. The PABC included packaging materials. DOE subsequently proposed a new approach for calculating and tracking the amounts of MgO backfill and CPR placed in WIPP to ensure that the required MgO safety factor of 1.67 is maintained on a room-by-room basis (US DOE 2004f).

In Section 6.0, the actinide oxidation states used for solubility modeling are reviewed. The same actinide oxidation states were assumed for the CRA PA as for the CCA PA and the PAVT. However, new data have become available since approval of the CCA, and questions have been raised regarding the assumption that plutonium will be present in the long-term WIPP repository brines in the (III) or (IV) oxidation states. The new data included results from Source-Term Waste Test Program (STTP) experiments that indicated the presence of plutonium(V) and plutonium(VI) in samples from a few experiments and literature reports of the formation of $PuO_{2+x}(s)$, which could increase plutonium concentrations in repository brines. The actinide oxidation states assumed by DOE in both the CCA PA and the CRA PA continue to be appropriate. Evidence that supports the selected actinide oxidation states includes: 1) the maintenance of reducing conditions by microbial degradation of CPR and anoxic corrosion of iron-based metal in the repository, 2) the results of the STTP experiments are not applicable to WIPP, and 3) other available experimental evidence indicating that plutonium(III) and plutonium(IV) will be the stable oxidation states in the equilibrium WIPP repository. Formation of $PuO_{2+x}(s)$ has not been observed under the reducing conditions expected in the WIPP repository, so this phase does not appear likely to control plutonium solubilities in the equilibrium repository.

Section 7.0 examines the assumption of homogeneity used in actinide solubility modeling. This assumption was evaluated because of the heterogeneous loading of waste observed in Panel 1 of the WIPP repository and because use of the Option D panel closure makes it less likely that brine in contact with waste in one panel of the repository will contact brine in another panel. However, because of the assumption of chemical equilibrium, heterogeneous distribution of the radionuclide inventory between the panels will not affect the calculated actinide solubilities. DOE appears to have made assumptions that adequately account for the effects of heterogeneous distribution of organic ligands between panels in the actinide solubility calculations, if the inventory of organic ligands in the repository is adequately bounded.

Section 8.0 addresses assumptions related to actinide solubility modeling calculations and reviews the modeling results. DOE's assumption that temperature effects will not significantly affect actinide solubilities is reasonable, provided wastes with heat-generating potential are not included in the WIPP inventory in quantities inconsistent with assumptions included in the CCA. For nonmicrobial PA vectors, DOE assumed that the brucite-calcite reaction will control carbon dioxide fugacities and that microbial colloid transport would not occur. Because of the increased probability of microbial degradation of CPR, DOE should assume control of carbon dioxide fugacity by the brucite-hydromagnesite$_{5424}$ reaction and that microbial colloid transport will occur in all PA vectors. DOE incorporated this change in the PABC.

DOE used uncertainties developed using the CCA thermodynamic database in actinide solubility calculations for the CRA PA; however, because of revisions to the thermodynamic database for the CRA, DOE has re-evaluated the actinide solubility uncertainties. These revised uncertainties should be used in PA calculations of the +III, +IV, and +V actinide solubilities. DOE did not consider all potentially relevant information that has been developed since the CCA to determine if the uranium(VI) concentration used in the CRA PA was still defensible and whether a uranium(VI) solubility model can be developed from the available data. Evaluation of the available data indicates that higher uranium(VI) concentrations should be used in PA. This review also indicated the need for additional experiments and model development efforts to determine appropriate uranium(VI) concentrations. DOE performed sensitivity calculations to determine whether organic ligand concentrations caused by uncertainties in the waste inventory or production of ligands during microbial degradation of CPR could significantly affect actinide solubilities. The results of this review indicated that some organic ligands have the potential to significantly affect actinide solubilities. Ligands such as acetate and lactate may form during microbial degradation of cellulosic materials and persist in solution; DOE performed a series of calculations to demonstrate that actinide solubilities are unlikely to be significantly affected by the production of ligands by microbial degradation of CPR. However, organic ligands were included in the CRA PA. DOE was also directed to update solubility uncertainty and to use a conservative value for the uranium(VI) solubility, 10^{-3} M, in the PABC.

In Section 9.0, the actinides that were included in the PA calculations and DOE's explanation for the selection of these actinides are evaluated. The Agency evaluated the potential importance of neptunium on PA (US EPA 2005), because of its potentially high solubility in the presence of organic ligands. The results of these calculations indicated that neptunium-237 would not contribute significantly to potential releases, and that its omission from the CRA PA was acceptable.

Section 10.0 provides a review of the changes DOE made to the distribution coefficients (K_ds) used in the calculation of actinide transport through the Culebra. No new experimental data are available for the actinide K_ds. DOE has used the lognormal distribution assumed by the Agency for the PAVT and corrected minor errors in the K_d values, which has resulted in more conservative (lower) values being used in the CRA PA. Because the changes to the K_d ranges are minor and conservative and these results have been previously reviewed by the Agency (US EPA 1998b), the values used in the CRA PA and the PABC are acceptable.

Section 11.0 summarizes the Agency's conclusions based on their review of chemistry-related CRA issues.

1.0 INTRODUCTION

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, is an underground facility designed for the permanent disposal of transuranic (TRU) defense-related waste. WIPP is located approximately 2,000 feet below ground in rooms mined within the Salado Formation, which is primarily composed of halite (NaCl) layers with interbedded anhydrite ($CaSO_4$). The U.S. Department of Energy (DOE) operates the WIPP repository under the oversight of the U.S. Environmental Protection Agency (the Agency). DOE submitted the Compliance Certification Application (CCA) to the Agency in 1996. After extensive review of the CCA and supplemental information provided by DOE, including performance assessment (PA) calculations referred to as Performance Assessment Verification Testing (PAVT), the Agency certified that DOE had met the regulatory requirements and WIPP began accepting waste in March 1999.

DOE is required to submit a Compliance Recertification Application (CRA) every 5 years after the initial receipt of waste at WIPP, and the first CRA was submitted to the Agency in March 2004 (US DOE 2004b). Waste characteristics and waste components must be analyzed and the results must be included in any certification application [40 CFR 194.24(b)] and those waste characteristics and components that could affect releases must be incorporated into performance assessment [40 CFR 194.32(a)]. All additional data collected since the most recent CCA or CRA must be included in the CRA [40 CFR 194.15(a)], including any geochemical information, analyses, or results of laboratory experiments that are relevant to the performance of the repository.

This report summarizes EPA’s review of chemistry-related issues important to actinide source term modeling and actinide transport in the Culebra Dolomite above the repository for the WIPP CRA PA. The principal documents included in this review were CRA Appendix PA Attachment SOTERM (US DOE 2004b) and the supporting references cited by this attachment, portions of CRA Appendix BARRIERS (US DOE 2004b) and its supporting references, and portions of CRA Appendix TRU WASTE (US DOE 2004b) and its supporting references. Additional information has been obtained from DOE’s responses to requests by the Agency for additional information and from the results of reviews of chemistry-related issues carried out by the Agency since the CCA.

As a result of the Agency’s review EPA directed DOE to change many parameters related to chemistry (EPA 2005b, see Docket A-98-49 Item II-B2-25). DOE implemented these changes in a new performance assessment, call the Performance Assessment Baseline Calculation or PABC. EPA reviewed these changes (EPA 2006, see Docket A-98-49 Item II-B1-16) and found that DOE adequately implemented then in the PABC.

Chemistry-related issues addressed in this report include the FMT geochemical modeling code and thermodynamic database used to model actinide solubilities (Section 2.0); changes in the Salado Formation brine chemistry used in actinide solubility calculations (Section 3.0); information related to microbial degradation of cellulosics, plastics and rubber (CPR) in the repository (Section 4.0); the ability of the MgO backfill to control chemical conditions (Section 5.0); actinide oxidation states assumed in source term modeling (Section 6.0); the effects of heterogeneous waste loading on chemical conditions in the repository (Section 7.0); a review of the actinide source term modeling calculations (Section 8.0); an assessment of the actinides included in PA (Section 9.0); and a review of changes to the distribution coefficients (K_ds) used in PA to model the release of actinides by transport through the Culebra member of the Rustler Formation (Section 10.0).

Results of this review indicate that although DOE adequately accounted for new information related to many chemistry-related issues in the CRA PA (US DOE 2004b), a number of chemistry-related issues required additional information or changes to the PA. These issues included: the need for a higher assumed probability of significant microbial degradation of CPR, lack of accounting for heterogeneous waste loading in calculations of the required amounts of MgO to maintain appropriate chemical conditions in the repository, DOE's assumption that methanogenesis would be the major pathway for microbial degradation of CPR despite the presence of abundant sulfate, lack of support for the assumption that the brucite-calcite reaction would control carbon dioxide fugacities in nonmicrobial vectors, inadequate information supporting the assumption that microbial colloid transport of actinides will not occur in the absence of significant microbial degradation of CPR, the need for recalculation of actinide solubility uncertainties used in PA, unresolved questions regarding the causes of differences in actinide solubilities calculated for the PAVT and CRA PA, questions regarding the sensitivity of actinide solubilities to organic ligand inventories, and whether DOE should develop a uranium(VI) solubility model or otherwise revise the uranium(VI) concentrations used in PA. DOE has provided responses to these issues, and the results of the review are incorporated in the new PABC.

2.0 FMT CODE AND DATABASE CHANGES

The Fracture Matrix Transport (FMT) code was used to model actinide solubilities in WIPP brines for the CCA PA, the PAVT, and the CRA PA. The FMT code was also used to model actinide solubilities for the revised CRA PA, also referred to as the Performance Assessment Baseline Calculation (PABC). The FMT code is used to calculate aqueous concentrations in WIPP brines based on aqueous speciation and solubility equilibria using the Pitzer activity coefficient model. The FMT model does not include reactions representative of redox processes, so the oxidation state of each actinide must be assumed for the calculations (Section 6.0).

FMT Version 2.4 was used for the CRA PA (Brush and Xiong 2003b). No revisions were made to the FMT code or conceptual models for the CRA PA, because the Agency accepted the conceptual models used in the CCA PA, and additional studies carried out since the CCA PA and the PAVT did not imply the need to make any revisions (Brush and Xiong 2003b). However, revisions were made to the FMT database since the PAVT. The FMT database used for the CRA PA was FMT_021120.CHEMDAT (CRA Appendix PA Attachment SOTERM-3.3). Changes to the FMT database since the PAVT are documented in Giambalvo (2002a, 2002b, 2002c, 2002d, 2002e, 2003), and these changes are reviewed below.

2.1 Sources of New Data

For the aqueous species, the main new sources of thermodynamic data were Fanghänel et al. (1999), Könnecke et al. (1997), Novak et al. (1997) and Al Mahamid et al. (1998). For the organic species, the main sources of updated parameter values were Choppin et al. (2001) and related documents that discuss data derived from the same experimental data. Most of the thermodynamic data used to update the FMT database relating to organic species are found in Tables 43 through 45 of Choppin et al. (2001). The experimental data that were used to derive the new thermodynamic data are presented in Tables 1 through 42. Some of the data listed in Tables 43 and 44 of Choppin et al. (2001) are based on earlier work, and so are not new experimental data.

2.2 Actinide Data Included in the Database

The thermodynamic database contains information for three actinide oxidation states, americium(III), thorium(IV), and neptunium(V), which are used as analogues to calculate the solubilities of the other actinide oxidation states, i.e., plutonium(III) and (IV), curium(III), neptunium (IV) and uranium(IV) (Section 6.0). A solubility model has not been developed for the (VI) actinides (Section 8.2), so data for this actinide oxidation state are not included in the thermodynamic database.

2.2.1 Americium(III) Data

Updated data for the speciation and solubility model for actinides in the +III oxidation state are derived essentially from americium(III) data, the exception being two hydrolysis constants and related Pitzer parameters. Aqueous americium(III) species included in the revised thermodynamic database were americium(III) hydrolysis species, the first two hydrolysis constants being derived from an experimental study involving curium(III), as well as americium-carbonate, -sulfate, and -chloride species (Giambalvo 2002a).

Changes to the database related to aqueous species since the PAVT included slight revisions to the americium-carbonate and americium hydrolysis species data and addition of the species $Am(CO_3)_4^{5-}$, $AmCl^{2+}$, $AmCl_2^+$, $AmSO_4^+$ and $Am(SO_4)_2^-$ to the thermodynamic database. The same americium solids were included in the revised database as in the PAVT database, including $AmOHCO_3(c)$, $Am(OH)_3(s)$, $NaAm(CO_3)_2{\bullet}6H_2O(c)$, and $AmPO_4(c)$. Thermodynamic data for $AmOHCO_3(c)$ and $Am(OH)_3(s)$ were revised slightly, but data for the other two americium(III) solids remained unchanged since the PAVT (Giambalvo 2002a). References were provided for all modifications and additions.

In updating the database, Giambalvo (2002a) addressed what appeared to be shortcomings of the PAVT +III actinide model: (i) inconsistencies in incorporating a hydrolysis model into the database, and (ii) the limited range of ionic strength over which certain data had been collected.

2.2.2 Thorium(IV) Data

Thorium(IV) aqueous species and thermodynamic data in the revised database had relatively few changes since the PAVT, except for a minor revision to the data for $Th(OH)_4(aq)$ and changes to the ternary interaction parameters (θ and ψ) describing the interaction of $Th(CO_3)_3^{6-}$ with Cl^- and Na^+(Giambalvo 2002c). Aqueous thorium(IV) species included in the thermodynamic database were thorium(IV) hydrolysis species, and thorium-carbonate, -hydroxycarbonate, and -sulfate species (Giambalvo 2002c). Thorium(IV) solids in the database included $ThO_2(am)$, $Th(SO_4)_2{\bullet}9H_2O(s)$, $Th(SO_4)_2{\bullet}8H_2O(s)$, $Th(SO_4)_2Na_2SO_4{\bullet}6H_2O(s)$, $Th(SO_4)_2K_2SO_4{\bullet}4H_2O(s)$, $Th(SO_4)_22K_2SO_4{\bullet}2H_2O(s)$, and $Th(SO_4)_23.5K_2SO_4(s)$. No changes were made to the thermodynamic data for these thorium(IV) solid species.

2.2.3 Neptunium(V) Data

The neptunium(V) aqueous and solid species included in the database have not changed since the PAVT. Aqueous species include neptunium(V) hydrolysis species as well as neptunium(V)-carbonate, and -hydroxy-carbonate species. Neptunium(V) solids include $NpO_2OH(aged)$, $NpO_2OH(am)$, $NaNpO_2CO_3{\bullet}3.5H_2O(s)$, $Na_3NpO_2(CO_3)_2(s)$, $KNpO_2(CO_3)(s)$ and $K_3NpO_2(CO_3)_2(s)$. Giambalvo (2002d) recommended minor revisions to some of the thermodynamic data.

2.2.4 Parameter Values for Organic Ligands - Actinide Complexation

Giambalvo (2002b) acknowledged Choppin et al. (2001) as the main source of updated thermodynamic parameter values for the protonation of organic ligands and complexation of organic ligands with actinides and with magnesium. Giambalvo (2002b) noted that differences between PAVT values and the new recommended values are due primarily to refinements in the fitting process to experimental data.

Giambalvo (2002b) discussed the basis for the selection of parameter values for an americium-lactate species ($AmLac^{2+}$) and thorium-acetate species ($ThAc^{3+}$) from the literature, where there is some uncertainty or inconsistency in some of the data available. Her analysis provided an acceptable resolution to this inconsistency. Giambalvo (2002b) also noted that satisfactory references were not available for thermodynamic parameter sets relating to species $AmAc^{2+}$, ThEDTA(aq), $MgAc^{2+}$, MgOx(aq), $MgCit^{-}$ and $MgEDTA^{2-}$. Consequently, Giambalvo (2002b) relied on experimental data provided by Choppin et al. (2001) to derive the relevant parameter sets. Review of this derivation indicated that the new recommended values are acceptable.

Giambalvo (2002e) also revised the thermodynamic data relating to oxalate solids solubility in brine, in order to be consistent with the complementary work on organic ligands. Again, the changes to the previous thermodynamic database are minor but provide consistency. In addition, modeling results compare favorably with measured solubility data.

2.3 Model Predictions Using the PAVT and Revised Database

Giambalvo (2003) compared the actinide solubilities of americium(III), thorium(IV) and neptunium(V) calculated using the PAVT database to the solubilities calculated using the revised database. Each database was used for four solubility calculations: 1) Brine A (representative of Salado brine) with organic ligands, 2) Brine A without organic ligands, 3) ERDA-6 (representative of Castile brine) with organics, and 4) ERDA-6 without organic ligands. However, organic ligand concentrations used in the calculations were equal to those used in the CCA PA and PAVT rather than the concentrations used in the CRA. Furthermore, no modeling was reported to be carried out using the GWB composition, which was used in the CRA PA to represent Salado brine. Thus, these solubility comparisons have some limitations. Giambalvo (2003) noted that the assumptions involving mineral equilibria and mineral suppression were the same as those used for the PAVT.

Using the results of solubility predictions for thorium(IV) and neptunium(V), Giambalvo (2003) showed that solubilities resulting from the PAVT database and from the revised database were essentially the same, with differences in the predicted solubilities of less than 7%.

In contrast, Giambalvo (2003) obtained significantly different solubilities for americium(III) predicted using the PAVT and revised thermodynamic databases. The new database resulted in solubilities calculated for Brine A, with and without organics, and ERDA-6 without organics, that were more than twice as high as solubilities calculated using the PAVT database. For

ERDA-6 with organic ligands present, the predicted solubility was approximately a factor of six smaller.

Giambalvo (2003) explained these differences in terms of the lack of consistency in the previous thermodynamic database, in which the solubility product and hydrolysis constants pertaining to americium hydrolysis species had been taken from different sources. In the absence of any additional modeling, such an explanation appears reasonable. In calculations with the new database, the solubility-controlling phase was $Am(OH)_3(s)$ instead of the solid phase $AmOHCO_3(c)$ that controlled americium(III) solubilities when the PAVT database was used. Where higher Am(III) solubilities were predicted with the revised database, $Am(OH)^{2+}$ was the dominant Am-species in solution, due to corrections to the Am(III) hydrolysis constants. In the case in which a lower Am(III) solubility was predicted using the revised database (ERDA-6 brine with organic ligands present), the dominant americium species in solution was $AmEDTA^-$, which had a concentration approximately 10 times smaller than the concentration calculated using the PAVT database.

2.4 Acceptability of the Revised Thermodynamic Database

The version of the FMT database used in CRA PA calculations is FMT_021120.CHEMDAT as described in Giambalvo (2003). Giambalvo (2003) summarizes previous documents (Giambalvo 2002a, 2002b, 2002c, 2000d, and 2002e), which are used to support the changes incorporated in the new database. The new database was reviewed and changes from the previous version were checked with the corresponding references and, in the case of updated data associated with organic ligand complexation, the data were compared to the information in Choppin et al. (2001). In general, the changes to both aqueous and organic species are minor, and all changes are well supported by the referenced documents. Where available, modeling results using the revised thermodynamic data were compared with experimental values as part of the recommendation process. For these reasons, the new database appears to be an acceptable update of the previous (FMT_970407.CHEMDAT) database and to contain as consistent a data set as possible.

Giambalvo (2003) notes that the Na^+/K^+ and Mg^{2+}/Ca^{2+} analogies have not been thoroughly tested but considers that theoretical considerations combined with limited experimental evidence indicate that such analogies should result in better model prediction compared with neglecting interactions involving the cation for which no data are directly available. While this argument is reasonable, Giambalvo (2003) recommends re-evaluating such analogies in the future as more data become available.

Giambalvo (2003) noted that most of the plutonium(III) species and those uranium(IV) species having parameters assigned by analogy with thorium(IV), have been de-activated from the new database. This action will not affect the solubility predictions used in PA calculations.

In terms of quality assurance of new thermodynamic data derived from experimental data, Giambalvo (2002b) carried out a verification exercise on key thermodynamic parameter values (normalized chemical potential and Pitzer parameter values) to compare the predicted apparent stability constant ($\log\beta_{101}$) values with experimental values. An error in the Choppin et al. (2001) $AmAc^{2+}$ $\log\beta_{101}$ value was identified from this process and this value was subsequently corrected before the data were included in the database (Giambalvo 2002b).

The FMT database was revised after the CRA PA, and the version FMT_050405.CHEMDAT was used to calculate actinide solubilities for the WIPP PABC (Brush 2005). Changes to the database between the versions used for the CRA PA and the PABC include addition of the calcium oxalate solid whewellite ($CaC_2O_4 \cdot H_2O$) to the database, correction of the molecular weight of oxalate ($C_2O_4^{2-}$) in the database, and correction of the μ^0/RT value for $Th(OH)_4(aq)$ species (Brush 2005, Brush and Xiong 2005). These changes were not reviewed as part of the current evaluation, but will be considered during the review of the PABC (see EPA 2006, Docket A-98-49 Item II-B1-16).

3.0 SALADO FORMATION BRINE CHEMISTRY

In the PAVT, the formulation referred to as Brine A was used to simulate intergranular Salado brines. However, a new Salado brine formulation referred to as Generic Weep Brine (GWB) was used in the CRA PA. Analysis Plan AP-098 (Brush and Xiong 2003b) discusses the use of both GWB and Brine A in the CRA PA to simulate intergranular Salado brines and provides the compositions of these brines (Table 3-1). A detailed discussion of GWB brine and a comparison of this brine to Brine A is provided by Snider (2003d).

GWB was developed based on chemical analyses of intergranular fluids that seep into the WIPP excavations from the disturbed rock zone (Snider 2003d). DOE developed the GWB formulation because of the potential effects of magnesium concentrations in the brine on the modeled and experimental chemical behavior of the MgO backfill; the concentration of magnesium in GWB is lower than in Brine A (Table 3-1). Snider (2003d) verified the calculations supporting the formulation of GWB and compared the concentrations of major cations and anions in several WIPP brines. The comparison between GWB and Brine A indicated that GWB has higher boron, sodium, bromide, chloride, and sulfate concentrations, and lower calcium, potassium, and magnesium than Brine A. Brine A has a relatively low reported inorganic carbon concentration, whereas none was reported for GWB (Table 3-1). The ionic strength of GWB is approximately 6.5 compared to approximately 5.9 for Brine A.

The composition of GWB as specified in Table 2 of Snider (2003d) differs slightly, but not significantly, from the composition specified in Table 4 of Brush and Xiong (2003b); the concentrations in Table 4 of Brush and Xiong (2003b) were provided before it was established that additional water - 15 g - needed to be added to dissolve all solids. However, the CRA PA solubilities were determined using the Snider (2003d) GWB composition, as stated in Brush and Xiong (2003a).

Brush and Xiong (2003b) stated that DOE would continue to use both GWB and Brine A to facilitate comparison of the actinide solubility modeling results with the CCA PA and PAVT. The results of FMT modeling calculations using Brine A and GWB are compared in Table 3-2. The results were obtained for both brine formulations assuming control of carbon dioxide fugacity by the brucite-hydromagnesite$_{5424}$ reaction and the presence of organic ligands. The results indicate slightly lower americium(III) concentrations and higher neptunium(V) concentrations using GWB instead of Brine A (Table 3-2). Thorium(IV) concentrations, pH, and carbon dioxide fugacities were essentially the same for the two brine formulations.

The formulation of GWB appears to have been adequately documented by Snider (2003d), which was one of the tasks specified in Brush and Xiong (2003b). The GWB formulation is reported to more closely match the composition of Salado intergranular brines than Brine A, which was reported to be representative of brines that have interacted with potassium and magnesium minerals before intruding into WIPP (Molecke 1983). Therefore use of the GWB formulation in place of Brine A for the CRA PA and future actinide solubility calculations is appropriate.

Table 3-1 Brine A and GWB Compositions (Brush and Xiong 2003a)

Component	**Brine A**	**GWB**[I]
Boron	0.020	0.155
Calcium	0.020	0.014
Potassium	0.770	0.458
Magnesium	1.44	1.00
Sodium	1.83	3.48
Bromide	0.010	0.026
Chloride	5.35	5.51
Sulfate	0.040	0.175
Total Inorganic Carbon	0.010	not reported
Specific Gravity (kg/L)	1.2	1.2
pH (standard units)	6.5	not reported
Total Dissolved Solids (mg/L)	306,000	not reported

[I] All units are moles/L solution, unless otherwise specified

Table 3-2 Comparison of FMT Modeling Results Obtained with Brine A and GWB Brine. In These Calculations, the Brucite-Hydromagnesite$_{5424}$ Reaction Was Assumed to Control Carbon Dioxide Fugacity and Organic Ligands Were Present in Solution

Component	Brine A	GWB	Ratio GWB/Brine A
Ionic Strength	7.405	7.540	1.02
pH	8.6896	8.6899	1.00
Carbon Dioxide Fugacity	3.135×10^{-6} atm	3.135×10^{-6} atm	1.00
Total Carbon	3.585×10^{-4} M	3.505×10^{-4} M	0.98
Sulfate	5.990×10^{-2} M	1.824×10^{-2} M	0.30
Chloride	5.793 M	5.431 M	0.94
Sodium	4.096 M	4.332 M	1.06

Calcium	2.632×10^{-2} M	1.103×10^{-2} M	0.42
Magnesium	0.4770 M	0.5818 M	1.22
Americium(III)	4.348×10^{-7} M	3.069×10^{-7}	0.71
Thorium(IV)	1.161×10^{-8}	1.186×10^{-6}	1.02
Neptunium(V)	5.813×10^{-7}	1.017×10^{-6}	1.75
FMT Output File	AP098_FMT_RUN008	AP098_FMT_RUN018	–

4.0 MICROBIAL EFFECTS ON REPOSITORY CHEMISTRY

Microbial processes that could significantly affect WIPP repository chemistry include:

- Microbial gas generation;
- Microbial production of organic compounds that form complexes with actinides in solution; and
- Mobilization of radionuclides by colloidal microbes.

Because of the MgO backfill and abundant ferrous iron in the WIPP repository, conditions such as pH, redox potential, and carbonate ion concentrations are expected to be controlled by abiotic processes and will not be significantly influenced by microbial processes (US EPA 1998c).

In the following subsections, the conceptual models related to microbial processes and implementation of these processes in the WIPP PA are described. Information that has been developed since the CCA PA and PAVT is reviewed, and the results of previous Agency reviews of microbial effects are summarized.

4.1 Conceptual Models and Implementation

The conceptual models and approach for including the effects of microbial processes in the WIPP PA are described for microbial gas generation, microbial colloids, and microbial production of organic ligands.

4.1.1 Microbial Gas Generation

The same conceptual model was used for microbial gas generation in the WIPP repository for both the CCA and CRA. In the conceptual model, it is assumed that microbial consumption of CPR may occur in the repository and produce methane (CH_4) and carbon dioxide (CO_2). The major pathways for microbial degradation of CPR are predicted to include the following reactions:

$$C_6H_{10}O_5 + 4.8\ H^+ + 4.8\ NO_3^- \rightarrow 7.4\ H_2O + 6\ CO_2 + 2.4\ N_2 \qquad (1)$$

$$C_6H_{10}O_5 + 6\ H^+ + 3\ SO_4^{2-} \rightarrow 5\ H_2O + 6\ CO_2 + 3\ H_2S \qquad (2)$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3\ CH_4 + 3\ CO_2 \qquad (3)$$

where $C_6H_{10}O_5$ is the chemical formula for cellulose. In reactions (1) and (2), one mole of carbon dioxide is produced for each mole of organic carbon consumed. Reaction (3), however produces only 0.5 moles of carbon dioxide per mole of organic carbon consumed. Reactions (1) to (3) are predicted to proceed sequentially according to the energy yield of the reactions (Wang and Brush 1996). As the denitrification and sulfate-reduction reactions (reactions 1 and 2, respectively) proceed, they are predicted to consume the limited amounts of nitrate and sulfate in the WIPP waste inventory. In both the CCA and the CRA, it was predicted that methanogenesis (reaction 3) would be the dominant reaction pathway and consequently, that approximately half of the organic carbon consumed would be converted to carbon dioxide (US DOE 1996, Appendix SOTERM Section 8.2.2; US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.2).

It was assumed that microbial consumption of CPR could be limited by the long-term viability of microbes in the repository, and whether microbes consume plastics and rubbers was also considered important in the conceptual model. The rate of microbial degradation was assumed to be dependent on brine saturation in DOE's conceptual model (US DOE 2004b, Appendix PA Attachment MASS).

The average-stoichiometry model is the mathematic model used to implement the gas generation conceptual model for the WIPP CCA PA and CRA PA. The average-stoichiometry model accounts for the formation of gas by anoxic corrosion of steels and other Fe-based alloys and by microbial consumption of CPR. In the average-stoichiometry model, gas is assumed to be generated at a rate dependent on the availability of brine in the computational cell. Gas can be generated by anoxic corrosion in all realizations. However, significant microbial gas production was assumed to occur in half the realizations for the CCA PA, PAVT, and CRA PA because of uncertainties associated with microbial processes. In one half of the realizations in which significant microbial consumption of CPR occurred (one quarter of all realizations), only cellulosics were assumed to be consumed by microbial activity. In the remaining half of the realizations with significant microbial consumption of CPR (one quarter of all realizations), all CPR materials, including plastics and rubber, were assumed to be consumed by microbial activity (US DOE 2004b, Section 6.4.3.3).

Microbial gas generation rates used in the average stoichiometry model were based on experimental data on the rates of gas generation from microbial consumption of papers under inundated and humid conditions (Wang and Brush 1996). A gas-generation rate is determined in BRAGFLO from the humid and inundated rates based on the effective liquid saturation (US DOE 2004b, Section 6.4.3.3). These gas generation rates were calculated from the initial linear part of the experimental curve of carbon dioxide as a function of time and have not changed since the CCA (US DOE 2004b, Appendix PA Attachment PAR; Wang and Brush 1996).

4.1.2 Microbial Colloids

Colloidal particles are expected to be generated in the repository by microbial degradation of CPR, corrosion of steel, hydrodynamic entrainment of colloidal-sized mineral fragments, and other mechanisms. These colloidal particles may sorb dissolved actinides, or dissolved actinides may form intrinsic colloidal particles. In addition, colloidal-sized microbes can participate in actinide transport because they can actively bioaccumulate actinides and act as sorption substrates for actinides. Actinide-bearing, colloidal-sized particles may be transported with dissolved actinides to the Culebra or through the fractured anhydrite interbeds of the Salado (US

DOE 2004b, Appendix PA Attachment SOTERM-6.0). In the CCA PA, the PAVT, and the CRA PA, the largest contributors to the mobile colloidal actinide source term were actinides associated with humic substances and microbes (US DOE 2004b, Appendix PA Attachment SOTERM Section 6.4). The conceptual model and implementation for the transport of actinides by humic substances is summarized in Section 4.1.3 (below).

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Microbial actinide accumulation was considered in the CCA PA, the PAVT and the CRA PA according to a relatively simple model. In this model, each radionuclide is distributed between microbially bound and aqueous phases according to a proportionality constant (PROPMIC), with a value (CAPMIC) that represents the maximum concentrations of actinides that could be associated with microbes.

4.1.3 Microbial Production of Macromolecules and Simple Organic Compounds

Through partial degradation of CPR or cell lysis (disruption of cellular integrity) microbes may produce macromolecules and simple organic compounds. These substances may form complexes with actinides in solution and affect actinide transport in brines and groundwaters (US EPA 1998c).

Macromolecules, also referred to as high-molecular-weight compounds, are expected to behave similarly to environmental humic acids. The same approach for estimating mobile actinide concentrations associated with humic colloids has been used for the CCA PA, the PAVT, and the CRA PA. Because of uncertainties and a lack of appropriate scientific information associated with the in situ formation of humic substances in the WIPP repository, the amounts of humic substances that may form in the repository were not directly estimated. The contribution of humic-bound actinides to the actinide source term was bounded by quantifying humic-actinide complexation and the solubilities of humic substances in WIPP brines (US DOE 2004b, Appendix PA Attachment SOTERM Section 6.3.3). The concentration of actinides bound to humic acids in solution were determined using proportionality constants (PHUMCIM and PHUMSIM) in combination with the actinide solubilities, as well as a maximum concentration of mobile actinides that could be associated with humic colloids (CAPHUM).

Low-molecular-weight organic compounds (also referred to as organic ligands), such as lactate, citrate, and acetate can be produced as metabolites by some microbial organisms. These compounds are generally preferred over cellulose as a microbial growth substrate, although some organisms are unable to degrade them. In many microbial communities, producers and consumers of these low-molecular-weight breakdown products coexist and maintain the compounds at steady state (US EPA 1998c). Actinide complexation by these types of organic ligands was not included in the CCA PA and PAVT solubility calculations because of inadequate thermodynamic data at high ionic strength. However, calculations carried out at low ionic strength indicated that other ions such as Ca^{2+} and Mg^{2+} would compete for the organic ligands and render the ligands unavailable for complexation with the actinides (US EPA 1998c). The CRA PA calculations included the effects of actinide complexation by acetate, citrate, EDTA, and oxalate based on a new thermodynamic database (Giambalvo 2003). The identities and concentrations of ligands included in the solubility calculations were based on their reported presence in the WIPP inventory. Lactate has not been reported in the WIPP inventory and therefore was not included in the calculations (US DOE 2004b, Appendix PA Attachment SOTERM Section5.0).

In the CRA, DOE mentions the possibility of microbial consumption of organic ligands, but does not address the possible production of organic ligands as microbial metabolites. Because of the uncertainty associated with the presence and viability of organisms that could degrade ligands in the WIPP repository environment, DOE did not include the possible microbial consumption of these compounds in the solubility calculations (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.2).

4.2 Information Developed Since the CCA

Since the CCA, additional experimental data have been developed related to microbial degradation rates and reaction products. However, no new experimental data have been provided related to mobilization of actinides by microbial colloids.

4.2.1 Microbial Gas Generation

Preliminary results from experiments designed to investigate gas generation caused by biodegradation of CPR in the WIPP repository environment were available at the time of the CCA (Francis and Gillow 1994). These experiments continued after approval of the CCA, and additional results from these experiments have been reported (Francis et al. 1997; Francis and Gillow 2000; Gillow and Francis 2001a; Gillow and Francis 2001b; Gillow and Francis 2002a; Gillow and Francis 2002b). The results of the experiments were recently summarized by Gillow and Francis (2003).

For these experiments, cellulosics were prepared from materials likely to be included in WIPP waste, including filter paper, paper towels and laboratory wipes. Granular bentonite clay was used in some of the experiments because this material was being considered as a potential repository backfill at the time these experiments began. A mixed inoculum was prepared from a variety of samples (Gillow and Francis 2003). These samples were selected to simulate various sources of microorganisms that could enter the WIPP, including:

- Sediment and brine from Nash Draw, which is located upwind of the WIPP repository and may be a representative source of halophilic and halotolerant bacteria that could be introduced to the WIPP environment by the ventilation system or movement of materials underground;
- Brine from the WIPP underground workings (G-Seep brine collected December 12, 1991); and
- Samples collected from a non-sterile laboratory at Brookhaven National Laboratories that were expected to be representative of the non-halophilic microorganisms originating at the waste generator sites that could be introduced with the WIPP waste.

Experiments were carried out under both inundated and humid conditions for cellulosic materials and under inundated conditions for both unirradiated and electron-beam irradiated plastic and rubber materials.

4.2.1.1 Inundated Experiments with Cellulose

Inundated experiments were carried out with G-Seep brine, a natural brine collected from a seep within WIPP. This brine was found to contain 10^4 to 10^6 bacterial cells per ml (Gillow and Francis 2003). A nutrient mixture was added to some of the experiments that included yeast extract, potassium phosphate dibasic (K_2HPO_4) and ammonium nitrate (NH_4NO_3). Excess potassium nitrate (KNO_3) was added to some nutrient-amended experiments as an additional electron acceptor. Experiments were prepared under anaerobic conditions as well as under initially aerobic conditions. Bentonite was added to some experiments.

Results from the inundated experiments with cellulose indicated that total gas production as well as carbon dioxide production occurred in nearly all experiments (Gillow and Francis 2003). The observation of gas production in the initially aerobic, unamended, uninoculated samples indicated that the microbial population naturally present in G-Seep brine could metabolize organic carbon. The only experiments in which total gas production and carbon dioxide production were not observed were those that were initially anaerobic, unamended, uninoculated, and without bentonite (Gillow and Francis 2003).

The inundated experiments were analyzed for methane after 9.5 years of reaction, and methane was detected in all treatments. The overall rate of methane production was slow relative to the production rate of carbon dioxide. Greater amounts of methane were produced in the anaerobic experiments than in the initially aerobic experiments (Gillow and Francis 2003).

After 6 years of incubation, the microbial population in anaerobic inundated samples was characterized by direct microscopy enumeration and DNA analysis. The results of these analyses indicated that a diverse assemblage of bacterial and archael microorganisms was present and that this assemblage was well populated with extreme halophiles (Gillow and Francis 2003).

4.2.1.2 Humid Experiments with Cellulose

Humid samples were prepared with cellulosics mixed with either crushed WIPP muck-pile salt, a mixture of muck-pile salt and bentonite, or reagent-grade salt. Samples were prepared with and without added nutrients; the nutrients consisted of ammonium nitrate solution, potassium phosphate, and yeast extract. Inoculum was prepared as previously described and pipetted onto the cellulose. Succinate or glucose was added with the nutrient amendment to selected samples to evaluate the effects of a readily metabolizable carbon source. Two of the succinate-amended treatments had added acetylene gas to examine N_2O production from denitrification. Both initially aerobic and anaerobic samples were prepared.

The results of the experiments indicated that the mixed inoculum biodegraded cellulose under humid conditions. Under humid conditions, addition of the nutrient amendment led to less gas production than in samples without nutrients. Bentonite enhanced gas production under humid conditions, and methane was detected only when bentonite was present (Gillow and Francis 2003).

Experiments to study microbial gas generation at water activities consistent with the presence of MgO in the repository were described by Gillow and Francis (2002a and 2002b), and a test plan for additional experiments was prepared by Wang (2002). However, data from these experiments have not been reported.

4.2.1.3 Inundated Experiments with Plastics and Rubbers

Both unirradiated and electron-beam irradiated plastic and rubber materials were tested to determine the rate and extent of gas generation caused by microbial degradation. The plastics tested were polyethylene and polyvinylchloride (PVC), and the rubber materials were neoprene, leaded hypalon, and unleaded hypalon. The irradiated plastics and neoprene received an absorbed dose of either 500 to 700 Mrad (low dose) or 4,000 to 6,000 Mrad (high dose). Only low-dose hypalon was tested because high-dose irradiation of the leaded sample caused extensive melting (Gillow and Francis 2003). Each sample bottle contained a piece of polymer and a mixture of G-Seep Brine, WIPP muck-pile salt slurry, and surficial lake brine/sediment slurry. Mixed inoculum was added to the experiments without dilution to maximize the potential plastic- or rubber-degrading microorganisms in each experiment. Some samples were amended with nutrients, using a pH 7 stock solution that contained ammonium nitrate, potassium phosphate, and yeast extract. Control samples without polymer and with and without nutrients were also prepared (Gillow and Francis 2003).

A small amount of gas production was observed in control samples because of microbial degradation of dissolved organic carbon and trace inorganic nutrients in the brine inoculum. Total gas production in most samples with polyethylene was only slightly higher than in control samples. Gillow and Francis (2003) attributed the higher gas production in these experiments to the use of polyethylene as a substrate for more effective utilization of dissolved organic carbon and trace nutrients in the inoculum rather than to degradation of the polyethylene.

Irradiated PVC generally had an inhibitory effect on total gas production. Based on the results of the experiments, Gillow and Francis (2003) concluded that there was little overall evidence for degradation of PVC in the experiments.

Total gas and carbon dioxide production data indicated long-term degradation of low-dose and high-dose irradiated neoprene in both initially aerobic and anaerobic experiments (Gillow and Francis 2003). Degradation also appeared to occur in experiments with unirradiated and irradiated neoprene, unleaded hypalon, and leaded hypalon. Irradiation of neoprene and hypalon appeared to enhance carbon dioxide production. The amount of methane produced during the experiments with the plastics and rubber materials was consistent with degradation of dissolved organic carbon in the inoculum/inundation fluids, and there was no evidence of methanogenesis caused by biodegradation of the polymers (Gillow and Francis 2003).

4.2.1.4 Argonne National Laboratory Microbial Degradation Experiments

Additional experiments related to microbial degradation of cellulosic materials under WIPP-relevant conditions were conducted by DOE at Argonne National Laboratory (Felicione et al. 2001). In these experiments, steel containers were filled with TRU wastes and synthetic WIPP brine (Brine A) inoculated with microbes typical of those found at WIPP. The containers were purged with inert gas and sealed, and gas samples were periodically extracted to determine the generation of gases from metal corrosion, microbial action, and radiolysis. Relatively small quantities of carbon dioxide, which may indicate microbial degradation, were observed in all tests that contained cellulosic waste materials, in one container with steel plus sludge, and in one container with sludge, rubber, and plastic. The maximum conversion rate of carbon to carbon dioxide was found to be 2.3×10^{-6} g-mol/y/g carbon (Felicione et al. 2001).

4.2.2 Microbial Colloids

There does not appear to be any new experimental data since the CCA PA and PAVT related to microbial colloids. PROPMIC and CAPMIC, the constant parameters used to predict the microbially bound actinide concentrations, are based on the results of laboratory experiments and have not changed since the CCA (US DOE 2004b, Appendix PA Attachment SOTERM Table SOTERM-11).

However, implementation of the microbial colloid model did change for the CRA PA. In a footnote to Table SOTERM-11 (US DOE 2004b, Appendix PA Attachment SOTERM), DOE noted that microbial colloids were not included in nonmicrobial vectors. In contrast, microbial colloids were included in all vectors for the CCA PA and the PAVT. Therefore, the assumption of only a 50% probability of significant microbial degradation of CPR in the repository affects the calculation of actinide transport by microbial colloids as well as the calculation of microbial gas generation.

4.2.3 Microbial Production of Organic Compounds

For the inundated microbial degradation experiments with cellulose, aqueous metabolites were characterized for both initially aerobic and anaerobic samples (Gillow and Francis 2003). Organic acids detected in the experimental solutions after 9.5 years of reaction included acetic, butyric, formic, fumaric, lactic, malonic, oxalacetic, oxalic, propionic, succinic, isobutyric, valeric, and isocaproic acids.

Acetic, formic, lactic and propionic acids were detected in inoculated and uninoculated initially aerobic samples that did not contain a nutrient amendment. After 9.5 years of reaction, lactic and propionic acids were consumed and concentrations of acetic and formic acids appeared to be decreasing (Gillow and Francis 2003). The addition of nutrients to the experiments, both with and without excess nitrate, affected the organic acids produced in the initially aerobic experiments. In these experiments, acetic, butyric, formic, fumaric, lactic, oxalacetic, propionic, succinic, and malonic acids were produced. Acetic acid concentrations increased throughout the experiments, and after 9.5 years reached higher concentrations (6.91 and 11.0 mM) than in unamended samples. Butyric, formic, lactic, propionic and succinic acids were detected in early samples from the nutrient-amended experiments, but were consumed after 9.5 years. Acetic, oxalacetic, and malonic acids were detected in solution at the end of the initially aerobic, nutrient-amended experiments; the sample without excess nitrate also contained fumaric acid. Addition of bentonite to the initially aerobic experiments had relatively little effect on the uninoculated, unamended experiments. However, bentonite increased the accumulation of acetic acid in the inoculated experiments without nutrient amendments, and slightly decreased acetic acid accumulation in the nutrient-amended experiments with and without excess nitrate (Gillow and Francis 2003).

Anaerobic conditions appeared to stimulate the mixed inoculum. Organic acid production in anaerobic samples followed trends similar to the aerobic samples; however, lactic, fumaric, formic, and butyric acids accumulated in the anaerobic samples in addition to acetic acid (Gillow and Francis 2003). Isocaproic acid was detected in the nutrient-amended sample with excess nitrate after 9.5 years.

Bryan and Snyder (2001a, 2001b) report experiments designed to examine the degradation of cellulosic materials under WIPP repository conditions and evaluate the potential production of isosaccharinic acid (ISA). The formation of ISA has been reported under alkaline conditions, and ISA can be a strong complexing agent for actinides. However, the possible formation of ISA has not been evaluated for WIPP repository conditions (Bryan and Snider 2001a). The experiments were commenced in August 2000 and samples were collected (Bryan and Snider 2001a; Bryan and Snider 2001b; Snider 2002). However, it was reported that samples were no longer being collected and the existing samples had not been analyzed because a gas chromatograph-mass spectrometer was not available (Snider 2002).

4.3 Previous Agency Reviews Related to Microbial Effects

The Agency reviewed information regarding microbial effects on WIPP repository chemistry during its review of the CCA, which was documented in a technical support document (US EPA 1998c). In addition, the Agency considered DOE's assessment of microbial gas generation during its review of DOE's request to allow disposal of Advance Mixed Waste Treatment Facility (AMWTF) waste in WIPP (US EPA 2004b; TEA 2004a).

4.3.1 CCA Source Term Model

The Agency reviewed microbial effects during their review of DOE's Source Term Model in the CCA. In their review of the CCA, the Agency (US EPA 1998c) noted the uncertainties associated with whether microbial communities capable of degrading CPR would be present in the hypersaline WIPP environment, and numerous factors that may limit microbial gas generation, including the concentrations of nutrient and toxic compounds and limitations imposed by temperature, salinity, Eh, pH and the availability of electron acceptors. The Agency observed that it is generally difficult to estimate the rate and extent of slow processes such as the degradation of CPR over long time periods by extrapolating the results of short-term studies. The Agency concluded that, based on the available evidence at that time, DOE's approach to addressing the probability of significant microbial gas generation was adequate (US EPA 1998c). The Agency also noted that the carbon dioxide production rates used in WIPP PA are likely to be conservative overestimates, and that the addition of MgO backfill to the WIPP repository made the carbon dioxide production rates unlikely to be of significant concern.

The Agency found that microbial processes are unlikely to affect actinide solubilities by influencing repository pH, redox potential and carbonate ion concentrations, because these properties are likely to be controlled by abiotic factors (US EPA 1998c). The Agency also found that high-molecular-weight compounds produced from cellulose degradation are unlikely to increase actinide concentrations in the aqueous phase for undisturbed scenarios. Low-molecular-weight compounds could increase actinide mobilization for scenarios in which WIPP brines are brought to the Culebra Dolomite or directly to the surface (US EPA 1998c), but limited data were available regarding whether these compounds were likely to form in the WIPP repository environment.

The Agency expressed concerns regarding the experimental determination of microbial actinide binding parameters (US EPA 1998c). However, the Agency found that DOE's formulation of microbial actinide accumulation in the CCA was appropriate, and the approach used in the CCA to estimate parameters for microbial binding of actinides was reasonable, given the available data (US EPA 1998c).

4.3.2 Microbial Gas Generation Evaluation During AMWTF Review

At the time of the CCA PA, DOE assumed that all carbon in CPR could potentially be converted to carbon dioxide and used this assumption to calculate the amount of MgO required in the backfill. Since the time of the CCA PA and PAVT, methanogenesis has been observed in some of the microbial degradation experiments (Gillow and Francis 2003). DOE stated that methane generation in the experiments demonstrates that methanogenesis will occur in the WIPP repository environment if microbial degradation of CPR occurs. DOE has also indicated that only limited amounts of CPR degradation will take place through denitrification and sulfate reduction (reactions 1 and 2) because of the relatively small amounts of sulfate and nitrate in the waste (Hansen et al. 2003a and 2003b). Consequently, after sulfate and nitrate inventories in the waste are consumed, CPR degradation will either cease or will proceed through methanogenesis (reaction 3 on page 12). Because methanogenesis produces only 0.5 moles of carbon dioxide for each mole of CPR carbon that is degraded, CPR degradation through methanogenesis would significantly reduce the amount of carbon dioxide that could be produced and the amount of MgO required to maintain the required chemical conditions in the repository.

TEA (2004a) reviewed the information supplied by DOE (Hansen et al. 2003a and 2003b; Kanney et al. 2004) and concluded that DOE’s consideration of the sulfate available for CPR degradation by sulfate reduction did not adequately account for sulfate that is present in the brine and in the Salado Formation. The Agency considered the available information and the uncertainty associated with possible microbial processes in the repository, and directed DOE to continue calculating required quantities of MgO backfill by assuming all CPR carbon could be converted to carbon dioxide unless new and convincing evidence was provided that methanogenesis would occur in the WIPP repository (US EPA 2004b, US EPA 2004c).

4.4 Probability of Microbial Degradation

DOE estimated the probability of microbial degradation in the CCA PA, the PAVT and the CRA PA by considering the uncertainties associated with the presence and activity of microbes in the repository capable of degrading CPR, whether sufficient electron acceptors will be present and available, and whether enough nutrients will be present and available (Wang and Brush 1996; US DOE 2004b, Appendix PA Attachment SOTERM-2.2.2). DOE assumed a 50% probability of significant microbial degradation of cellulosics, and in those vectors that had significant microbial degradation of cellulosics, DOE assumed a 50% probability of significant microbial degradation of plastics and rubbers.

Additional information has been developed since the CCA PA and PAVT that necessitated reevaluation of the probability of microbial degradation of CPR for the CRA PA. The Agency requested that DOE evaluate whether the assumed probability of significant microbial degradation of CPR should be increased based on the currently available information (US EPA 2004a, Comment G-9). The Agency also requested that DOE assess the potential impact of a higher probability of significant microbial degradation of CPR on microbial colloid formation and mobilization of actinides and the potential effects on microbial gas generation rates

DOE (US DOE 2004a) responded with information based on an analysis by Brush (2004). Brush (2004) considered seven factors that could affect the probability of significant microbial degradation of CPR in the WIPP repository. These factors, which were originally considered by Brush (1995) for the CCA, are whether:

- Microorganisms will be present in the repository when it is filled and sealed;
- Sterilization of the waste and other contents of the repository will prevent microbial activity;
- Microbes will survive for a significant fraction of the 10,000 years of repository performance;
- Sufficient water will be present;
- Sufficient quantities of biodegradable substances will be present;
- Sufficient electron acceptors will be present and available; and
- Enough nutrients, especially nitrogen and phosphorous, will be present and available.

These factors are considered below.

4.4.1 Presence of Microorganisms

The inoculum prepared for the experiments summarized by Gillow and Francis (2003) was designed to replicate potential sources of microbial populations in the repository. The results of the degradation experiments indicate that these microbial populations are capable of degrading cellulosics and some rubber materials. DNA analysis of samples from inundated experiments indicates the presence of a diverse population of microbes, many of which are halophilic (Gillow and Francis 2003). Inundated, initially aerobic samples that contained only the microbes naturally present in G-Seep brine also exhibited evidence of microbial degradation of cellulose. Therefore, it appears relatively likely that microbes capable of consuming CPR will be present and active in the repository, at least during the period immediately following repository closure. Brush (2004) concluded that the new information has eliminated this issue as a source of uncertainty, thereby increasing the probability of significant microbial activity.

4.4.2 Sterilization of Waste

Brush (1995) discussed the possibility of sterilizing WIPP waste by irradiation, autoclaving, use of biocides, or filtration and concluded that such measures would not reduce the uncertainty associated with significant microbial degradation in the repository. Brush (2004) referred to studies indicating the potential biocidal or inhibitory properties of MgO; these studies and the potential effects of MgO on microbial degradation were summarized in the CRA (US DOE 2004b, Appendix BARRIERS-2.3.4.2.2). DOE noted that the cited experimental results suggest that MgO might reduce the rate of microbial gas generation in the WIPP (US DOE 2004b, Appendix BARRIERS-2.3.4.2.2), but concluded that in the absence of repository-specific data, it was not possible to reduce the microbial gas generation rates used in PA. Brush (2004) stated in the text that the information on the potential biocidal or inhibitory effects of MgO reduces the probability of significant microbial degradation of CPR in the WIPP repository; however, in the accompanying table, Brush (2004) indicated that this information has no effect on microbial degradation probability.

The cited references regarding the potential biocidal properties of MgO have not been independently reviewed. However, DOE acknowledges that there is a lack of repository-specific data on this subject (US DOE 2004b, Appendix BARRIERS-2.3.4.2.2). Because it is not clear that MgO will have biocidal or inhibitory effects on the bacteria likely to be present in the WIPP repository, this information does not change the probability of significant microbial degradation.

4.4.3 Viability of Microorganisms and Presence of Sufficient Biodegradable Substrate

Considerable uncertainty remains regarding the long-term viability of microbial populations in the repository. Brush (1995) acknowledges the virtual impossibility of conducting experiments that will test the long-term survivability of microorganisms in the WIPP repository environment. However, Brush (2004) cites the slowing or possible cessation of microbial gas generation in experiments described by Gillow and Francis (2003) as evidence that microbes are less likely to survive long enough to affect repository performance. Brush (2004) also states that the slowing or possible cessation of microbial gas generation in these experiments indicates that microbial degradation may not consume all of the cellulosic materials in the repository.

Gas production rates in the experiments summarized by Gillow and Frances (2003) were typically rapid during the initial stages of the experiments, then slowed considerably. It is possible that this reaction rate reduction was caused by the complete consumption of degradable cellulosics or by a lack of long-term viability of the microorganisms. However, it is also possible that the reaction rates slowed because of other factors in the experiments that may not occur in the repository, such as the consumption of nutrients or electron acceptors. It is also possible that the slower reaction rates may have proven to be nonzero over a longer time period. Another consideration is whether long-term nonradiolytic inorganic processes might convert cellulosics to a more readily biodegradable form, as cited by Brush (1995) in a discussion of the biodegradability of plastics and rubber. Thus, there does not appear to be any conclusive evidence that a significant portion of the cellulosics in the WIPP waste will be unavailable for microbial degradation.

Vreeland et al. (2000) identified the existence of viable microbes in Salado Formation salt, and observed that these microbes appeared to have survived since the end of the Permian Period (251 Ma). Brush (2004) noted that there is some disagreement regarding the significance of the results of this study. Nevertheless, some evidence exists that viable microorganisms can exist in salt formations that are millions of years old (e.g., McGenity et al. 2000). Thus, there is no new evidence indicating that viable bacteria cannot survive for significant periods in the WIPP environment, and in fact there appears to be some evidence, albeit controversial, of the survival of halophilic subsurface microorganisms for millions of years.

4.4.4 Presence of Sufficient Water

The presence of water in the repository is likely to be important for the transport of nutrients and electron acceptors to the substrates (Brush 1995). Brush (2004) noted that implementation of the Option D panel closure system has decreased the water content of the waste in PA during undisturbed performance assessment periods. In addition, reaction of MgO to form brucite [$Mg(OH)_2(s)$] will consume water, which is not currently accounted for in PA. Therefore, Brush (2004) concluded that the presence of sufficient water appears to be less likely than at the time of the CCA, making the probability of significant microbial degradation also less likely. Brine saturation is taken into account in PA when calculating microbial degradation rates, based on the presence of humid or inundated conditions (US DOE 2004b, Appendix PA).

4.4.5 Presence and Availability of Electron Acceptors and Nutrients

Electron acceptors such as sulfate are likely to be present and available for reaction in the WIPP repository because of sulfate present in the waste, in the brine, and in solid phases in the Salado Formation (Section 4.3.2). Because of the sulfate present in the brine, in the anhydrite interbeds, and dispersed in the halite of the Salado Formation, it is possible that sufficient sulfate will be available for all CPR in the repository to degrade via the sulfate reduction reaction (reaction 2). The availability of sufficient nutrients in the repository to sustain microbial degradation is less certain. The estimates of phosphate in the waste have increased since the CCA. Current inventory estimates include 1.05×10^5 kg of phosphate (Leigh and Sparks-Roybal 2003), which indicates some nutrients will be present in the repository.

4.4.6 Effects on Probability of Significant Microbial Degradation

Evaluation of information that has become available since the CCA indicates:

- An increased probability that microorganisms will be present in the repository when it is filled and sealed.
- There is insufficient evidence to show that MgO will prevent microbial activity in the WIPP repository environment, and there is no change since the CCA regarding the factor related to waste sterilization.
- Evidence exists that microbes have survived in subsurface environments for millions of years, although this evidence is controversial. In addition, there is no repository-specific evidence that MgO will interfere with the long-term viability of microbes. Therefore,

there appears to be no new evidence indicating that microbes will not survive for a significant fraction of the 10,000 years of repository performance, and there is some new evidence making their long-term viability more likely than it appeared at the time of the CCA.

- The incorporation of the Option D panel closure system and the consumption of water by the hydration of brucite may decrease the amount of water available to transport nutrients and electron acceptors within the repository. However, DOE has not demonstrated that the amount of water in the undisturbed repository will be so low that it prevents microbial degradation of CPR and the presence of humid or inundated conditions are accounted for in PA. Therefore, this factor remains unchanged since the CCA.

- Sufficient quantities of biodegradable substances will be present, which is unchanged since the CCA.

- Sufficient electron acceptors will be present and available, which is unchanged since the CCA.

- It is likely that nutrients, such as nitrogen and phosphorous, will be present in the repository. The amount of phosphate reported in the inventory has increased since the CCA, making the microbial degradation of CPR in the repository appear more likely.

The overall balance of information developed since the CCA indicates that microbial degradation of cellulosic materials may be more likely than previously assumed. Results from DOE’s experiment also indicate that rubber materials may be microbially degraded in the WIPP repository environment. On the other hand, no evidence was found in the DOE experiments of microbial degradation of polyethylene or PVC. Based on this information, it appears that the probability of significant microbial degradation of cellulosic materials should be higher than the 50% assumed for the CCA PA, PAVT, and the CRA PA. Because only limited degradation of rubber materials was observed and no degradation of plastics was observed, there is no evidence that the probabilities of plastics or rubber degradation assumed for the CCA PA and PAVT should be revised.

DOE evaluated the potential effects of a higher probability of significant degradation of CPR on microbial gas generation rates by comparing gas volumes and repository pressures for vectors with (biological) and without significant microbial activity (nonbiological) using BRAGFLO simulation results (US DOE 2004a). The gas generation rate and repository pressure at early times is larger for biological vectors, as is the maximum cumulative gas generation and repository pressure over the 10,000-year regulatory period. The maximum cumulative gas generation and the range in the amount of gas generated for the biological vectors is approximately 1.4 to 1.5 times the values observed for nonbiological vectors (US DOE 2004a).

The effects of the assumed probability of microbial degradation of CPR were assessed by comparing total radionuclide mobilization for microbial and nonmicrobial vectors, based on

PANEL output for Scenarios S1 and S3 (US DOE 2004a). For Scenario S1 (Salado brine), the range of mobilized radionuclides is similar for the microbial and nonmicrobial vectors, although the central tendency appears higher for the microbial vectors. For Scenario S3 (Castile brine), the range of concentrations for the biological vectors are higher than for nonbiological vectors. These higher concentrations have the potential to influence releases through the Culebra and direct brine releases because these release modes are associated with intrusions (US DOE 2004a).

For biological and nonbiological vectors, DOE compared releases through the Culebra, direct brine releases, spall releases, and total releases to assess the possible effects of microbial activity. The comparison indicated that releases through the Culebra were minimally affected, most likely because the probability of such releases is low. Higher releases were observed in biological vectors for direct brine releases and for spall releases. However, total releases were not significantly higher for biological vectors than nonbiological vectors because of the importance of cuttings and cavings to total releases, and cuttings and cavings should not be significantly affected by microbial activity (US DOE 2004a).

4.5 Evaluation of Microbial Degradation Rates

The ranges of microbial degradation rates used in BRAGFLO for the CCA PA, the PAVT and the CRA PA were determined using initial results from the WIPP microbial degradation experiments with cellulose (Wang and Brush 1996). The rates were determined from experiments that did not contain bentonite: inclusion of bentonite in the experiments typically increased the amounts and rates of carbon dioxide production in initially anaerobic inundated and humid samples (Figures 4 and 16 of Gillow and Francis 2003). Bentonite appeared to affect carbon dioxide and total gas production by providing nutrients or alternate electron acceptors (Gillow and Francis 2003). Although bentonite will not be used as backfill in the repository, the bentonite in the experiments could have the same effects as waste soils and other solid materials in the repository. Consequently, the microbial degradation experiments obtained with bentonite could have some applicability to reactions in the repository.

Maximum inundated rates were determined by Wang and Brush (1996) from experimental results up to 411 days in initially anaerobic experiments that were inoculated, and that included nutrients and nitrate amendments. Minimum inundated rates were determined from initially anaerobic, inoculated experiments up to 1,034 days without nitrate or nutrient amendments. If maximum carbon dioxide production rates are calculated over the same time period (69 to 411 days) using the same methods from the experiments with bentonite, the maximum rate would be 0.48 moles/kg cellulose/y instead of the reported 0.3 moles/kg cellulose/y.

Similarly, maximum carbon dioxide production rates can be calculated from humid experiments that contained bentonite and nutrient amendments. The initial rapid rate from 6 to 140 days in the bentonite-containing experiment can be calculated using data reported in Gillow and Francis (2003). The maximum rate in the humid experiment with bentonite is 1.13 mole/kg/year, compared to the maximum value of 0.04 mole/kg/year used in the CCA PA, the PAVT, and the CRA PA.

Wang et al. (2003) recalculated inundated and humid microbial degradation rates using lower, longer-term carbon dioxide generation rates from the experiments. Although Wang et al. (2003) asserted that these lower rates were more representative of rates likely to occur in the WIPP repository, the microbial gas generation rates used in the CRA PA were the same, higher rates as those used in the CCA PA and the PAVT.

DOE used a two-step process to simulate microbial gas production rates in the WIPP repository for the PABC (Nemer et al. 2005, EPA 2006). The initially rapid rates of microbial gas production will be simulated by increasing the initial pressure in the BRAGFLO input file. This “precharging” of the repository gas pressure will be combined with the use of lower gas generation rates determined from long-term experimental data. The rate used for humid conditions will be constrained to be less than the inundated microbial degradation rate. DOE has reported that this proposed implementation of lower long-term microbial degradation rates reduces both the rate of pressurization and the pressure in the undisturbed repository (Nemer et al. 2005). This implementation also results in slightly higher brine saturation for the undisturbed repository. For the disturbed repository, pressures are relatively unchanged by the different rates, but the disturbed brine saturation is higher using the lower long-term rates.

DOE’s planned implementation of an initially rapid microbial degradation rate followed by slower long-term rates is likely to be more representative of repository conditions. Assuming a rapid initial rate followed by slower long-term rates is more consistent with the experimental data and with general patterns of microbial processes. A consequence of this change is likely to be longer persistence of microbial gas-generating processes and higher brine saturations in both the disturbed and undisturbed repository scenarios. DOE’s implementation of this change for the PABC was found adequate by the EPA (see EPA 2006).

4.6 Microbial Degradation Products

DOE has maintained that the relatively small amounts of nitrate and sulfate in the waste will limit the denitrification and sulfate reactions (reactions 1 and 2 on page 12) that can occur in the repository. However, DOE does not account for the sulfate naturally present in the brine (Brush and Xiong 2003a) and in the Salado Formation (Lambert 1992; Pfeifle and Hurtado 1998). Sulfate present in the brine will be available for microbial degradation of CPR via reaction (2). As sulfate is consumed by the reaction, the assumption of equilibrium within the repository requires that sulfates present in the Salado Formation dissolve to maintain equilibrium between the minerals in the Salado and brine in contact with the waste. Therefore, it is possible that sufficient sulfate will be available for complete CPR degradation through reactions (1) and (2), which convert all carbon in the CPR to carbon dioxide.

The observation of methane in samples from inundated cellulose experiments indicates that methanogenesis may occur if electron acceptors such as nitrate have been consumed (Gillow and Francis 2003). However, the experiments do not appear to have demonstrated that methanogenesis will occur in the presence of excess sulfate, which may be present in the WIPP environment from sulfate dissolved in brine and in sulfate minerals in the Salado Formation. Therefore, there is no conclusive evidence that methanogenesis will occur in the WIPP repository.

Production of organic acids has been observed in the inundated experiments with cellulose. Acids that accumulated in some of the experiments included acetic acid and lactic acid (Gillow and Francis 2003). These acids are important for modeling actinide solubilities because they are likely to dissociate to acetate (CH_3COO^-) and lactate ($CH_3CHOHCOO^-$). Acetate and lactate formation during microbial degradation could increase the inventory of ligands in the WIPP repository, possibly leading to an increase in actinide solubilities. Concentrations of acetic acid up to 0.039 M were observed in the most recent samples from the cellulose microbial degradation experiments. This concentration is greater than the concentration of acetate used to calculate actinide solubilities for the CRA (0.005 M, US DOE 2004b, Appendix PA Attachment SOTERM Table SOTERM-4). The maximum lactic acid concentration in the most recent samples from the cellulose degradation experiments was 0.003 M. Although this concentration is relatively low compared to the acetic acid concentrations, the possible significance of this concentration of lactate was unknown because lactate was not been identified in the WIPP inventory and was therefore not included in the actinide solubility calculations (Appendix PA Attachment SOTERM Section 5.0). However, DOE has carried out sensitivity calculations to determine the potential effects of lactate on actinide solubilities (Section 8.6.3). The results of these calculations indicated that lactate, at the concentrations that may be produced by microbial degradation of CPR, is unlikely to significantly affect actinide solubilities.

4.7 Conclusions

Based on the available data from microbial degradation experiments, the occurrence of at least small amounts of microbial degradation of CPR in the WIPP repository is highly probable. However, based on the available experimental data, humid and inundated rates could slow considerably after this initial amount of reaction. DOE's proposed implementation of higher initial rates followed by lower long-term rates appears to be a reasonable approach for simulating microbial degradation processes and is consistent with the available experimental data.

Because sulfate is present in brines and in the Salado Formation anhydrite interbeds and halites, sufficient sulfate may be available for all CPR in the repository to degrade via denitrification or sulfate reduction. Therefore, DOE should continue to assume for the purposes of calculating the amounts of MgO backfill that all carbon in CPR could potentially be converted to carbon dioxide.

Ligands such as acetate and lactate may form during microbial degradation of cellulosic materials and persist in solution. Consequently, the Agency requested that DOE perform bounding actinide solubility calculations that appropriately account for ligand concentrations that may be achieved through microbial degradation of CPR (US EPA 2004c, Comment G-13). DOE's response to this request for additional information is discussed in Section 8.6.

5.0 BACKFILL EFFICACY

MgO backfill was included in the WIPP repository design to control chemical conditions and limit gas pressures by sequestering CO^2. Selection of MgO as an engineered barrier was based on an analysis described in the CCA (US DOE 1996 Appendix EBS). The backfill was designed to control repository chemical conditions and thereby minimize actinide solubilities in the postclosure repository (US DOE 1996 Appendix BACK Section 1).

5.1 Conceptual Model and Implementation

Expected performance of the MgO backfill was described in the CCA (US DOE 1996 Appendices BACK and SOTERM). Additional information was provided by DOE during the Agency's review of the CCA (US EPA 1997).

5.1.1 MgO Reactions in the Repository

MgO backfill is expected to control actinide solubilities in brine within the post-closure repository by consuming carbon dioxide produced by microbial degradation of CPR and buffering brine pH at moderately alkaline values. MgO will initially react with brine to form brucite:

$$MgO(s) + H_2O \rightleftharpoons Mg(OH)_2(s) \qquad (4)$$

and brucite dissolution is expected to buffer brine pH in the repository:

$$Mg(OH)_2(s) + 2\,H^+ \rightleftharpoons Mg^{2+} + 2\,H_2O \qquad (5)$$

Microbial degradation of CPR will produce carbon dioxide, which can react with brucite to form magnesium-carbonate phases such as magnesite [$MgCO_3(s)$]:

$$Mg(OH)_2(s) + CO_2(g) \rightleftharpoons MgCO_3(s) + H_2O \qquad (6)$$

hydromagnesite, for which two chemical formulas have been reported:

$$5\,Mg(OH)_2(s) + 4\,CO_2(g) \rightleftharpoons Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O(s)^{II} \qquad (7)$$

$$4\,Mg(OH)_2(s) + 3\,CO_2(g) \rightleftharpoons Mg_4(CO_3)_3(OH)_2 \bullet 3H_2O(s) \qquad (8)$$

[II] Hydromagnesite of this formula has been designated by DOE in some documents as hydromagnesite$_{5424}$; to prevent confusion between the different possible formulas, this notation is also used in the present report.

or nesquehonite [$MgCO_3 \bullet 3H_2O(s)$]:

$$Mg(OH)_2(s) + CO_2(g) + 2\ H_2O \rightleftharpoons MgCO_3 \bullet 3H_2O(s) \qquad (9)$$

Because of the high energy of hydrolysis of the magnesium ion, magnesite does not precipitate directly from low-temperature solutions. Instead, metastable formation of hydrated magnesium carbonate phases such as hydromagnesite and nesquehonite is more likely to occur. Because these phases are not thermodynamically stable under repository conditions, they are expected to eventually dehydrate to form magnesite, e.g.:

$$Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O(s) + CO_2(g) \rightleftharpoons 5\ MgCO_3(s) + 5\ H_2O \qquad (10)$$

At equilibrium in the repository, magnesite is expected to be the most stable magnesium-carbonate phase (US EPA 1998c).

The magnesium-carbonate phase(s) that form in the repository will control the carbon dioxide partial pressure. In the CCA PA, DOE assumed that the brucite-magnesite reaction (6) would control carbon dioxide partial pressure (US DOE 1996 Appendix SOTERM). The Agency reviewed experimental data on magnesium-carbonate formation in WIPP brines (SNL 1997) and found that nesquehonite formed initially in the experiments, but nesquehonite converted within a few days to a solid similar in composition to protohydromagnesite [$(MgCO_3)_4 \bullet Mg(OH)_2 \bullet 4H_2O(s)$] (US EPA 1998c). The formation of hydromagnesite was observed in other scoping experiments (SNL 1997). There was no evidence of hydromagnesite conversion to magnesite in the experiments reviewed by the Agency (US EPA 1998c).

Based on a review of the literature (US EPA 1998c), the Agency developed the following conceptualization of the sequence and time scales of reactions between infiltrating brine and MgO backfill in the WIPP repository:

1. Rapid reaction of MgO with brine to produce brucite (hours to days);
2. Rapid carbonation of brucite to produce nesquehonite and possibly hydromagnesite (hours to days);
3. Rapid conversion of nesquehonite to hydromagnesite (days to weeks);
4. Slow conversion of hydromagnesite to magnesite (hundreds to thousands of years).

The Agency found that brucite in combination with the different magnesium carbonates buffered carbon dioxide fugacities at different values, with the highest value observed for nesquehonite, intermediate values for the two different forms of hydromagnesite, and the lowest fugacities for magnesite (US EPA 1998c). Higher carbon dioxide fugacities generally increase actinide solid solubilities because of the formation of aqueous actinide-carbonate complexes. Verification calculations indicated that the form of hydromagnesite [either $Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O(s)$ or $Mg_4(CO_3)_3(OH)_2 \bullet 3H_2O(s)$] had little effect on predicted actinide concentrations (US EPA

1998c). Errors in the thermodynamic database used for the CCA PA were corrected for the PAVT (US EPA 1998c). The verification calculations indicated that because of the database errors, the actinide solubilities predicted in the CCA PA using the brucite-magnesite buffer were higher than the likely repository concentrations, even if brucite-nesquehonite buffers carbon dioxide partial pressures (US EPA 1998c).

5.1.2 Placement of MgO Backfill

MgO emplaced in the repository is obtained from the supplier in a dry granular form (WTS 2003). This form was selected to minimize dusting in case of a premature bag rupture, ensure sufficient permeability for access of brine for reaction, reduce possible entrainment of MgO in brine flow, and provide sufficient density so adequate amounts can be placed in the repository (US DOE 1996, Appendix BACK Section 2; US DOE 2004b, Appendix BARRIERS Section 2.2). Adequate reactivity of supplied MgO is tested using a laboratory procedure (Krumhansl et al. 1997; WTS 2003).

MgO was initially placed in the repository in 4,200 pound supersacks and 25 pound minisacks. The supersacks were placed on top of various combinations of waste containers (Standard Waste Boxes, 7-packs of 55 gallon drums, TDOPs, 4-packs of 85 gallon overpack drums, and 3-packs of 100 gallon drums), whereas the minisacks were placed among the waste containers and between the waste containers and the sides of the disposal rooms. However, DOE requested the Agency's approval to eliminate the MgO minisacks to enhance worker safety; the Agency approved this change in January 2001 (US DOE 2004b, Appendix BARRIERS; US EPA 2001a and 2001b). The MgO supersacks are constructed of woven polypropylene material and are designed to provide a barrier to atmospheric moisture and carbon dioxide (WTS 2003). The supersacks are provided with a support sheet, which remains under the supersacks after placement on the waste containers (WTS 2003).

At the time of the CCA, DOE calculated the required amount of MgO by assuming that all CPR carbon in the repository could be converted to carbon dioxide; DOE determined that the amount of MgO required to react with this amount of carbon dioxide would be 43,700 tons (US EPA 1997). The MgO safety factor is defined as the moles of MgO divided by the maximum moles of carbon dioxide that could be generated by the waste. An appropriate safety factor was included in the engineered barrier design by setting the amount of MgO at 85,000 tons. This quantity was based on the density of the MgO, the volume of the backfill packages, and the amount of space available in the repository for the backfill. The amount of MgO backfill in the CCA provided a safety factor of 1.95 (US EPA 1997). Elimination of MgO minisacks decreased the safety factor to 1.67 (US EPA 2001a).

5.2 Information Developed Since the CCA

DOE has continued to study the potential reactions of MgO in the WIPP repository. Results reported since the CCA PA and PAVT include Source-Term Waste Test Program (STTP) results, characteristics of the MgO currently used in the repository, and results from ongoing WIPP experiments related to MgO hydration and carbonation reactions.

5.2.1 STTP Experiments

The STTP experiments were designed to provide data on the concentrations of actinides, actinide-containing colloids, complexing agents, and other chemical reactants in simulated WIPP brine in contact with candidate backfill materials and actual transuranic (TRU) wastes (Villarreal 1996). Experiment L-28 from the STTP was designed to evaluate actinide concentrations in Salado brine in contact with direct oxide reduction (DOR) pyrochemical salt wastes. This experiment contained DOR waste (containing plutonium and americium); soluble salts of thorium, uranium, neptunium, and neodymium; iron mesh; Brine A (Salado brine), and an anaerobic inoculum. Experiment L-28 was pressurized to 60 bar with carbon dioxide gas to simulate the relatively high carbon dioxide partial pressures that could be generated by microbial degradation of CPR in the absence of MgO backfill. At the time this experiment began, MgO was not a planned backfill material.

Experiment L-28 was first sampled in August 1995, with three additional samples obtained between January 1996 and January 1997. In February 1997, Experiment L-28 was briefly depressurized, a slurry of MgO prepared from Brine A was added, the experiment was resampled, and the reaction vessel was repressurized to 60 bar with carbon dioxide gas. A constant carbon dioxide partial pressure of 60 bars was maintained and periodic sampling continued until May 1999. Addition of the MgO slurry was expected to increase the pH of samples from the experiment. However, after an initial increase in pH to 7.7, the pH decreased to values consistent with those observed before MgO addition, in the range from approximately 5 to 5.5.

DOE attributed the apparent failure of MgO to buffer pH values in Experiment L-28 to solidification of the MgO, which isolated the MgO hydration products from reaction with carbonate in the brine (US DOE 2000). DOE indicated that the results of Experiment L-28 had no relevance to WIPP conditions, because of the high carbon dioxide overpressure and relatively low pH (US DOE 2000; US DOE 2004b, Appendix PA Attachment SOTERM-4.8).

The Environmental Evaluation Group (EEG) contended that there is significant uncertainty regarding the length of time nesquehonite will persist under repository conditions. The persistence of nesquehonite would increase actinide solubilities, so EEG indicated that additional investigation was necessary to establish the likely magnesium-carbonate phases that will form in the repository (Oversby 2000). Because the addition of MgO to Experiment L-28 did not bring about the expected decrease in plutonium concentrations in solution, EEG questioned whether MgO backfill in the repository would decrease plutonium solubilities as predicted by DOE

(Oversby 2000). The Agency reviewed the results of the STTP experiments and EEG's concerns and determined that the experiment with MgO was not relevant to repository conditions because of the high carbon dioxide partial pressure (SCA 2000).

5.2.2 Characterization of Premier MgO

WIPP MgO backfill is currently obtained from Premier Chemicals. Premier MgO is generated using a different process, has a different texture, and contains higher percentages of potentially reactive impurities than the MgO initially used as WIPP backfill (Bryan and Snider 2001b). Premier MgO is manufactured from mined sedimentary magnesite that is calcined to expel all carbon dioxide (US DOE 2004b, Appendix BARRIERS-2.3.1). This material has been characterized by X-ray diffraction (XRD) and found to contain primarily periclase (MgO), along with minor phases such as forsterite (Mg_2SiO_4), lime (CaO), monticellite ($CaMgSiO_4$), spinel ($MgAl_2O_4$), and ulvospinel ($FeTi_2O_4$). Periclase and lime, which are expected to be reactive, made up approximately 90 wt% of the Premier MgO, with the unreactive constituents forming the remaining 10 wt% (Snider 2003c). Particle-size analysis has been carried out for two batches of Premier MgO (Bryan and Snyder 2001a; US DOE 2004b, Appendix BARRIERS Section 2.3.1). The particle-size distribution of these two batches varied considerably: one batch had a bimodal distribution, with most MgO falling into the higher or lower size ranges, whereas the other batch had a single distribution of particle sizes centered at the middle of the range.

5.2.3 MgO Hydration and Carbonation Experiments

DOE has conducted a series of experiments to evaluate the hydration and carbonation of MgO in the WIPP repository (Bryan and Snider 2001a; Zhang et al. 2001; Snider 2001; Bryan and Snider 2001b; Snider 2002; Snider 2003c; Snider and Xiong 2002; Xiong and Snider 2003; US DOE 2004b, Appendix BARRIERS). Experiments have been carried out by Sandia National Laboratories at their Albuquerque and Carlsbad, New Mexico locations.

5.2.3.1 Albuquerque Hydration Experiments

Experiments designed to evaluate hydration rates under humid and inundated conditions were carried out using salt solutions or simple mixtures instead of WIPP brines (Zhang et al. 2001). The MgO in the experiments was the backfill material used during the early stages of waste disposal at WIPP (supplied by National Magnesia Chemicals).

Humid-condition experiments were carried out at temperatures from 30° to 90°C by suspending MgO pellets over saturated salt solutions that provided relative humidity values ranging from 35% to 95%. The extent of reaction was determined gravimetrically, by assuming that carbonation reactions were negligible and hydration was the only significant reaction. Inundated-condition experiments were carried out at temperatures from 30° to 90°C by immersing MgO samples in deionized water and various salt solutions. For these experiments, the extent of hydration was determined using a quantitative XRD technique. In both humid and inundated experiments, hydration initially proceeded slowly as brucite nucleated, then more rapidly after this initial phase. At high extents of hydration, hydration rates again slowed, resulting in an S-shaped profile when the extent of hydration was plotted against time (Zhang et al. 2001).

Inundated experiments were also carried out using high-purity MgO in deionized water (Zhang et al. 2001; Snider 2001). However, because of inconsistencies in the results of the experiments with high-purity MgO, these results will not be used in the WIPP PA (Snider 2001).

5.2.3.2 Carlsbad Hydration Experiments

Experiments to measure hydration rates were carried out at SNL-Carlsbad. The experiments were carried out under humid and inundated conditions using MgO obtained from Premier Chemicals, the current supplier of WIPP backfill material.

Humid hydration experiments were carried out at 25°, 40°, 60°, and 80° C and relative humidities of 35%, 50%, 75% and 95%. Uncrushed Premier MgO was placed in trays for each experiment, and these trays were placed in a container with a saturated salt solution to provide the appropriate relative humidity. Sample analysis was through loss by ignition, assuming that MgO hydration to brucite was the only reaction that occurred (Bryan and Snider 2001b). Hydration rates were found to increase with temperature and humidity, with essentially complete (over 80%) hydration in higher-humidity samples at 80°C (Snider 2002; Snider 2003c). No evidence of hydration was observed in experiments carried out at 35% relative humidity at temperatures ranging from 25° to 80°C. DOE stated that brucite was the only reaction product identified in the experiments carried out in humid conditions (US DOE 2004b, Appendix BARRIERS-2.3.2.1), although Snider (2003c) indicated that the production of brucite was assumed because the MgO was not in contact with any reactant except water vapor and XRD analysis had not yet been performed. Therefore, DOE has not presented analysis data demonstrating the formation of only brucite in the humid experiments.

Inundated experiments are being conducted with Premier MgO in deionized water, 4 M NaCl, GWB brine, and ERDA-6 brine at 25°, 50°, 70° and 90°C. In deionized water, NaCl, and ERDA-6 brine, brucite was the only hydration phase detected by XRD. Hydration occurred relatively rapidly and ceased in samples from the deionized water experiments at 90°C after approximately 85% of the Premier MgO was converted to brucite. No periclase was identified in the reaction products, which indicated that hydration was complete and nonreactive materials made up the remaining portion of the MgO (Snider 2003c). Experiments carried out in NaCl and brine proceeded more slowly than in deionized water, and reaction rates increased with increasing temperature (Snider 2003c).

In inundated hydration experiments with GWB, a magnesium-chloride-hydroxide hydrate phase formed initially, with brucite becoming the stable hydration phase only at higher extents of reaction (Snider 2002). Higher volumes of brine used in the experiments led to higher fractions of the magnesium-chloride-hydroxide hydrate in the reaction products (Snider 2002). Although this phase could not be identified by XRD in higher-temperature experiments, the phase

$Mg_3Cl(OH)_5{\cdot}4H_2O$ was detected in some experiments at 25°C (US DOE 2004b, Appendix BARRIERS-2.3.2.1). This phase has been detected in higher-temperature experiments using scanning electron microscope (SEM) examination (Snider 2003c). In longer-term experiments, there is XRD evidence that this material was slowly being replaced by brucite (Snider 2003c; US DOE 2004b, Appendix BARRIERS-2.3.2.1).

"Cemented cake" experiments have also been conducted by DOE. These experiments consisted of three different thicknesses of MgO immersed in GWB or ERDA-6 brine, in which the samples are not agitated; experiments were carried out at 25°, 50°, 70° and 90°C (Bryan and Snider 2001b). The intent of these experiments was to determine whether thicker layers of MgO would result in slower hydration rates. In all experiments with ERDA-6 brine, layer thickness did not appear to affect hydration rates (Snider 2002). Layer thickness also did not affect hydration rates in GWB at 50°, 70° and 90°C. However, at 25°C, the hydration rates for the three thicknesses evaluated were significantly different, and hydration rates were relatively low (Snider 2002).

The results of agitated and unagitated hydration experiments were compared for experiments conducted at 70° and 90°C (Snider 2002). In ERDA-6 brine, a greater extent of reaction was observed in agitated experiments, which seemed to indicate cementation was slowing the reaction rate. However, visual examination of the solids indicated that they were friable. In GWB experiments, agitated and unagitated results were very similar, even though some cementation of the unagitated solids appeared to occur (Snider 2002).

5.2.3.3 MgO Carbonation Experiments at Atmospheric Carbon Dioxide Concentrations

MgO carbonation experiments were carried out under inundated conditions using four different solutions: deionized water, 4 M NaCl, GWB brine, and ERDA-6 brine. These experiments were conducted using Premier MgO as the solid starting material. Humidified room air was bubbled through the samples to maintain atmospheric carbon dioxide partial pressure (Bryan and Snider 2001b). Results of these experiments indicated that after approximately 1 year of reaction, carbonation was proceeding slowly in all solutions. Higher extents of reaction were observed in deionized water, intermediate amounts were observed in 4 M NaCl and ERDA-6 experiments, and the lowest extent of reaction was observed in the GWB experiments. Evaluation of the extent of reaction as a function of time indicated that increasing ionic strength decreased the conversion rate (Xiong and Snider 2003). Hydromagnesite$_{5424}$ and calcite were detected by XRD in all four sets of experiments after 327 days of reaction, and there was no evidence of nesquehonite formation (Snider and Xiong 2003).

Additional experiments were carried out with Premier MgO in either deionized water or 4 M NaCl at atmospheric carbon dioxide concentrations. In these experiments, solution concentrations were determined for hydrogen ion, calcium, magnesium, potassium, and sodium. Results of the solution analyses were used to calculate saturation indices for brucite, hydromagnesite$_{5424}$, nesquehonite, and periclase to determine the potential for formation of these phases. Based on the modeling results, it was suggested that nesquehonite would not form at the low carbon dioxide partial pressures expected in WIPP. Consequently, the reaction path was believed to be periclase ⇒ brucite ⇒ hydromagnesite$_{5424}$ in the WIPP backfill (Snider and Xiong 2002).

DOE compared the rates of carbon dioxide uptake at room temperature and atmospheric carbon dioxide partial pressure to the predicted rate of carbon dioxide production by microbial degradation of CPR. Based on this analysis, it appeared that carbon dioxide uptake rates are likely to exceed carbon dioxide production rates by several orders of magnitude and high carbon dioxide partial pressures are therefore unlikely to occur in the repository (Xiong and Snider 2003).

5.2.3.4 MgO Carbonation Experiments at Higher Carbon Dioxide Concentrations

Experiments have also been carried out using an atmosphere that contained 5% carbon dioxide (5×10^{-2} atm, Snider and Xiong 2002). Experiments were conducted using ERDA-6 and GWB brines and one of four solids: Premier MgO, Premier MgO that was hydrated to form brucite, reagent-grade MgO, or reagent-grade MgO that was hydrated to form brucite (Snider and Xiong 2002). These experiments showed relatively high carbonation rates compared to equivalent experiments carried out with atmospheric carbon dioxide concentrations.

XRD analysis indicated that reagent grade MgO and brucite from reagent-grade MgO initially formed nesquehonite in experiments carried out with ERDA-6 brine. In the experiments with brucite, the nesquehonite converted to hydromagnesite$_{5424}$ within the initial 3 weeks of the experiments. Nesquehonite was still present after 3 months in experiments that began with reagent-grade MgO, although some evidence of hydromagnesite$_{5424}$ formation was observed (Snider and Xiong 2002).

In ERDA-6 experiments with brucite generated from Premier MgO, nesquehonite was formed initially. However, within about 2 months of the start of the experiment, nesquehonite had converted to hydromagnesite$_{5424}$. In experiments with ERDA-6 and Premier MgO, hydromagnesite$_{5424}$ formed within 3 weeks, with only a poorly developed peak observed for nesquehonite. After about 36 days, this peak had disappeared and the nesquehonite had apparently converted to hydromagnesite (Snider and Xiong 2002).

GWB samples did not appear to form nesquehonite, and hydromagnesite$_{5424}$ was the only magnesium-carbonate reaction product observed using XRD. However, the hydromagnesite$_{5424}$ peak was not well developed after 91 days of reaction (Snider and Xiong 2002).

5.3 Agency Reviews Related to MgO Efficacy

Since the CCA, the Agency has reviewed information related to MgO efficacy in the WIPP repository on a number of occasions. In response to questions raised by the results of the STTP experiments regarding the ability of MgO to lower actinide solubilities (Section 5.2.1), the Agency reviewed the implications of these experimental results and concluded that the STTP experiments were not relevant to WIPP conditions because of the high carbon dioxide partial pressure (SCA 2000).

The Agency also reviewed information related to MgO efficacy in WIPP and the formation of magnesium-carbonate phases on a number of additional occasions since the CCA. The Agency reviewed the uncertainty regarding the persistence of nesquehonite in the repository and concluded that no new evidence had been developed since the CCA to demonstrate that the MgO backfill would not behave as expected in the repository (TEA 2000; TEA 2001).

5.4 Evaluation of Reaction Products and Reaction Rates

Expected MgO hydration and carbonation reactions in the WIPP repository are described in US DOE 2004b, Appendix BARRIERS Section 2.3.2 and inclusion of these reactions in PA calculations of actinide solubilities is summarized in US DOE 2004b, Appendix PA Attachment SOTERM Section 3.5. DOE states that brucite is expected to be the only MgO hydration product that will form in the WIPP repository under humid conditions and under inundated conditions in the presence of ERDA-6 brines. However, in inundated experiments with GWB, the MgO hydration reaction produced both brucite and an amorphous or crystalline Mg-Cl-OH-H_2O phase. DOE states that modeling calculations with the FMT thermodynamic speciation and solubility code indicates that both brucite and $Mg_2Cl(OH)_3{\bullet}4H_2O$ are stable in GWB, but that long-term experiments with GWB suggest that brucite may be replacing the amorphous Mg-Cl-OH-H_2O phase (US DOE 2004b, Appendix BARRIERS Section 2.3.2.1).

Brush and Xiong (2003b) state that the solids in equilibrium with GWB included brucite and $Mg_2Cl(OH)_3{\bullet}4H_2O$ in actinide solubility calculations used in the CRA PA calculations for both microbial and nonmicrobial vectors. In US DOE 2004b, Appendix BARRIERS Section 2.3.2.3, DOE included $Mg_2Cl(OH)_3{\bullet}4H_2O$ in the discussion of the solids in equilibrium with GWB that would control carbon dioxide fugacities in the case of significant microbial activity. However, in US DOE 2004b, Appendix BARRIERS Section 2.3.2.4, DOE does not list the reaction of MgO with GWB to form $Mg_2Cl(OH)_3{\bullet}4H_2O$ as potentially buffering pH. Similarly, in US DOE 2004b, Appendix PA Attachment SOTERM Section 3.5, DOE does not include $Mg_2Cl(OH)_3{\bullet}4H_2O$ as an equilibrium solid phase in the calculations with GWB. However, based on the calculations reported in Brush and Xiong (2003a and 2003b), it appears that formation of $Mg_2Cl(OH)_3{\bullet}4H_2O$ in equilibrium with GWB was appropriately considered in PA solubility calculations.

Carbonation reactions involving MgO and brucite have been investigated by DOE under inundated conditions and at carbon dioxide pressures ranging from atmospheric to 5%. Nesquehonite formation (reaction 9 on page 31) was only observed at the highest carbon dioxide partial pressure, and nesquehonite apparently was being replaced by hydromagnesite$_{5424}$ as these experiments progressed (US DOE 2004b, Appendix BARRIERS Section 2.3.2.2). In all GWB and ERDA-6 inundated experiments with Premier MgO at atmospheric carbon dioxide partial pressures, hydromagnesite$_{5424}$ was the only magnesium-carbonate phase detected. DOE noted that magnesite appears to be the most stable magnesium-carbonate phase under WIPP repository conditions. However, because of the lack of experimental evidence of magnesite formation and the formation of hydromagnesite$_{5424}$ in the experiments conducted to date, DOE concluded that hydromagnesite$_{5424}$ will be the dominant magnesium-carbonate phase in the WIPP repository during the regulatory period (US DOE 2004b, Appendix BARRIERS Section 2.3.2.2). In the actinide solubility calculations for the CRA PA, DOE assumed that brucite-hydromagnesite$_{5424}$ would buffer carbon dioxide fugacities in PA vectors with significant microbial activity (US DOE 2004b, Appendix PA Attachment SOTERM Section 3.5). In PA vectors without significant microbial activity, DOE assumed that carbon dioxide fugacities would be buffered by brucite-calcite (Section 8.1.1).

DOE has adequately accounted for information developed since the CCA in their consideration of the magnesium-carbonate phases most likely to control pH and carbon dioxide fugacities in the WIPP repository. Based on the experimental results, the formation of nesquehonite appears to be transient and hydromagnesite$_{5424}$ is likely to be the most important magnesium-hydroxycarbonate phase in the repository during the regulatory time period. The formation of phases used in the actinide solubility modeling calculations, i.e., brucite, $Mg_2Cl(OH)_3{\bullet}4H_2O$, and hydromagnesite$_{5424}$ have been observed in experiments carried out by DOE under inundated and humid conditions. Thus, these phases are likely to form in the repository within the regulatory time period.

5.5 MgO Safety Factor Calculations

In the CCA, DOE assumed that all carbon in the repository was available for the formation of carbon dioxide (US EPA 1997). The amount of MgO to be placed in the repository was determined by DOE based on the assumed configuration of the waste and the calculation that approximately 4,000 lbs of MgO would be placed in the repository per linear foot of waste; this amount of MgO was calculated to be 8,560 tons per panel and 85,600 tons in the entire repository (US DOE 1996 Section 3.3.3). DOE determined that the total moles of MgO required to react with the maximum possible amount of carbon dioxide that could be generated was 9.85×10^8 moles, which is equivalent to 43,700 short tons of MgO (US EPA 1997). The Agency calculated the safety factor for the MgO backfill as the moles of MgO in the backfill divided by the maximum moles of carbon dioxide that could be produced; this safety factor was equal to 1.95 (US EPA 1997). The safety factor decreased to 1.67 when MgO minisacks were no longer placed with the waste (US EPA 2001a).

DOE cited the concept of sequential use of electron acceptors (US DOE 2004b, Appendix BARRIERS-2.5.1), in which nitrate and sulfate are successively consumed by microbial degradation reactions (Section 4.1.1). Because the quantities of nitrate and sulfate in the waste are limited, DOE stated that the majority of CPR degradation will take place by methanogenesis, in which CPR carbon is converted to equimolar amounts of carbon dioxide and methane (US DOE 2004b, Appendix BARRIERS Section 2.5.1); thus, DOE is now assuming that only approximately one-half of the total carbon in the repository could be converted to carbon dioxide. DOE cited experimental evidence of the formation of methane during CPR degradation (Section 4.2.1). Using this assumption of sequential use of electron acceptors, the CRA inventory of CPR, and assumptions regarding the numbers of various waste packages (e.g., TDOPs, standard waste boxes, etc.), DOE calculated an MgO safety factor of 2.45 for the CRA inventory (US DOE 2004b, Appendix BARRIERS Section 2.5.2; Table BARRIERS Section 3; Snider 2003a).

DOE's safety factor calculations only accounted for sulfate that is present in the waste and did not include the effects of sulfate that naturally occurs in the Salado Formation. Because anhydrite is dispersed in the halite interbeds and is present as interbeds in the Salado Formation, abundant sulfate will be available to repository brines. In fact, abundant sulfate minerals were assumed by DOE for FMT modeling of actinide solubilities, which were carried out assuming equilibrium of the brines with anhydrite (US DOE 2004b, Appendix PA Attachment SOTERM Section 3.5). Because of the sulfate present in the Salado Formation, the possibility that microbial degradation of CPR could take place only through denitrification and sulfate reduction, thereby converting all carbon in the repository to carbon dioxide, cannot be ruled out. Although microbial degradation experiments carried out for WIPP have generated methane, these experiments were not performed with excess sulfate and therefore do not show that methanogenesis will definitely occur in the WIPP repository. Snider (2003a) calculated the safety factor for the WIPP repository assuming that all CPR carbon could form carbon dioxide (the EPA safety factor). This safety factor was 1.30, a significant reduction from the Agency-approved value of 1.67.

The CRA safety factor calculations were carried out assuming homogeneous waste loading in the repository (Snider 2003a). However, waste loading in Panel 1 of the repository has not been homogeneous. Because shipments of waste placed in Panel 1 included an intensive campaign from Rocky Flats, 54% of the waste in Panel 1 was from this site (Leigh 2003). DOE has stated that this situation could be representative of waste shipments from the Advanced Mixed Waste Treatment Facility (AMWTF) when this site begins shipping compressed waste (Hansen 2003), and it is reasonable to assume it could also be representative of shipments from other sites. Compressed waste from the AMWTF has significantly higher CPR densities than non-AMWTF waste (Leigh and Lott 2003; Leigh 2003); therefore, the CRA safety factor calculations should account for the possibility that high proportions of compressed waste may be loaded into individual rooms in each panel.

DOE attempted to account for heterogeneous loading of high-CPR AMWTF waste in safety factor calculations described in a reference cited by the CRA (Snider 2003a). In these calculations, it was assumed that supercompacted and uncompacted waste from the AMWTF would be shipped to the repository in amounts proportional to their total volumes (Conservative Panel X Scenario). Based on information provided by DOE at an Agency/DOE technical exchange meeting (October 21 and 22, 2003), shipments of uncompacted AMWTF waste are likely to be completed several years before shipments of supercompacted waste. During the last few years of operation of the AMWTF, it is likely that only supercompacted waste will be generated, and this waste will be placed in WIPP with waste from other generator sites. This latter scenario is likely to result in significantly lower MgO safety factors than the scenario considered by DOE (Snider 2003a), because average non-AMWTF contact-handled waste has significantly higher CPR densities than uncompacted AMWTF waste. An MgO safety factor of 1.05 was calculated for the "conservative Panel X" scenario assuming that methanogenesis did not occur (Snider 2003a). This safety factor is significantly less than the previously approved value of 1.67; if non-AMWTF contact-handled waste is included in the calculations instead of uncompacted AMWTF waste, the MgO safety factor will be less than 1.05.

In the MgO safety factor calculations presented in the CRA, Snider (2003a) assumed one supersack would be placed on top of each TDOP. This assumption was based on one TDOP occupying the space of three seven-packs of 55-gallon drums. However, one TDOP occupies the space of only two seven-packs (Triay 2004). Erroneously assuming that one TDOP takes up the space of three seven-packs caused a lower ratio of waste to MgO in the safety factor calculations, and resulted in an overestimation of the MgO safety factor.

Snider (2003a) used a value of 0.846 in the safety factor calculations to correct for the proportion of reactive MgO in the Premier MgO. This proportion was based on the maximum extent of reaction observed in inundated MgO hydration experiments carried out at 90°C in deionized water and humid MgO hydration experiments carried out at 80°C and 95% relative humidity (Snider 2003b). This fraction is consistent with the reported presence of approximately 10% unreactive impurities based on XRD analysis of Premier MgO (Snider 2003c).

When calculating the amount of CPR in the repository for the CRA PA, DOE did not take into account the materials external to the waste containers, such as shrink wrap placed around the 55-gallon drum seven-packs or the support sheets and packaging materials used for the MgO supersacks (US EPA 2004a, Comment G-2). DOE assessed the quantities of emplacement materials relative to the quantities of CPR reported in the CRA and found that accounting for these material would increase the CPR inventory by 12.7% (US DOE 2004d). DOE stated that PA calculations had been carried out with 250% of the CPR quantity used in the CRA PA, and comparison of the results with the CRA PA had indicated that the results of the increase were relatively minor. Therefore, DOE concluded that the omission of the CPR materials external to the waste packages was unlikely to have had a significant effect on the conclusions of the CRA PA (US DOE 2004d).

The Agency pointed out that the MgO safety factor had not been appropriately computed for the CRA (US EPA 2004a, Comment C-23-5). The Agency reiterated the condition that DOE must maintain a 1.67 MgO safety factor, and requested that DOE provide a plan for implementing this condition (US EPA 2004a, Comment G-4). DOE responded that they would take the necessary measures to ensure that necessary amounts of MgO are emplaced within the repository, and committed to providing the plan requested by the Agency (US DOE 2004e, US DOE 2004f).

Because of its importance in calculating the MgO safety factor, the Agency requested that DOE provide new and convincing evidence that methanogenesis will be the dominant reaction by which CPR degradation occurs. The Agency stated that in the absence of such new evidence, DOE must assume that microbial degradation of CPR will take place through denitrification and sulfate reduction when calculating the MgO safety factor (US EPA 2004c). DOE provided additional information at a technical information exchange meeting in October 2004 indicating that the MgO safety factor would be calculated assuming that all CPR carbon could be converted to carbon dioxide (TEA 2004b).

5.6 Conclusions and Key Issues

Review of Appendix BARRIERS to the CRA (US DOE 2004b) has indicated that DOE's incorporation of new information regarding MgO hydration and carbonation reactions is adequate. The MgO hydration and carbonation reactions used in the CRA actinide solubility calculations are consistent with data developed since the CCA. MgO will react to form brucite and possibly $Mg_2Cl(OH)_3 \cdot 4H_2O$; MgO and brucite will react with carbon dioxide to produce hydroxymagnesite. The most likely formula for hydromagnesite is $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O(s)$, based on the results of experiments conducted by DOE since the CCA. Although transient formation of nesquehonite has been observed in some experiments, this phase does not appear likely to persist. Even though magnesite is the most thermodynamically stable magnesium-carbonate phase, it may not form under WIPP repository conditions during the relevant time frame. Therefore, DOE appropriately used metastable hydromagnesite$_{5424}$ as the magnesium-carbonate phase most likely to form in the repository and control carbon dioxide partial pressures.

The MgO safety factor calculated by DOE in US DOE 2004b, Appendix BARRIERS is not conservative because methanogenesis may not occur. MgO safety factor calculations should account for the possibility that all carbon in the repository could be converted to carbon dioxide because of the availability of sulfate in the Salado Formation and WIPP brines. DOE now plans to calculate MgO safety factors assuming the potential for complete conversion of CPR carbon to carbon dioxide (TEA 2004b). Waste loading in Panel 1 has demonstrated that waste placement in the repository is likely to be heterogeneous. Tight panel seals could prevent brine mixing between panels, so enough MgO should be included in each room of each panel to ensure an adequate safety factor under heterogeneous waste loading conditions, such as those that may occur when supercompacted AMWTF waste is preferentially loaded in a panel with non-AMWTF contact-handled waste.

If future MgO safety factor calculations include assumptions regarding the space occupied by the waste packages, it should be assumed that a TDOP only takes up the space of two 55-gallon drum seven-packs, not three, as was assumed for the CRA. Future MgO safety factor calculations also should take into account the CPR in the repository from shrink wrap placed around waste packages and support sheets and packaging materials used for the MgO supersacks. DOE has proposed to track the amounts of MgO backfill and CPR as they are emplaced in each room to ensure that the required MgO safety factor of 1.67 is maintained on a room-by-room basis (US DOE 2004f). DOE has corrected this issue in the safety factor calculation in the CRA.

6.0 ACTINIDE OXIDATION STATES

The actinide oxidation states assumed in the CRA PA were unchanged since the CCA (US DOE 2004b, Appendix PA Attachment SOTERM Section 4.0). The actinide oxidation states were determined based on the assumption that reducing conditions would be established relatively quickly in the WIPP repository (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.3), combined with a literature review and experimental investigations (US DOE 2004b, Appendix PA Attachment SOTERM Section 4.0). The stable oxidation states in the WIPP repository environment were determined to be:

- Americium(III), curium(III) and thorium(IV);
- Plutonium(III) and plutonium(IV);
- Neptunium(IV) and neptunium(V); and
- Uranium(IV) and uranium(VI).

The FMT model does not include calculations to determine redox states, therefore for plutonium, neptunium, and uranium, each of which may be present in two oxidation states, an oxidation-state parameter (OXSTAT) was sampled uniformly (US DOE 2004b, Appendix PA Attachment PAR). The lower oxidation states of these constituents were assumed for half of the PA calculations, and the higher oxidation states were assumed for the other half of the calculations.

6.1 Actinide Oxidation State Information Developed Since the CCA

Grambow et al. (1996) evaluated the sorption and reduction of uranium(VI) from brine solutions on iron corrosion products, including hydrous iron(II)-magnesium oxides and magnetite, under anoxic conditions. Addition of uranium(VI) to experiments with brine and iron corrosion products produced a rapid decrease in aqueous uranium concentrations. Most of the uranium associated with the solid phases appeared to be uranium(VI) rather than uranium(IV), so sorption of uranium(VI) appeared to be the dominant process for removing uranium from solution. In the solution phase, reduction of uranium(VI) to uranium(IV) was observed, but to a lesser extent than predicted by thermochemical calculations. The cause of this discrepancy was not determined.

The Actinide Source-Term Waste Test Program (STTP) included a series of experiments conducted with WIPP brines in contact with actual TRU waste (Villarreal et al. 2001). The experiments were designed to simulate anticipated repository conditions based on the conceptualization of the WIPP repository at the time the experiments began. The presence of plutonium(V) and plutonium(VI) was detected in samples from a few STTP experiments (US DOE 2004b, Appendix PA Attachment SOTERM- Section 4.8). Plutonium(V) was observed in two of the experiments, but the plutonium(V) concentrations decreased with time, consistent with the assumption that plutonium would be present in the repository as plutonium(III) and plutonium(IV) oxidation states over the long term. Concentrations of plutonium(VI) that did not decrease with time were observed only in two experiments with high carbon dioxide overpressures (60 bars) and pH values of approximately 5. DOE maintained that these conditions are not representative of the WIPP repository because of the presence of MgO backfill, and that these experiments and the observation of plutonium(VI) that persisted in solution are not relevant to WIPP repository conditions (US DOE 2004b, Appendix PA Attachment SOTERM Section 4.8).

Haschke et al. (2000) reported that PuO_{2+x}, (in which x is less than or equal to 0.27) is the stable binary plutonium oxide phase in air. This phase contains a significant amount of plutonium(VI) in addition to plutonium(IV) in its structure. Previous investigations indicated that PuO_2, which contains only plutonium(IV), is the most stable plutonium oxide. Because plutonium(IV) solids are relatively insoluble, plutonium is generally considered to be relatively immobile under most environmental conditions. Based on the Haschke et al. (2000) article, Madic (2000) stated that the presence of plutonium(VI) in PuO_{2+x}, which could increase plutonium mobility in the environment, should be considered in safety evaluations of long-term plutonium storage.

The formation of the higher oxide PuO_{2+x} occurs by reaction of PuO_2 with water in moist air or moist oxygen:

$$PuO_2(s) + x\ H_2O(\text{adsorbed}) \rightarrow PuO_{2+x}(s) + x\ H_2(g)$$

over the temperature range of 25 to 350°C (Haschke et al. 2000). The progress of this reaction was monitored by evaluating the formation of hydrogen gas. This reaction occurs via a catalytic cycle, in which adsorbed water reacts with the plutonium oxide solid to form PuO_{2+x}, and in the presence of O_2, atomic hydrogen on the solid surface reacts to re-form H_2O. However, this reaction has not been demonstrated to occur in brines or in the presence of reductants such as iron metal.

Xia et al. (2001) investigated the distribution of plutonium, neptunium, and uranium oxidation states in synthetic ERDA-6 WIPP brine in the presence of powdered metallic iron. These experiments were carried out under an inert (argon) atmosphere over a pH range from approximately 8 to 12. The results of these experiments indicated that the effects of adding iron powder on the plutonium(VI) concentrations in solution (initially 2.5×10^{-4} M) depended on pH. At pH values less than 9, iron addition resulted in decreased Eh values and plutonium(VI) decreased to concentrations ranging from 10^{-5} to 10^{-8} M. However, at pH values of 9 to 12, iron addition produced only small decreases in Eh values and plutonium(VI) concentrations. Xia et al. (2001) attributed this limited effect at higher pH to the formation of coatings that limited the availability of the iron metal to the brine. To confirm the formation of coatings as the cause of the limited effects of the powdered iron, a second addition of iron powder was carried out in the higher-pH experiments. This second iron addition reduced measured Eh and plutonium concentrations in the brine solution at pH values of approximately 9 and 12, although the effects at pH 10 were small. Spectroscopic examination of the brines indicated that 85-90% of the plutonium remaining in solution was present in the +V oxidation state. Xia et al. (2001) interpreted these results to mean that more iron was required to maintain reducing conditions in higher-pH brine solutions. Absorption spectroscopy was used to determine that plutonium(VI) disappeared in brine solutions with added iron powder. Xia et al. (2001) suggested that the plutonium in solution could be plutonium(V) in equilibrium with $PuO_2 \cdot xH_2O(s)$, although the concentration of plutonium(V) in the monitored solution was below the detection limit for spectrophotometric determination.

In experiments carried out by Xia et al. (2001) with neptunium(V) in synthetic ERDA-6 brine, iron addition decreased neptunium solution concentrations and appears likely to have reduced neptunium(V) to neptunium(IV). In experiments with uranium(VI) in ERDA-6 brine, iron addition did not result in the reduction of uranium(VI) to uranium(IV), probably because of the effects of the brine on the reducing capacity of iron powder (Xia et al. 2001).

Reed et al. (1997) reported experimental results related to the effects of oxalic acid, citric acid, and EDTA on the stability of neptunium(VI) and plutonium(VI) in brine solutions. These complexing agents are important because they have been reported in the WIPP inventory (Section 8.6). A mixture of EDTA, citrate, and oxalate were added to ERDA-6 brine at pH values of 8 and 10 with 10^{-4} M carbonate, to ERDA-6 brine at pH 10 without carbonate, and to G-Seep brine at pH 5 and 7 without carbonate. In the G-Seep brine, the plutonium(VI) was rapidly reduced to form plutonium(V) and plutonium(IV) organic complexes. The presence of carbonate in the ERDA-6 brine at pH 8 slowed the reduction rate of plutonium(VI) to plutonium(IV) and plutonium(V) species. At pH 10 in the presence of carbonate, no reduction was observed and the plutonium(VI)-carbonate complex predominated in solution. In the absence of carbonate at pH 10 in ERDA-6 brine, slow reduction of plutonium(VI) was observed. Based on these results, it appears that hydrolytic and carbonate species stabilize plutonium(VI) with respect to reduction by the organic ligands. The addition of iron coupons to these experiments caused the reduction of plutonium(VI) to plutonium(IV) and the consequent reduction of plutonium concentrations in solution (ANL 1997).

In experiments with citrate, oxalate, and EDTA at pH 5 and 7 in G-Seep brine, neptunium(VI) was rapidly reduced to neptunium(V) (Reed et al. 1997). There was no evidence of further reduction of neptunium(V) to neptunium(IV) after two months duration. The presence of carbonate complexes at pH values of 8 and 10 in ERDA-6 brine slowed the rate of neptunium(VI) reduction. In the absence of carbonate at pH 10, neptunium(VI) was rapidly removed from solution to form neptunium(IV) and (V) organic complexes and precipitates.

Humic acids are likely to form in the WIPP repository as a product of microbial degradation of CPR (US DOE 2004b, Appendix PA Attachment SOTERM-2.2.2). The reduction of plutonium(V) by humic acids was investigated in 5 m NaCl in the presence and absence of divalent cations (calcium and magnesium) at pcH[III] values of 5.7 and 8 (André and Choppin

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[III] pcH = $-\log(M_{H^+})$, where M_{H^+} is the molar concentration of the hydrogen ion in solution

2000). Increasing concentrations of divalent cations and humic acid increased the rates and percentages of plutonium(V) reduced by the humic acid.

6.2 Agency Reviews Related to Actinide Oxidation States

The Agency reviewed and agreed with the expected oxidation states used in the CCA PA and PAVT. At the time of the CCA, most stakeholder questions related to actinide oxidation states concerned the possible persistence of plutonium(VI) in the WIPP repository. The Agency (US EPA 1998c) considered a number of experimental studies that indicated reductants, including soluble iron, metallic iron, humics, and other organic ligands, would reduce plutonium to the (III) and (IV) oxidation states under equilibrium conditions in the repository (Weiner 1996; Felmy et al. 1989; Rai and Ryan 1985; Choppin 1991).

Questions were raised by EEG regarding whether higher oxidation states of plutonium might persist in repository brines. The evidence cited by EEG included the observation of higher plutonium oxidation states in solution samples from the STTP experiments and the possible formation of $PuO_{2+x}(s)$ in the WIPP repository, which could increase plutonium concentrations in repository solutions (Haschke et al. 2000; Oversby 2000). EEG also believed that the equilibrium model for calculating plutonium solubility was inadequate and proposed a model based on kinetics (TEA 2001; Haschke and Oversby 2001).

The Agency reviewed the STTP results and the evidence cited by EEG on a number of occasions to determine whether this evidence contradicted the assumption that plutonium would be present in the (III) and (IV) oxidation states in the equilibrium WIPP repository (MFG 2000; TEA 2001; TEA 2002). The Agency concluded that the observation of plutonium(V) and plutonium(VI) in the STTP experiments does not challenge the assumptions of lower plutonium oxidation states (III and IV) in the repository. The observations of plutonium(V) and (VI) in the STTP solution samples were sometimes transient, the redox conditions and carbon dioxide partial pressures in the STTP experiments were inconsistent with the conditions expected in WIPP repository environment, and the plutonium(V) and (VI) detected in the experiments may have been caused by oxidation of the solutions after the samples were removed from the tests (MFG 2000). Therefore, the STTP experimental results do not appear to be reliable indicators of equilibrium plutonium oxidation states or actinide solubilities in the WIPP repository environment.

The Agency considered the possible formation of $PuO_{2+x}(s)$ in the WIPP repository and concluded that no experimental evidence of its formation was available in brines or in the reducing conditions anticipated in the repository (MFG 2000; TEA 2002). On the other hand, the Agency observed that experimental studies (Grambow et al. 1996; Slater et al. 1997) in addition to the studies previously considered for the CCA have shown that iron metal and iron corrosion products reduce actinide oxidation states and actinide solution concentrations in brines (MFG 2000; TEA 2001).

6.3 Conclusions

The available information regarding microbial degradation of CPR and anoxic corrosion of iron-based metal indicates that reducing conditions will be maintained in the WIPP repository. No new evidence has been developed since the CCA related to the assumptions that americium(III), curium(III), and thorium(IV) will be the only stable oxidation states of these actinides at equilibrium.

The Reed et al. (1997) data were considered in interim form during the CCA (Reed et al. 1996). The results of this investigation indicated that both neptunium(IV) and neptunium(V) could be present in the repository because of the stabilization of neptunium(V) by organic ligands. The results of Xia et al. (2001) indicate that in the absence of ligands, neptunium(V) may be reduced to neptunium(IV) by metallic iron in the WIPP repository environment. Because of the uncertainty regarding whether neptunium will be present in repository brines in the +IV or +V oxidation state, DOE has continued to assume that either oxidation state is equally likely for the purposes of PA.

The information available at the time of the CCA regarding uranium oxidation states, as well as the data from the investigation by Xia et al. (2001) indicates that it may be possible for uranium(VI) to persist in the repository environment. Therefore, uranium(IV) was assumed to be the dominant oxidation state for half the CRA PA vectors, and uranium(VI) was assumed to be the dominant oxidation state for the other half of the CRA PA vectors.

The available evidence continues to support the assumption that plutonium(III) or plutonium(IV) oxidation states will be present in the equilibrium WIPP repository. The results of the STTP experiments, which seemed to indicate the possible persistence of plutonium(V) and plutonium(VI) species under repository conditions (Villareal et al. 2001), are not applicable to WIPP. In addition, the formation of $PuO_{2+x}(s)$ (Haschke et al. 2000) has not been observed under the reducing conditions expected in the WIPP repository or in brines. However, questions have been raised regarding the possible persistence of plutonium(V) in the long-term WIPP repository. Plutonium(V) was the dominant oxidation state observed in some experiments with ERDA-6 brine and metallic iron, probably because coatings formed on the iron metal and limited its reducing capacity (Xia et al. 2001). Reed et al. (1997) observed that carbonate and hydrolytic complexes of plutonium(VI) slowed down or prevented its reduction by citrate, oxalate, and EDTA. However, in these experiments, the addition of iron metal coupons to the brines resulted in plutonium(VI) reduction to plutonium(IV) and the precipitation of plutonium(IV) solids (ANL 1997). The reasons for the different effects of iron metal in the experiments reported by ANL (1997) and Xia et al. (2001) are unclear. Despite this inconsistency, most of the evidence indicates that plutonium(III) and plutonium(IV) are the appropriate oxidation states in the long-term WIPP repository.

7.0 EFFECTS OF HETEROGENEOUS WASTE LOADING

In solubility calculations for the CCA PA, PAVT and CRA PA, it was assumed that waste would be homogeneously loaded in the repository. At the time of the CCA, no information was available regarding the potential patterns of waste loading that might occur, and this assumption was appropriate. However, information now available about Panel 1 waste loading indicates that it has not been homogeneous. Because shipments of waste placed in Panel 1 included an intensive campaign of waste shipments from Rocky Flats, 54% of the waste in Panel 1 was from this site (Leigh 2003). In addition, inclusion of the Option D panel closure makes it less likely that brine in contact with waste in one panel of the repository will contact brine in another panel. Therefore, it is necessary to consider the potential effects of waste heterogeneity on the results of PA.

Heterogeneous waste loading has the potential to affect actinide solubility calculations. Heterogeneous waste loading also may have a significant effect on the MgO safety factor calculations, which was addressed in Section 5.5 of this report.

EEG has questioned whether the assumption of homogeneous chemical conditions in the repository is appropriate (Oversby 2000). As an alternative to the approach used by DOE, EEG recommended calculating releases that would occur if a small number of waste drums containing relatively high concentrations of actinides and organic ligands are intersected by a borehole. This waste could be leached by drilling fluid, and if this borehole then reached an underlying brine pocket, EEG maintained that an unacceptable release of actinides could result. EEG recommended that DOE assess repository performance by calculating the range of actinide concentrations that could be released under this scenario, and multiplying by the probability of the scenario. The Agency considered the approach suggested by EEG on several occasions (US EPA 1998a, TEA 2000, TEA 2001). The Agency observed that performance assessments for the CCA and PAVT were based on a probabilistic approach rather than the calculation of solubilities associated with a worst-case scenario as suggested by EEG, and this probabilistic approach had been peer-reviewed and found to be acceptable. The Agency found that the effects of waste heterogeneity on PA were adequately addressed by the uncertainties assigned to the actinide solubilities (US EPA 1998a, TEA 2000, TEA 2001).

Information regarding waste loading in Panel 1 of the WIPP repository has indicated that waste is unlikely to be homogeneously distributed throughout the repository. In addition, tight panel seals are likely to limit mixing of brine between panels in an inundated repository. Consequently, the Agency requested that DOE address the potential effects of heterogeneous waste loading on the assumption of homogeneous chemical conditions throughout the entire repository (US EPA 2004c, Comment G-12).

DOE responded to this request for additional information with an assessment of the potential effects of higher amounts of plutonium in Panel 1 than would be expected based on homogeneous emplacement throughout a 10-panel repository (US DOE 2004c). DOE stated that the only likely effect of this higher-than-expected loading of plutonium in Panel 1 would be increased radiolysis that could cause plutonium to speciate as plutonium(V) or plutonium(VI) instead of the reduced oxidation states predicted for the repository (Section 6.0). However, because of microbial consumption of CPR and the amounts of metallic iron in the repository, including the large amounts of stainless steel in the pipe overpacks in Panel 1, DOE believes that reducing conditions and lower plutonium oxidation states will still be maintained in Panel 1.

Heterogeneous waste loading is unlikely to affect actinide solubilities if a relatively high proportion of the actinide inventory is present in a single panel because of the assumption of chemical equilibrium. However, the placement of waste with a high proportion of the organic ligand inventory in a panel could affect actinide solubilities. DOE has accounted for this possibility in the actinide solubility calculations by assuming that the entire organic ligand inventory is dissolved in the minimum amount of brine necessary for a release from the repository (US DOE 2004b, Appendix PA Attachment SOTERM-5.0). This approach ensures that the effects of heterogenous waste placement are adequately accounted for in the actinide solubility calculations, provided that the inventory of organic ligands is adequately bounded.

8.0 ACTINIDE SOURCE TERM MODELING

A number of assumptions used in actinide source term modeling for the CRA PA remain unchanged since the CCA PA and PAVT, as well as the PABC, including:

- Use of end-member Salado and Castile brine compositions to represent the range of brine compositions that may occur in the repository;
- Brine in the repository is well-mixed with waste;
- The dissolved concentrations of the actinides are limited by solubility-controlling solids in WIPP brines;
- FMT calculations of the solubility of americium(III), thorium(IV), and neptunium(V) are used for the solubilities of other actinides in these oxidation states, i.e., plutonium(III), plutonium(IV), uranium(IV), and neptunium(IV). This was referred to in the CCA and CRA as the oxidation state analogy;
- Repository brines are in equilibrium with halite and anhydrite, but equilibrium with respect to oxidation-reduction (redox) reactions is not assumed; and
- Salado or Castile brine compositions are maintained throughout the 10,000 year regulatory period at the compositions attained after equilibration with MgO

(US DOE 2004b, Appendix PA Attachment SOTERM Sections 2.2.1 and 3.3). However, some changes in assumptions related to actinide source term modeling have been implemented since the CCA. These changes include:

- Salado brine composition (Section 3.0);
- No microbial colloidal transport of actinides in PA vectors without significant microbial activity; and
- The mineral assemblage that buffers carbon dioxide fugacity in the absence of significant microbial activity.

Changes in modeling assumptions, new information related to actinide source term modeling, and the apparent effects on modeled actinide solubilities are addressed in the following sections.

8.1 Modeling Assumptions in the Absence of Significant Microbial Activity

For the CRA PA, DOE assumed a probability of 0.5 for the occurrence of significant microbial degradation of CPR in the WIPP repository, meaning that in one-half the PA vectors, no significant microbial degradation occurred and significant microbial degradation occurred in the other one-half of the PA vectors (US DOE 2004b, Appendix PA Attachment SOTERM-2.2.2).

This assumed microbial degradation probability has remained unchanged since the CCA. However, as addressed in Section 4.4 of this report, significant additional information has become available since the CCA that indicates a relatively high probability of microbial degradation of CPR in the WIPP repository.

In the CRA PA, the assumed probability of microbial degradation affected the amounts of gas generation modeled for different PA vectors, and also affected actinide source term modeling. In PAVT solubility calculations, DOE assumed that carbon dioxide fugacities were controlled by the brucite-hydromagnesite$_{5424}$ reaction and microbial colloid formation was assumed to contribute to the actinide source term. These assumptions remained unchanged in the CRA PA for vectors that included significant microbial degradation of CPR. However, for CRA PA vectors that did not include significant microbial degradation of CPR, DOE assumed that carbon dioxide fugacities were controlled by the brucite-calcite reaction:

$$\mathrm{Mg(OH)_2 + Ca^{2+} + CO_2(aq\ or\ g) \rightleftharpoons CaCO_3 + Mg^{2+} + H_2O(aq\ or\ g)} \qquad (11)$$

(US DOE 2004b, Appendix PA Attachment SOTERM Sections 2.2.2 and 3.5) and also assumed microbial colloids did not contribute to the actinide source term (Table SOTERM-11).

8.1.1 Control of Carbon Dioxide Fugacities

DOE addressed the different reactions likely to buffer carbon dioxide fugacity in the CRA (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.2; US DOE 2004b, Appendix BARRIERS Section 2.3.2.4). DOE stated that calcite is stable under WIPP conditions and has been observed to form readily at low temperatures in GWB and ERDA-6 brines because of the rapid carbonation of lime or portlandite [$Ca(OH)_2(s)$] (US DOE 2004b, Appendix BARRIERS Section 2.3.2.4). In PA vectors with significant microbial production of carbon dioxide, DOE stated that the amount of calcium ion available is likely to be overwhelmed by the amount of carbon dioxide, so the brucite-calcite reaction (11) was suppressed to allow the brucite-hydromagnesite$_{5424}$ reaction to control carbon dioxide fugacities. However, in the absence of significant microbial carbon dioxide production, DOE stated that sufficient calcium ion would be available to allow control of carbon dioxide fugacities by the brucite-calcite reaction (US DOE 2004b, Appendix BARRIERS Section 2.3.2.4).

The FMT modeling runs used in the CRA PA are listed in Table 8-1. The pH values and carbon dioxide fugacities calculated for the different microbial vectors and the nonradioactive solid phases in equilibrium with the brines are summarized in Table 8-2. In the CRA PA calculations with ERDA-6 (Castile) brine, the brucite dissolution reaction buffered the pH, brucite-hydromagnesite$_{5424}$ buffered the carbon dioxide fugacity in microbial vectors, and brucite-calcite buffered carbon dioxide fugacity in nonmicrobial vectors. The presence of $Mg_2Cl(OH)_3{\bullet}4H_2O(s)$ in the GWB (Salado) phase assemblage indicates that pH was buffered by both brucite and $Mg_2Cl(OH)_3{\bullet}4H_2O(s)$ dissolution reactions, both brucite-hydromagnesite and $Mg_2Cl(OH)_3{\bullet}4H_2O(s)$-hydromagnesite$_{5424}$ buffered the carbon dioxide fugacity in microbial vectors, and both brucite-calcite and $Mg_2Cl(OH)_3 \cdot 4H_2O(s)$-calcite buffered carbon dioxide fugacity in nonmicrobial vectors (Brush and Xiong 2003a).

For the GWB (Salado) nonmicrobial vector calculations, the carbon dioxide fugacity was very similar to the value calculated for the microbial vector. However, for the ERDA-6 (Castile) brine, the carbon dioxide fugacity was significantly lower for the nonmicrobial vector than the microbial vector (Table 8-2). The reason for this difference is not readily apparent. Examination of the FMT output file for the nonmicrobial GWB calculations (FMT run 12) indicates that the precipitation of hydromagnesite$_{5424}$ was prevented. There does not appear to be a valid reason for suppressing hydromagnesite$_{5424}$ formation, because hydromagnestite$_{5424}$ has been observed to form readily in low-temperature experiments (Section 5.2.3).

Comparison of the actinide solubilities calculated for the microbial and nonmicrobial CRA PA vectors indicates that the lower carbon dioxide fugacity that resulted from assuming control by the brucite-calcite buffering reaction had negligible effects on the actinide solubilities for the GWB (Salado) brine and on (III) actinide solubilities for the ERDA-6 (Castile) brine. However, the lower carbon dioxide fugacity in the nonmicrobial vector affected the (IV) and (V) actinide solubilities calculated for Castile brine (Table 8-2): (IV) actinide concentrations were lower and (V) actinide concentrations were higher in the nonmicrobial vectors. Because the (IV) actinide solubilities appear to be more significant for PA, the effects of assuming the lower carbon dioxide fugacities associated with the brucite-calcite reaction appear to have been nonconservative for Castile brine.

DOE did not provide adequate information to support the assumption that brucite-calcite reaction would control the carbon dioxide fugacity in nonmicrobial vectors. In particular, DOE did not adequately define “the absence of significant microbial activity in the WIPP” (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.2). DOE does not state that the amounts of microbial degradation will be zero in these vectors, but that the amount will be small. However, even if a small amount of CPR degradation occurs when judged in terms of the volume of gas generated, it is possible that the effects on the chemistry of the system could be important. DOE did not perform a mass-balance calculation to indicate how much or how little degradation would be required to produce amounts of carbon dioxide sufficient to essentially remove all calcium in the brines and result in buffering by the brucite-hydromagnesite reaction (7). However, because microbial degradation probability has been increased, essentially including some microbial degradation in all vectors (Section 4.4), the assumption that brucite-calcite will buffer carbon dioxide fugacities in some vectors is not included in the PABC calculations (Brush 2005).

8.1.2 Microbial Colloids

The formulation of the colloidal actinide source term calculations presented in the CRA appears to be unchanged since the CCA. The Agency previously reviewed DOE’s approach for modeling the colloidal actinide source term and found it to be adequate for use in PA (US EPA 1998c).

A potentially significant change in the implementation of the colloidal actinide source term was DOE's assumptions regarding the contribution of microbial colloids to the actinide source term in the case of PA vectors without significant microbial degradation. For all PA vectors in the CCA PA and the PAVT, DOE assumed that microbial colloids would contribute to the actinide source term (US DOE 2004b, Appendix TRU WASTE Section 2.4.2). However, for CRA nonmicrobial vectors, DOE assumed that microbial colloid transport would not occur. The elimination of microbial colloid transport of actinides in the nonmicrobial vectors could have significantly affected the total actinide concentrations calculated for the CRA actinide source term, because the actinide concentrations associated with microbial colloids can be several multiples of the dissolved actinide concentrations (US DOE 2004b, Appendix TRU WASTE Section 2.4.2).

Relatively small amounts of microbial degradation may occur in nonmicrobial vectors, and DOE has not defined the level of degradation necessary for microbial colloid formation to significantly affect the actinide source term. Because microbial degradation will be assumed to occur in all vectors for the PABC, microbial transport of actinides is included in all PABC vectors.

8.2 Uranium(VI) Solubility

DOE has not developed a solubility model for uranium(VI). DOE has stated that the hydrolysis behavior of uranium(VI) in basic solutions is complicated, and a satisfactory solubility model is therefore unavailable. Hobart and Moore (1996) estimated that the appropriate uranium(VI) concentration was 1×10^{-5} m, based on an assessment of the limited experimental data available at the time. The selected concentration was not a conservative estimate; instead, this value was selected because it was within the range of the available experimental values.

The uranium(VI) solubility used in the CCA PA, the PAVT, and the CRA PA was 8.8×10^{-6} M (US DOE 1996, Appendix SOTERM Table SOTERM-2; US DOE 2004b, Appendix PA Table PA-8 and Appendix PA Attachment SOTERM Table SOTERM-2). However, the text in both the CCA and the CRA erroneously states that Hobart and Moore (1996) estimated the solubility of uranium(VI) at pH 10 in the absence of carbonate to be 8.8×10^{-5} M. In addition to this typographical error, DOE appears to have created some confusion related to the concentration units used for the uranium(VI) concentrations. Both molal (moles/kg) and molar (moles/liter) units are used. For dilute solutions, these units are roughly equivalent because at 25°C, 1 liter of aqueous solution should have a weight of approximately 1 kilogram. However, the density of the WIPP brines is approximately 1.2 kg/liter (US DOE 2004b, Table 2-6). Thus, if the uranium(VI) concentration is 1×10^{-5} m (Hobart and Moore 1996), multiplication by the specific gravity would yield a concentration of 1.2×10^{-5} M. Instead, DOE appears to have divided by the specific gravity, resulting in the use of a smaller uranium(VI) concentration.

8.2.1 Agency's CCA Review of Uranium(VI) Solubility

The Agency reviewed DOE's predictions of uranium(VI) solubilities, including the information in the CCA and supporting documents (Hobart and Moore 1996; Novak and Moore 1996), and additional information that became available after the CCA (US EPA 1998c). The Agency noted two assumptions that DOE relied on in selecting this uranium(VI) concentration for PA. One of DOE's assumptions was that carbonate would be completely absent from repository brines, when in fact the brucite-hydromagnesite$_{5424}$ reaction will control carbonate concentrations at relatively low, but non-zero levels. Another assumption was that a model for uranium(VI) could not be developed because of uncertainties regarding uranium(VI) hydrolysis species; the Agency noted that the dominant species in the pH range relevant to the WIPP repository are likely to be carbonate complexes such as UO_2CO_3, $UO_2(CO_3)_2^{2-}$, and $UO_2(CO_3)_3^{4-}$ (US EPA 1998c). Therefore, precise knowledge of the stabilities of the hydrolysis species may not be necessary to model uranium(VI) speciation under the expected repository conditions, because only a small fraction of the total dissolved uranium(VI) exists as hydrolysis species. However, the Agency accepted the use of a single uranium(VI) concentration in PA because it was consistent with the available data presented in Reed and Wymans (1997) as well as Hobart and Moore (1996), and because these data were used with the actinide solubility uncertainty range developed for the CCA.

8.2.2 Review of Currently Available Uranium(VI) Solubility Data

DOE (2004b) did not evaluate new data since the CCA regarding the solubility of the +VI actinides. The Agency requested additional information from DOE regarding relevant actinide solubility data developed outside the WIPP program since the CCA (US EPA 2004c, Comment C-23-14). In their response, DOE cited data that were included in the FMT database for the +III, +IV, and +V actinides, but did not address the +VI actinides (US DOE 2004c).

The available data related to uranium(VI) solubility in NaCl brines were reviewed to determine whether the uranium(VI) concentration used in the CRA PA is still justified. Although solubility data are available for uranium(VI) solids from a number of sources, many of these data are not applicable to the high ionic strength NaCl brines and moderately alkaline pH conditions in the repository. The relevant carbonate ion (CO_3^{2-}) concentrations for the WIPP repository in equilibrium with hydromagnesite$_{5424}$ and brucite are listed in Table 8-2 for GWB (run 18) and ERDA-6 brine (run 28); these carbonate concentrations are important for the evaluation of the available solubility data. The pcH values obtained from these FMT output files are also listed in Table 8-2.

The available uranium(VI) solubility data for WIPP-relevant pH and ionic strengths are summarized in Table 8-3. Díaz Arocas and Grambow (1998) investigated uranium(VI) solubilities in up to 5 M NaCl solutions in the absence of carbonate. The experiments were conducted from oversaturation. In experiments above pH 7.5, a poorly-crystalline sodium-uranate solid solution phase was formed. The results of Díaz Arocas and Grambow (1998) indicate that the solubility of this phase is 3×10^{-5} M in the absence of carbonate at pH 8.9 in 5

M NaCl. This concentration is somewhat higher than the value used in the CCA PA, the PAVT, and CRA PA (8.8×10^{-6} M). The presence of carbonate ions in WIPP brines would likely increase uranium(VI) concentrations to higher levels than those observed in the Díaz Arocas and Grambow (1998) experiments. On the other hand, determining the solubility only from oversaturation may have resulted in an overestimation of the solubility of the sodium uranate solid. In addition, the small crystal sizes and poorly crystalline nature of the solids formed in the experiments may have increased solubilities relative to equilibrium phases that may form over the longer time periods applicable to the WIPP repository.

Lin et al. (1998) also evaluated uranium(VI) solubilities in solutions with up to 5 M NaCl, but their experiments included a range of carbonate ion (CO_3^{2-}) concentrations. This study was described in an extended meeting abstract rather than in a peer-reviewed publication, so only a limited amount of information is presented. At carbonate ion concentrations greater than 10^{-7} M, as are expected in the WIPP repository, $UO_2(CO_3)_3^{4-}$ was the dominant uranium(VI) complex in solution. At higher carbon dioxide partial pressures, the solubility-controlling solid phase was found to be UO_2CO_3(s), whereas at lower partial pressures, sodium uranate was identified as the solid phase in NaCl-saturated solutions. However, the carbon dioxide partial pressure for this phase transformation was not stated. The reported solubility of UO_2CO_3(s) at a carbonate ion concentration of 10^{-5} m was approximately 5×10^{-3} m. This concentration is likely to be an overestimation of uranium(VI) concentrations because a phase that is less soluble than UO_2CO_3(s) is more likely to be stable under WIPP repository conditions.

Solubility data described in an interim report by Reed and Wygmans (1997) were considered by the Agency during its review of the CCA (US EPA 1998c). In this investigation, Reed and Wygmans (1997) reported uranium(VI) concentrations from ERDA-6 solubility experiments with 10^{-4} M carbonate that ranged from 1.1×10^{-8} M at pH 8 to greater than 10^{-4} M at pH 10 (Table 8-3). Because the results of these experiments vary so widely and are either lower pH or higher pH with higher carbonate than expected WIPP repository conditions, they provide little information regarding expected uranium(VI) concentrations at pH 9 and carbonate concentrations of approximately 10^{-5} M.

The experimental results reported by Reed and Wygmans (1997) appear to be from the same experiments for which preliminary results were reported by Reed et al. (1996), and that were used by DOE to establish the uranium(VI) solubility for the CCA PA and CRA PA (Hobart and Moore 1996). Hobart and Moore (1996) also reported results from experiments in WIPP brines based on personal communication from Palmer (1996). At pH 9.8 in the absence of carbonate, Palmer (1996) observed a uranium(VI) solubility of 2.8×10^{-6} m in equilibrium with a phase that appears to be $UO_2(OH)_2$(s). Hobart and Moore (1996) also reported uranium(VI) concentrations from the STTP experiments, but because the STTP experiments have been determined not to be relevant to WIPP conditions (Section 6.2), these results are not considered in the present analysis. Yamazaki et al. (1992) conducted uranium(VI) solubility experiments from both oversaturation and undersaturation in synthetic WIPP brine at pcH values ranging from 6.4 to 12.4. The results obtained at the pcH conditions closest to WIPP repository conditions are listed in Table 8-3. Relatively high uranium(VI) concentrations were observed in the pcH 8.4

experiments, which contained carbonate approximately in equilibrium with the atmosphere and in which schoepite ($UO_3 \cdot 2H_2O$) was the solubility-controlling solid phase. Much lower uranium(VI) concentrations were observed in the pcH 10.4 experiments, in which nitrogen gas was passed over the solutions to minimize carbon dioxide concentrations and potassium diuranate ($K_2U_2O_7$) and brucite were found to have precipitated from solution. Modeling calculations indicated that the high solubility at pcH 8.4 was caused by the formation of the aqueous $UO_2(CO_3)_3^{4-}$ species. Yamazaki et al. (1992) observed that the solubility-controlling solid phase was schoepite below pcH 9.3 and potassium diuranate above this pcH.

Solubility-controlling solids that have been identified in the experimental studies include schoepite, $UO_2(OH)_2(s)$, $UO_2CO_3(s)$, sodium uranate, and potassium diuranate. Based on the results of Yamazaki et al. (1992) and Lin et al. (1992), it appears that a potassium-, sodium-, or calcium-uranate phase is the most likely solubility controlling solid at the conditions expected in the WIPP repository. Fanghänel and Neck (2002) also observed the formation of a sodium uranate phase [clarkeite, $NaUO_2O(OH) \cdot H_2O(c)$] in 5 M NaCl experiments at pH values of approximately 8. Consequently, the most likely solubility controlling solid for uranium(VI) in the long-term WIPP repository is likely to be sodium uranate.

The dominant uranium(VI) aqueous species at repository conditions of pH and carbonate ion concentration is likely to be the triscarbonate complex [$UO_2(CO_3)_3^{4-}$], according to information presented by Lin et al. (1998) and Millero (1999). The zero-ionic-strength speciation data presented by Wall and Wall (2004) in their evaluation of uranium(VI) complexation by organic ligands also indicates that the triscarbonate complex will be the dominant uranium(VI) aqueous species. In fact, calculations of uranium(VI) speciation performed by the Agency with these data at anticipated WIPP repository carbonate ion concentrations (Section 8.6.4) indicate that over 99% of uranium(VI) in solution could be either the triscarbonate complex or biscarbonate complex [$UO_2(CO_3)_2^{2-}$]. These calculations indicate that the presence of free carbonate ion at the concentration calculated for GWB (2.16×10^{-5} M, run 18) would increase uranium(VI) concentrations by a factor of 250 relative to the concentration without carbonate.

A solubility of 3×10^{-5} M has been reported for sodium uranate in 5 M NaCl brine for pH 8.9 in the absence of carbonate (Díaz Arocas and Grambow 1998). This concentration is probably a reasonable upper limit for the solubility of an alkali or alkaline-earth uranate solid in NaCl brines in the absence of carbonate. To make this upper limit consistent with the carbonate concentrations expected in the WIPP repository, this concentration should be adjusted upwards by approximately two orders of magnitude, based on the speciation calculations using low-ionic-strength data mentioned above. Thus, a reasonable upper limit for uranium(VI) solubility in WIPP brines would be approximately 10^{-3} M. This concentration is approximately two orders of magnitude higher than the midrange value used in the CCA PA, PAVT and CRA PA and exceeds the upper limit of the solubility uncertainty range used in these assessments. However, it is reasonable that the upper limit should be considerably higher than the value estimated by Hobart and Moore (1996), because their value was for systems without carbonate and was a midrange rather than an upper-limit estimate. The selected upper limit value is also reasonably consistent with the 0.50 fractile estimate (2×10^{-3} M) made by the expert panel for moderate-pH systems in the presence of carbonate (Hobart et al. 1996).

8.2.3 Uranium(VI) Model Development

DOE continues to assert that no satisfactory predictive model for uranium(VI) solubility is available for WIPP conditions (US DOE 2004b, Appendix PA Attachment SOTERM-3.4.4). However, DOE does not consider evidence that carbonate species are likely to be much more important than hydrolysis species under WIPP repository conditions, which makes precise knowledge of hydrolysis speciation less important for the development of an adequate model. In addition, DOE has not provided an assessment of whether development of such a model is now possible, given the additional data that have become available since the CCA PA and PAVT (e.g., Brown 2002, Rai et al. 2002).

A study in which Pitzer parameters for uranium were estimated has become available since the PAVT (Plyasunov et al. 1998). DOE did not address whether these estimated Pitzer coefficients are sufficient for the development of an FMT solubility model or whether this type of approach could be used to develop a model. The utility of an FMT solubility model was illustrated by DOE's use of zero-ionic-strength thermodynamic data to address questions related to the sensitivity of uranium(VI) solubility to organic ligand concentrations (Wall and Wall 2004).

Because of the scarcity of uranium(VI) solubility data relevant to WIPP repository conditions and the lack of a thermodynamic model for uranium(VI), a fixed upper-limit value for the uranium(VI) concentration in the long-term WIPP repository was selected by EPA and required to be used in the PABC. This value is expected to provide a reasonably conservative estimate of the upper limit of uranium(VI) concentrations for use in PA. Obtaining solubility data at WIPP-relevant conditions combined with the development of a uranium solubility model would likely have a number of benefits. For example, uranium(VI) solubility could be dealt with in the same manner as other actinide oxidation states for PA, a lower and more realistic uranium(VI) concentrations could probably be used in PA, and questions regarding issues such as the sensitivity of uranium(VI) solubilities to ligand concentrations could be addressed in a direct manner without unnecessary assumptions and approximations.

8.3 Actinide Solubility Uncertainties Used in PA

For the CCA PA and the PAVT, DOE addressed uncertainties related to actinide solubilities by calculating the solubilities of the +III, +IV, and +V actinides in Castile and Salado brines under the conditions expected in the WIPP repository. The uncertainty in these values was then accounted for by sampling a cumulative distribution function representing uncertainty and multiplying the solubilities by the sampled value to determine the actinide concentrations used in PA. The determination of the actinide solubility uncertainty distribution used in the CCA PA and PAVT is described in detail by US EPA (1998c). To obtain this distribution, DOE compared experimentally measured solubility data used to develop the solubility models in FMT to the concentrations predicted by curve-fitting with the code NONLIN (Babb 1996). DOE also compared solubilities reported in the literature with concentrations predicted using FMT for the conditions of the experiments. The population of errors from these comparisons were accumulated and used to generate a cumulative distribution. DOE excluded data for the +IV and +VI actinides from their evaluation because they determined that these data sets were inconsistent or technically deficient. The remaining data consisted of +III solubility measurements (139 values) and +V solubility measurements (11 values). A single distribution was determined, which ranged on a log scale from -2.0 to 1.4 with a median value of -0.09 (US DOE 2004b, Appendix PA Attachment SOTERM). This distribution was used to represent the uncertainties associated with the solubilities for all four actinide oxidation states.

The uncertainties determined for the CCA PA and PAVT were used to represent the actinide solubility uncertainties for the CRA PA (US DOE 2004b, Appendix PA Attachment SOTERM Section 3.6). Because the available solubility data and the FMT thermodynamic database have changed since the CCA PA and PAVT (Section 2.0; Brush and Xiong 2003b), the Agency requested that DOE re-evaluate the uncertainties associated with the actinide solubilities using the currently available actinide solubility data (US EPA 2004c, Comment C-23-16).

DOE re-evaluated the uncertainties associated with actinide solubilities (US DOE 2005; Xiong et al. 2004). The database used for this evaluation was FMT_040628.CHEMDAT. This database was modified from the version used for the CRA PA (FMT_021120.CHEMDAT) by correcting the molecular weight of oxalate and adding solid calcium oxalate to the database (Xiong 2004). Because none of the calculations used in the uncertainty evaluation involved oxalate or other ligands, using either database should yield the same results (Xiong et al. 2004).

Separate evaluations were carried out for the +III, +IV, and +V actinide oxidation states. Solubility data used to develop the thermodynamic data in the FMT database, as well as literature data were evaluated. For each data point, the predicted solubility was calculated for the relevant experimental conditions using FMT. The base 10 logarithm of the difference was then calculated by subtracting the predicted solubility from the measured solubility. These difference values were used to develop histograms and cumulative distribution functions. The +III evaluation was based on 243 measured and calculated solubilities, the +IV evaluation included 159 solubilities, and the +V evaluation included 136 solubilities (Xiong et al. 2004).

The sources of the data used in the evaluation are listed in Table 1 of Xiong et al. (2004). Comparison of these data with the data in FMT_040628.CHEMDAT and the discussion of these data in Giambalvo (2002a, 2002c, 2002d) indicate that not all of the data used to develop the database were included in the uncertainty analysis. For example, solubility data for $AmOHCO_3(s)$ (Felmy et al. 1990; Fanghänel et al. 1999) were included in the FMT database, but were not included in the uncertainty analysis (Xiong et al. 2004). The reasons these and other data were omitted were not provided by DOE. However, data for the solubility-controlling solids under WIPP repository conditions, as determined by FMT modeling (Section 8.5), were included in the uncertainty analysis.

For the +III actinides, the logarithm of the differences between measured and predicted solubilities ranged from -2.85 to +2.85 (Xiong et al. 2004). The median value was slightly less than 0, indicating that the FMT calculations predicted a higher concentration than the measured solubility slightly more often than the calculations underpredicted the measured solubility. The data used to generate the uncertainty distribution were primarily for neodymium phases, but included some solubility data for americium phases. This uncertainty range is broader than the range used previously for the CCA PA, PAVT, and CRA PA. Because it now includes only data for +III actinides and neodymium, which is expected to exhibit analogous solubility behavior, it is probably a more reasonable representation of uncertainty associated with the modeled +III actinide solubilities.

The logarithms of the observed differences for the +IV actinides ranged from -2.85[IV] to +3.3, with a median value between 0.6 and 0.75. This positive median value indicates that in the majority of comparisons, the measured solubility was higher than the concentration predicted by the FMT calculations. DOE did not discuss any potential reasons for this bias in the calculated values, such as varying degrees of solids crystallinity in the different experiments. An alternative explanation is provided by Fanghänel and Neck (2002), who observed a relatively large amount of scatter in the reported solubilities of amorphous thorium(IV) precipitates under alkaline conditions, which appeared to be caused by incomplete separation of colloids from the experimental solutions.

DOE carried out an additional evaluation of the +IV actinide solubility model to determine the cause of the underprediction of the experimental data (Nowak 2005, Xiong et al. 2005). Nowak (2005) re-evaluated the thorium(IV) thermodynamic data in the FMT database and recommended a revision to the μ^0/RT data for $Th(OH)_4(aq)$. This revision to the thermodynamic data was found by Xiong et al. (2005) to result a significant improvement in the ability of the +IV actinide solubility model to predict the available solubility data at high ionic strength. These revisions to the FMT database and +IV actinide uncertainty distribution were not reviewed as part of the current evaluation, but will be considered during the review of the PABC (see EPA 2006).

The range of logarithms of the differences between calculated and measured +V actinide solubilities ranged from -1.8 to +1.95, with a median value slightly less than 0. DOE also combined the three data sets to form a single distribution for the +III, +IV, and +V actinide solubilities. This distribution ranged from -3.0 to + 3.3, with a median value slightly above 0. The slightly positive median value indicated that for a small majority of cases, the FMT calculations slightly underpredicted the measured solubilities.

DOE does not propose to use the uncertainty distribution for the +V actinides in PA because neptunium is the only actinide expected to be present in the +V oxidation state in the equilibrium

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[IV] Figure 3 and Table 2 of Xiong et al. (2004) indicate that one value of -4.95 was observed; however, the text indicated that this value was in error and should have been 0.65.

WIPP repository (Section 6.0). Neptunium solubility will not be considered in future PA calculations because the inventory of neptunium is insufficient to affect the long-term performance of the repository regardless of its solubility (Brush et al. 2005).

DOE proposed to use the combined uncertainty distribution calculated with the +III, +IV, and +V solubility data in combination with the estimated uranium(VI) concentration from Hobart and Moore (1996) for PA (Brush et al. 2005). However, based on the evaluation of the available data regarding uranium(VI) solubility under long-term repository conditions (Section 8.2) and the lack of a basis for using the combined uncertainty distribution for the +VI actinide concentration uncertainty, a single value selected to represent the upper end of the solubility range that could be anticipated under repository conditions would be more defensible for use in PA. The evaluation of this upper limit value for uranium(VI) is described in Section 8.2.

The uncertainty distributions developed by DOE for use with the +III and +IV actinide solubilities have some potentially important limitations, for example, none of the solubilities were measured in experiments with ligands (Xiong et al. 2004) and DOE apparently did not include all data used to develop the FMT thermodynamic database in the uncertainty analysis. In addition, no data related to +VI actinides were evaluated because of the lack of a thermodynamic model for this oxidation state. However, the uncertainty ranges for the +III and +IV actinides are greater than the single range used in the CCA PA and PAVT, are based on larger data sets than were previously used, and only data relevant to the specific oxidation state were used to generate the distributions. Therefore, these uncertainty ranges appear to be adequate for use in PA. These new uncertainty ranges are used in the PABC.

8.4 Temperature Effects on Actinide Solubilities

The potential effects of temperature on actinide solubilities in the WIPP repository are assumed to be negligible based on calculations performed at the time of the CCA (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.4). DOE has not revised these calculations in the CRA to account for the potential effects of inventory changes since the CCA and non-uniform waste loading, e.g., the high proportion of pipe overpack waste in Panel 1. Although DOE has not quantitatively assessed the possible effects of these changes, it is reasonable to assume that repository temperature will not be significantly affected by these changes and that the effects of temperature on actinide solubilities can continue to be discounted (US DOE 2004b, Appendix PA Attachment SOTERM Section 2.2.4). However, in the event that heat-source plutonium or wastes containing significant heat-generating fission products are placed in WIPP in excess of the amounts assumed during the CCA, the validity of the CCA calculations that were used to estimate temperature increases may require re-evaluation.

8.5 Comparison of PAVT and CRA PA Actinide Solubilities

The actinide solubilities calculated for the CCA PA, the PAVT, and the CRA PA are summarized in Table 8-2. Comparison of the CRA actinide solubilities with the PAVT solubilities indicates that relatively minor changes were observed for the solubility of +III actinides in Salado brine, but larger changes of nearly an order of magnitude were observed in the +III solubilities in Castile brine. For the Salado and Castile brines, the only significant difference between the CRA PA and PAVT calculations of the +IV actinides was for the nonmicrobial vector in Castile brine (Table 8-2). The solubilities of the +V actinides calculated for the CRA PA were all higher than the solubilities calculated for the PAVT. No changes were observed in the +VI actinide solubilities because these concentrations were not modeled using FMT, but were instead fixed at a selected value (Section 8.2).

The CRA PA +III actinide solubilities in Salado brine are similar to those calculated for the PAVT. However, for the Castile (ERDA-6) brine calculations, the CRA PA solubilities are approximately one order of magnitude higher than concentrations calculated for the PAVT (Table 8-2). Information in the output files from the CRA PA FMT calculations (Table 8-1) indicates that the principal aqueous species in both the ERDA-6 and GWB brines were the americium hydrolysis species [$Am(OH)_2^+$, $AmOH^{2+}$, $Am(OH)_3(aq)$] and the aqueous organic complex $AmEDTA^-$. Comparison of the americium(III) concentrations calculated with organic ligands (FMT Runs 12, 18, 22, and 28) to concentrations calculated without organic ligands (FMT runs 11, 17, 21, and 27) indicated that the formation of the $AmEDTA^-$ aqueous complex significantly increased the calculated americium(III) concentrations, with $AmEDTA^-$ constituting approximately 26% of the aqueous americium(III) in GWB and 48% in ERDA-6 in the calculations that included organic ligands. This higher percentage of $AmEDTA^-$ calculated for ERDA-6 brine is the likely cause of the increased americium(III) concentrations relative to the PAVT concentrations for this brine. The solubility-controlling solid for americium(III) changed from $AmOHCO_3(s)$ in the PAVT calculations to $Am(OH)_3(s)$ in the CRA PA calculations, probably because of changes in the thermodynamic data for americium (Section 2.3).

The CRA PA +IV actinide solubilities were essentially unchanged since the PAVT for microbial and nonmicrobial vectors for Salado brine, and for the microbial vector for the Castile brine. However, the nonmicrobial Castile brine (ERDA-6) vector +IV actinide solubility was nearly an order of magnitude lower for the CRA PA than for the PAVT. The principal aqueous species for thorium(IV) was $Th(OH)_3CO_3^-$, with smaller proportions (approximately 3 to 13%) of $Th(OH)_4(aq)$ in the GWB and ERDA-6 FMT calculations with organic ligands. Significant complexation of thorium(IV) by organic ligands was not calculated. The relatively low carbon dioxide partial pressure calculated for ERDA-6 brine in the nonmicrobial vectors resulted in less complexation of thorium(IV) by carbonate ions in solution, and hence lower thorium solubilities compared to the other CRA PA vectors. The solubility-controlling solid for thorium(IV) was $ThO_2(am)$ for the CRA PA, which is unchanged from the PAVT.

The +V actinide solubilities in the Salado and Castile brines were 4 to 44 times higher for the CRA PA than the solubilities calculated for the PAVT. Comparisons of the neptunium(V) concentrations calculated with organic ligands (runs 12, 18, 22, and 28) to concentrations calculated without organic ligands (runs 11, 17, 21, and 27) indicated that the inclusion of organic ligands had a significant effect on neptunium(V) solubilities. Neptunium(V) was strongly complexed by oxalate, with the aqueous species $NpO_2oxalate^-$ constituting 73 to 94% of dissolved neptunium(V). Relatively smaller proportions of dissolved neptunium(V) (approximately 1 to 3%) were complexed by acetate [$NpO_2acetate^-$]. The solubility-controlling solid for neptunium(V) was $KNpO_2CO_3$(s), which is unchanged from the PAVT calculations. The neptunium(V) concentration in equilibrium with this phase will increase with decreasing carbonate concentrations; consequently, the nonmicrobial ERDA-6 vector, which has the lower carbon dioxide fugacity, also has the highest predicted neptunium(V) solubility.

8.6 Effects of Organic Ligands on Actinide Solubilities

DOE used inventory estimates available at the time of the CCA to identify four organic ligands that could affect actinide solubilities: acetate, citrate, EDTA, and oxalate (DOE 2004b, Appendix PA Attachment SOTERM Section 5.0). DOE (2004b) did not address whether new inventory information, such as new waste streams included since the CCA, might affect identification of complexing agents such as organic ligands that should be addressed in the calculations. Reported inventories of the four ligands evaluated for the CRA have changed since the CCA, including increased concentrations of acetate, changes in oxalate and citrate inventories that appear to have been caused by transposing the data during the CCA, and a decrease in the estimated inventory of EDTA (US DOE 2004b, Appendix PA Attachment SOTERM Table SOTERM-4).

8.6.1 FMT Calculations of the Effects of Organic Ligands

DOE stated that

acetate, citrate, EDTA, and oxalate will not significantly affect the +III and +IV actinide solubilities (US DOE 2004b, Appendix PA Attachment SOTERM Section 5.0). Comparison of FMT calculations with and without organic ligands indicates that this is true for the +IV actinides. However, comparisons of FMT output files for calculations with and without organic ligands indicate that higher +III actinide solubilities are observed in runs with organic ligands than in runs without organic ligands (Section 8.5). These higher concentrations occurred because $AmEDTA^-$ constituted approximately one-quarter to one-half of the aqueous americium(III) species in FMT runs with organic ligands. These comparisons also indicated that oxalate complexation significantly increased neptunium(V) solubilities.

8.6.2 CCA Low-Ionic-Strength Calculations

DOE cited calculations originally presented in the CCA that were used to evaluate the competition of transition metals, including iron and nickel, with actinide species for EDTA (US DOE 2004b, Appendix TRU WASTE Section 2.4.1.3). Because thermodynamic data for organic ligand complexation of actinides is now included in the FMT database, the Agency requested that DOE address whether these calculations are still valid (US EPA 2004c, Comment C-23-17).

Using the results of the calculations presented in the CCA, DOE concluded that 99.8% of EDTA will be complexed by nickel in the WIPP repository environment, rendering EDTA unavailable for complexation with actinides. The Agency reviewed these calculations at the time of the CCA (US EPA 1998c), and questioned their applicability because of the high nickel concentration assumed in the solution and because DOE had not supported its assertion that both nickel and iron would have relatively high solubilities in high-ionic-strength solutions relative to low-ionic strength conditions. The Agency instead assessed the relative importance of ligands on actinide solubilities by evaluating the effects of EDTA on the solubility of ThO_2(am) at lower ionic strength (US EPA 1998c). The results of these calculations indicated that thorium was not significantly complexed by EDTA in the higher pH range expected in the WIPP repository, and EDTA was primarily present as Ca^{2+} and Mg^{2+} complexes. Because DOE has now included thermodynamic data for organic ligand complexation of actinides in the FMT database, the results obtained using the low-ionic-strength calculations performed by the Agency have been confirmed for the +IV actinides at high ionic strength. However, it appears that the +III and +V actinide solubilities are affected by EDTA and oxalate complexation, respectively.

DOE responded to the Agency's request for additional information regarding the low-ionic-strength calculations cited in Appendix TRU WASTE (US DOE 2004b) and acknowledged that these calculations were superceded by the FMT calculations with organic ligands (US DOE 2004c). DOE had removed statements regarding these calculations in Appendix PA Attachment SOTERM (US DOE 2004b), but had not updated Appendix TRU WASTE to be consistent with the current understanding of the effects of organic ligand complexation on actinide solubilities. DOE acknowledged that such a change should have been made to Appendix TRU WASTE (US DOE 2004c).

8.6.3 Sensitivity of +III, +IV, and +V Actinide Solubilities to Organic Ligand Concentrations

DOE stated that no upper or lower limit is required for the quantities of organic ligands in the repository because organic ligand concentrations in the solubility calculations had an insignificant impact on actinide solubility (US DOE 2004b, Appendix TRU WASTE Section 3.8). However, review of the CRA did not indicate that a sensitivity analysis was conducted to establish the likely effects of variations in the organic ligand concentrations. The Agency therefore requested that DOE conduct such a sensitivity analysis (US EPA 2004c, Comment C-23-15).

Experimental investigation of microbial degradation of CPR has indicated that ligands including acetate, lactate, and oxalate can be produced by the degradation reactions (Gillow and Francis 2003). In many of the inundated experiments, measurable concentrations of these ligands persisted after nearly 10 years of reaction. For example, in anaerobic inundated experiments with cellulose, acetate concentrations ranged from 2×10^{-4} M in unamended samples to 6.99×10^{-3} M in amended and inoculated samples after 9.8 years of reaction; these concentrations are significant when compared to the acetate concentration of 5.05×10^{-3} M used in the CRA solubility calculations. In the same experiments, lactate concentrations ranged from below detection to 3.03×10^{-3} M. The production of lactate in the microbial degradation experiments is potentially significant because lactate has not been reported in the WIPP inventory and therefore was not included in the actinide solubility calculations (US DOE 2004b, Appendix PA Attachment SOTERM-5.0). Therefore, the Agency requested that DOE assess whether the production of organic ligands during microbial degradation of CPR could have significant effects on actinide solubilities (US EPA 2004c, Comment G-13).

In their response to the Agency's request for additional information regarding microbial production of organic ligands, DOE pointed out that although the potential production of organic ligands by microbial degradation of CPR was not accounted for in the CCA or CRA, neither was the potential consumption of organic ligands by microbes (US DOE 2004c). In their response, DOE cited a number of studies indicating that consumption of organic ligands such as acetate may occur in the WIPP repository. DOE also pointed out that the production of organic ligands during microbial degradation of CPR would be inconsistent with the Agency's specification of the assumption that all carbon in the CPR inventory could be converted to carbon dioxide for the purposes of calculating the MgO safety factor.

DOE incorporated thermodynamic data for acetate, citrate, EDTA, lactate, and oxalate with the +III, +IV, +V, and +VI actinides in the FMT database (Section 2.0). Data were also included for complexation of these ligands with Mg^{2+} to assess the effects of competition of Mg^{2+} and Ca^{2+} (by analogy to Mg^{2+}) on actinide complexation by these ligands. Therefore, DOE had the necessary thermodynamic data to carry out sensitivity calculations with FMT for the +III, +IV, and +V actinides to determine whether variations in the quantities of ligands present in the repository and the potential presence of lactate from microbial degradation could affect actinide solubilities (US DOE 2005). Details of these calculations are provided in Brush and Xiong (2004).

FMT solubility calculations were carried out for both GWB and ERDA-6 brines and for microbial and nonmicrobial vectors. DOE carried out these calculations assuming four potential concentrations for organic ligands:

- No organic ligands;
- Organic ligand concentrations equal to those used in the CRA PA FMT calculations;
- Organic ligand concentrations equal to those used in the CRA PA FMT calculations plus added lactate and acetate equal to the mean concentrations produced by microbial degradation of cellulose in the Gillow and Francis (2003) experiments; and
- Organic ligand concentrations an order of magnitude greater than the CRA PA FMT concentrations plus additional lactate and acetate.

The FMT results for the microbial vector calculations, in which brucite-hydromagnesite$_{5424}$ buffered carbon dioxide fugacity, are summarized in Tables 8-4 and 8-5 for GWB and ERDA-6 brine, respectively.

Including the CRA PA concentrations of organic ligands in the FMT calculations increased the +III actinide concentrations by factors of 1.36 and 1.95 for GWB and ERDA-6, respectively, compared to the concentrations without organic ligands (Tables 8-4 and 8-5). The increased +III actinide concentrations were predicted because of the formation of $AmEDTA^-$ in the calculations with CRA PA concentrations of organic ligands. Because the +III actinides are not significantly complexed by acetate or lactate at the concentrations estimated from the microbial degradation experiments, increasing these ligand concentrations had no detectable effect on the predicted +III actinide concentrations. For the calculations with an order of magnitude higher ligand concentrations, calculated +III actinide concentrations increased by factors of 3.97 and 10.6 for GWB and ERDA-6, respectively, compared to concentrations calculated with no organic ligands. For the FMT calculations with the highest ligand concentrations, the principal aqueous americium(III) species were $AmEDTA^-$ and $Am(OH)_2^+$ in both GWB and ERDA-6. Thus, the solubilities of the +III actinides appear to be sensitive to the assumed concentration of EDTA.

The results of the FMT calculations indicate that the varying concentrations of organic ligands did not change the +IV actinide concentrations. Examination of the FMT output files established that the +IV actinides are relatively insensitive to organic ligand concentrations because $Th(OH)_3CO_3^-$ and $Th(OH)_4(aq)$ were the only significant thorium(IV) aqueous species, even at the highest organic ligand concentrations evaluated.

The +V actinide solubilities appear to be strongly affected by organic ligand complexation, which DOE acknowledged (US DOE 2004c) in their response to the Agency's request for additional information regarding the effects of ligands on the +V actinides (US EPA 2004c). Concentrations of +V actinides in the FMT calculations with CRA PA concentrations of organic ligands increased by factors of 4.32 and 9.44 for GWB and ERDA-6, respectively, compared to calculations with no organic ligands (Tables 8-3 and 8-4). These increased concentrations were observed because of the complexation of neptunium(V) by oxalate. Increasing acetate and lactate concentrations by amounts estimated for microbial production of ligands did not significantly affect predicted +V actinide concentrations. However, increasing these organic ligand concentrations by an additional order of magnitude increased predicted +V actinide concentrations by factors of 32 and 67 for GWB and ERDA-6, respectively compared to calculations without organic ligands. In the calculations with the highest concentrations of organic ligands, the principal neptunium(V) aqueous species were $NpO_2oxalate^-$ and $NpO_2acetate(aq)$.

The results of these sensitivity calculations indicate that the predicted +IV actinide solubilities are not affected by the evaluated range of organic ligand concentrations. However, predicted +III and +V actinide solubilities were affected by changes in the estimated organic ligand concentrations. The results of these calculations indicate that the solubilities of the +III actinides are sensitive to EDTA concentrations in the WIPP repository, and the +V actinide concentrations are sensitive to the oxalate and possibly the acetate concentrations in the repository. Over the range of evaluated concentrations for citrate and lactate, no significant effects on the solubilities of the +III, +IV or +V actinides are predicted.

8.6.4 Possible Effects of Ligands on Uranium(VI) Concentrations in WIPP Brines

The Agency requested that DOE assess the potential effects of ligand complexation on the +VI actinides (US EPA 2004c, Comment C-23-13). Because only uranium is expected to be present in the +VI oxidation state in the equilibrium repository, the response to this request addressed the possible effects of ligands on uranium(VI) solubility in repository brines (US DOE 2004c). Thermodynamic data for complexation of uranium(VI) by acetate, citrate, EDTA, lactate, and oxalate in brines have been determined (Choppin et al. 2001). However, DOE has not developed a thermodynamic model for uranium(VI) in brines (Section 8.2), so this assessment could not be performed using FMT calculations.

Wall and Wall (2004) addressed the possible effects of organic ligands on uranium(VI) solubility. Wall and Wall (2004) used thermodynamic data at zero ionic strength from the updated OECD review (Mompean et al. 2003) for uranium species, zero-ionic-strength chemical potential data from the FMT database for non-uranium species, and zero-ionic-strength data for uranium(VI) complexes with acetate, citrate, EDTA, and oxalate from Choppin et al. (2001). Wall and Wall (2004) used these data to calculate equilibrium constants for zero-ionic-strength conditions. These equilibrium constants were then used with the pH, carbonate ion concentrations, and uncomplexed organic and inorganic ligand concentrations obtained from the high-ionic-strength FMT calculations (runs 12, 18, 22 and 28, Table 8-1) to estimate the various proportions of the different uranium(VI) species in the solutions. These calculations were repeated for the present analysis using the concentrations from FMT output file FMT_CRA1V_ORGS_014.OUT (Table 8-6) to include the possible effects of lactate and the UO_2HEDTA^- species. The speciation results reported by Wall and Wall (2004) and the results in Table 8-6 indicate that organic ligand complexes of uranium(VI) are likely to constitute a very small fraction of total uranium(VI) in solution. The results of these calculations indicate that carbonate species, in particular $UO_2(CO_3)_3^{4-}$ and $UO_2(CO_3)_2^{2-}$, are likely to be the dominant uranium(VI) species in solution at WIPP repository conditions.

The limitations associated with this calculation include the use of zero-ionic-strength thermodynamic data for high-ionic-strength calculations. Carbonate complexes are likely to be the most important uranium(VI) species under WIPP repository conditions, followed in importance by hydrolysis species (Table 8-6). Stability constants for the complexation of UO_2^{2+} by organic ligands at high ionic strength data are available (Choppin et al. 2001), as are high-ionic-strength stability constant data for the hydrolysis species (Bronikowski et al. 1999). Therefore, the relative proportions of UO_2^{2+}-ligand species compared to hydrolysis species can be assessed. Bronikowski et al. (1999) carried out this type of calculation to illustrate the ability of citrate to compete with hydrolysis species for uranium(VI) and provided hydrolysis constants of $10^{-4.97}$ for UO_2OH^+ and $10^{-12.77}$ for $UO_2(OH)_2(aq)$ in 5M NaCl. They developed the following equation based on the definitions of the stability constants for calculating the fraction (X) of the total UO_2^{2+}-ligand and UO_2^{2+}-hydrolysis species that would be complexed by an organic ligand:

$$X = \frac{\beta_{101}\,[\text{ligand}]}{\beta_{101}\,[\text{ligand}] + \beta_1^{OH}\,[H^+]^{-1} + \beta_2^{OH}\,[H^+]^{-2}} \qquad (12)$$

where:

β_{101} = stability constant for the aqueous 1:1 uranyl:ligand species
β_1^{OH} = stability constant for UO_2OH^+
β_2^{OH} = stability constant for $UO_{2(}OH)_2$
[ligand] = ligand concentration in solution
$[H^+]$ = hydrogen ion concentration in solution

These calculations were carried out using the conditions modeled for the microbial production of acetate and lactate ion in GWB (FMT_CRA1V_ORGS_014), which had a modeled pcH of 9.4. The results of these calculations indicated that UO_2EDTA^{2-}, which had the highest calculated fraction among the organic ligand species, would be present at a concentration equal to approximately 10% of the total uranium(VI) hydrolysis and ligand species. Because uranium(VI)-carbonate species are expected to be present in much greater concentrations than the hydrolysis species, UO_2EDTA^{2-} will constitute an even smaller percentage of the total dissolved uranium species under WIPP conditions. Therefore, these calculations indicate that organic ligands are unlikely to complex uranium(VI) to an extent that will significantly affect uranium(VI) solubilities in the WIPP repository environment.

Wall and Wall (2004) evaluated the assumption that only free ligand concentrations could be considered in their calculations, i.e., that UO_2^{2+} ions could not effectively compete for ligands with the metal ions that account for the majority of ligand concentrations. Because thermodynamic data are available for magnesium-ligand complexes, they compared the ability of UO_2^{2+} to compete with Mg^{2+} for organic ligands via the reaction:

$$MgL^{2-n} + UO_2^{2+} \rightleftharpoons Mg^{2+} + UO_2L^{2-n} \qquad (13)$$

where L represents an organic ligand. The equilibrium constant (K) for equation (13) is:

$$K = \frac{[Mg^{2+}][UO_2L^{2-n}]}{[UO_2^{2+}][MgL^{2-n}]} \qquad (14)$$

and the stability constants of formation for the 1:1 complexes of a ligand with UO_2^{2+} and Mg^{2+} are:

$$\beta_{UO_2^{2+}} = \frac{[UO_2L^{2-n}]}{[UO_2^{2+}][L^{n-}]} \qquad (15)$$

$$\beta_{Mg^{2+}} = \frac{[MgL^{2-n}]}{[Mg^{2+}][L^{n-}]} \quad (16)$$

Equations 14, 15, and 16 can be combined to yield the ratio of the 1:1 ligand complexes with uranium(VI) and magnesium ion as a function of the magnesium ion and UO_2^{2+} ion concentration:

$$\frac{[UO_2L^{2-n}]}{[MgL^{2-n}]} = \frac{\beta_{UO_2^{2+}}\,[UO_2^{2+}]}{\beta_{Mg^{2+}}\,[Mg^{2+}]} \quad (17)$$

Using the magnesium ion concentrations and organic ligand concentrations for the CRA PA solubility calculations with organic ligands (runs 12, 18, 22, and 28, Table 8-1) and the UO_2^{2+} concentration estimated from schoepite solubility at zero ionic strength and pH 9 (10^{-13} M), the results of the Wall and Wall (2004) calculations indicated that only very small ratios of the UO_2^{2+}-ligand species would be present, compared to the Mg^{2+}-ligand species. These results demonstrated that under the modeled WIPP repository conditions, UO_2^{2+} would not be able to effectively compete for ligands with Mg^{2+} and the use of the free ligand concentrations from the FMT output files was justifiable.

The evaluation of the effects of ligands on uranium(VI) solubilities under WIPP repository conditions is hampered by the lack of a solubility and aqueous speciation model at high ionic strength. However, the Wall and Wall (2004) calculations using low-ionic-strength data indicate that the uranium(VI)-ligand species concentrations will be negligible compared to carbonate and hydrolysis species concentrations. Additional calculations using 5 M NaCl stability constants for UO_2^{2+}-ligands complexes and UO_2^{2+}-hydrolysis species also indicate that UO_2^{2+}-ligands complexes are unlikely to form a significant fraction of uranium(VI) aqueous species under WIPP repository conditions. Uranium(VI) does not appear to be significantly affected by organic ligand complexation because of the relatively strong complexation of UO_2^{2+} by carbonate species to form $UO_2(CO_3)_3^{4-}$ and $UO_2(CO_3)_2^{2-}$ and to a lesser extent, by hydrolysis of the UO_2^{2+} ion under WIPP repository conditions.

8.6.5 Conclusions Regarding the Importance of Organic Ligand Concentrations for Estimating Actinide Solubilities

The Agency requested that DOE provide additional information regarding the possible effects of organic ligands concentrations on actinide solubilities in the WIPP repository (US EPA 2004c). In their response, DOE described the results of a series of calculations designed to determine the sensitivity of +III, +IV, and +V actinide solubilities to increases in organic ligand concentrations and the possible effects of microbially produced acetate and lactate (US DOE 2005). The results of these calculations show that the concentrations of the +III and +V actinides could be significantly affected if the concentrations of EDTA or oxalate in the repository significantly increased. These calculations illustrated that the +IV actinides were relatively insensitive to organic ligands over the range of evaluated concentrations, and that microbially produced lactate is unlikely to significantly affect actinide solubilities at the concentrations expected based on the microbial degradation experiments. The effects of EDTA concentrations on the modeled +III actinide concentrations indicates that the assumed concentrations, and hence the inventory, of organic ligands is potentially important for PA. However, the potential effects of oxalate and possibly acetate on the solubility of the +V actinides are less important, because neptunium is the only actinide assumed to be present in the equilibrium WIPP repository in the +V oxidation state, and the neptunium inventory is too low to significantly contribute to radionuclide releases (US EPA 2005).

8.7 Conclusions and Key Issues

Review of the CRA indicated that DOE's assumption that temperature effects will not significantly affect actinide solubilities is reasonable, provided wastes with large heat-generating potential, such as heat-source plutonium or wastes with high fission product concentrations, are not included in the WIPP inventory in excess of the quantities assumed in the CCA. However, other potentially important assumptions made by DOE (2004b) related to actinide solubilities in WIPP brines may not have been adequately supported.

Because DOE assumed that significant microbial degradation will occur in all PABC vectors (Section 4.0), the assumption that the calcite-brucite reaction will control carbon dioxide fugacities in the absence of significant microbial activity will no longer be included in PA. Similarly, DOE's assumption that microbial colloid transport will not occur in nonmicrobial vectors will no longer be an issue because all vectors will include significant microbial degradation. Therefore, DOE assumed that carbon dioxide fugacity will be controlled by the brucite-hydromagnesite$_{5424}$ reaction and that microbial colloid transport will occur in all vectors for the PABC (Brush and Xiong 2005).

The results of this review also indicated that recalculated uncertainties for the +III, +IV, and +V actinide solubilities based on the currently available thermodynamic data will be used in the PABC calculations instead of the single uncertainty range developed for the CCA. Sensitivity calculations also show that variations in organic ligand concentrations could significantly affect actinide solubilities, particularly the +III and +V actinides. Because of the importance of the +III actinide solubilities to PA, estimates of the quantities of ligands should continue to be included in the WIPP inventory.

The available data regarding uranium(VI) solubility under likely WIPP repository conditions remains limited. However, new data have become available since the CCA PA and PAVT indicating that a revised, higher uranium(VI) concentration should be used in PA. Because of the limited data and the lack of a uranium(VI) solubility model, there is a great deal of uncertainty associated with the uranium(VI) solubility that should be used in PA. Consequently, a relatively high uranium(VI) concentration is used in the PABC. Based on an evaluation of the available data, the Agency determined that a uranium(VI) solubility of 10^{-3} M be used as an upper-limit estimated value in the PABC calculations. Additional experimental data should be obtained at WIPP-relevant pH, ionic strength, and carbonate concentrations to reduce the uncertainty associated with the uranium(VI) solubility.

DOE has stated that a uranium(VI) solubility model cannot be developed because of uncertainties associated with the hydrolysis species. However, as previously pointed out in this report, carbonate speciation is likely to be much more important at WIPP-relevant conditions. During the expert panel evaluation of WIPP actinide solubilities, a uranium(VI) solubility model was apparently developed based on the panelists' expert judgement (Hobart et al. 1996; Millero 1999). In addition, Pitzer parameters for uranium were developed that are stated to be applicable to ionic media up to at least 4 m (Plyasunov et al. 1998); DOE does not appear to have evaluated this approach to determine whether it could be used at the ionic strengths relevant to WIPP. The development of a uranium(VI) solubility model will be important for understanding any new experimental data. Because the understanding of likely WIPP repository conditions may continue to evolve, a uranium(VI) solubility model would minimize the number of additional experiments that must be carried out and would also minimize uncertainty regarding the factors that are likely to be most important for controlling uranium(VI) solubility.

Table 8-1 Selected CRA PA FMT Output Files

Run Identifier	**Brine**	**Carbon Dioxide Buffer**	**Organic Ligands**	**File Name**
Run 11	GWB	Brucite-calcite	No	AP098_FMT_RUN011.OUT
Run 12	GWB	Brucite-calcite	Yes	AP098_FMT_RUN012.OUT
Run 17	GWB	Brucite-hydromagnesite$_{5424}$	No	AP098_FMT_RUN017.OUT
Run 18	GWB	Brucite-hydromagnesite$_{5424}$	Yes	AP098_FMT_RUN018.OUT
Run 21	ERDA-6	Brucite-calcite	No	AP098_FMT_RUN021.OUT
Run 22	ERDA-6	Brucite-calcite	Yes	AP098_FMT_RUN022.OUT
Run 27	ERDA-6	Brucite-hydromagnesite$_{5424}$	No	AP098_FMT_RUN027.OUT
Run 28	ERDA-6	Brucite-hydromagnesite$_{5424}$	Yes	AP098_FMT_RUN028.OUT

Table 8-2 Results of FMT Modeling of Actinide Solubilities

Property or Actinide Oxidation State	CRA Microbial Vectors, with Organic Ligands		CRA Nonmicrobial Vectors, with Organic Ligands		PAVT All Vectors, No Organic Ligands		CCA All Vectors, No Organic Ligands	
Brine	Salado	Castile	Salado	Castile	Salado	Castile	Salado	Castile
pH	8.69	9.02	8.69	8.99	8.69	9.24	8.69	9.24
pcH	9.40	9.72	9.40	9.69	--	--	--	--
Log carbon dioxide fugacity	-5.50	-5.50	-5.48	-6.15	-5.50	-5.50	-6.90	-6.90
Carbonate ion (M)	2.16×10^{-5}	6.88×10^{-5}	2.28×10^{-5}	1.39×10^{-5}	--	--	--	--
III (M)	3.07×10^{-7}	1.69×10^{-7}	3.07×10^{-7}	1.77×10^{-7}	1.2×10^{-7}	1.3×10^{-8}	5.82×10^{-7}	1.3×10^{-8}
IV (M)	1.19×10^{-8}	2.47×10^{-8}	1.24×10^{-8}	5.84×10^{-9}	1.3×10^{-8}	4.1×10^{-8}	4.4×10^{-6}	6.0×10^{-9}
V (M)	1.02×10^{-6}	5.08×10^{-6}	9.72×10^{-7}	2.13×10^{-5}	2.4×10^{-7}	4.8×10^{-7}	2.3×10^{-6}	2.2×10^{-6}
VI (M)	8.7×10^{-6}	8.8×10^{-6}	8.7×10^{-6}	8.8×10^{-6}	8.7×10^{-6}	8.8×10^{-6}	8.7×10^{-6}	8.8×10^{-6}
Equilibrium Nonradioactive Solid Phases, Salado Brine	anhydrite, halite, brucite, hydromagnesite$_{5424}$, $Mg_2Cl(OH)_3$• $4H_2O(s)$	anhydrite, halite, brucite, hydromagnesite$_{5424}$	anhydrite, halite, calcite, brucite, $Mg_2Cl(OH)_3$•$4H_2O(s)$	anhydrite, halite, brucite, calcite, glauberite	anhydrite, halite, brucite, hydromagnesite$_{5424}$, $Mg_2Cl(OH)_3$• $4H_2O(s)$	anhydrite, halite, brucite, glauberite, hydromagnesite$_{5424}$	anhydrite, halite, magnesite, brucite, $Mg_2Cl(OH)_3$• $4H_2O(s)$	anhydrite, halite, brucite, glauberite, magnesite
Equilibrium Radioactive Solid Phases	$Am(OH)_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$		$Am(OH)_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$		$AmOHCO_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$		$Am(OH)_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$	

Table 8-3 Experimental Uranium Solubility Data at High Ionic Strength

Uranium(VI) concentration	**pH**	**Carbon Dioxide**	**Solution**	**Solid**	**Reference**
3×10^{-5} M	8.9	Absent	5 m NaCl	$Na_{0.68}UO_{3.34} \cdot 2.15H_2O(s)$	Díaz Arocas and Grambow (1998)
9×10^{-5} M	7.6	Absent	5 m NaCl	$Na_{0.45}UO_{3.23} \cdot 4.5H_2O(s)$	Díaz Arocas and Grambow (1998)
~ 5×10^{-3} m	not specified[a]	10^{-5} [CO_3^{2-}]	5 M NaCl	$UO_2CO_3(s)$	Lin et al. (1998)
4.5×10^{-7} and 2×10^{-6} M[b]	7	10^{-4} M carbonate	G-Seep brine	Not determined	Reed and Wygmans (1997)
5.0×10^{-7} and 2×10^{-6} M[b]	7	Absent	G-Seep brine	Not determined	Reed and Wygmans (1997)
1.1×10^{-8} M	8	10^{-4} M carbonate	ERDA-6 brine	Not determined	Reed and Wygmans (1997)
5.5×10^{-7} M	10	Absent	ERDA-6 brine	Not determined	Reed and Wygmans (1997)
> 1×10^{-4} M	10	10^{-4} M carbonate	ERDA-6 brine	None formed	Reed and Wygmans (1997)
2.8×10^{-6} m	9.8	Absent	5.2 m WIPP brine	UO_2OH_2[c]	Palmer (1996)[d]

[V] Probably less than 7

[VI] The lower concentration was reported on page 4 of the text, but a higher concentration was illustrated in Figure 1A

[VII] Solid should probably have been identified as $UO_2(OH)_2(s)$, uranium(VI) concentration as cited by Hobart and Moore (1996)

[VIII] Hobart and Moore (1996) table cites Palmer et al. (1996), but reference list cites Palmer (1996) personal communication

Table 8-3 Experimental Uranium Solubility Data at High Ionic Strength (continued)

Uranium(VI) concentration	**pH**	**Carbon Dioxide**	**Solution**	**Solid**	**Reference**
1.82×10^{-3} M	8.4 (pcH)	$10^{-3.5}$ atm	3.8	Schoepite (oversaturation)	Yamazaki et al. (1992)
1.81×10^{-3} M	8.4 (pcH)	$10^{-3.5}$ atm	3.8	Schoepite (oversaturation)	Yamazaki et al. (1992)
1.4×10^{-3} M	8.4 (pcH)	$10^{-3.5}$ atm	3.8	Schoepite (undersaturation)	Yamazaki et al. (1992)
1.8×10^{-3} M	8.4 (pcH)	$10^{-3.5}$ atm	3.8	Schoepite (undersaturation)	Yamazaki et al. (1992)
3.8×10^{-7} M	10.4 (pcH)	Low	3.8	$K_2U_2O_7$ (oversaturation)	Yamazaki et al. (1992)
3.1×10^{-7} M	10.4 (pcH)	Low	3.8	$K_2U_2O_7$ (oversaturation)	Yamazaki et al. (1992)
1.8×10^{-7} M	10.4 (pcH)	Low	3.8	$K_2U_2O_7$ (undersaturation)	Yamazaki et al. (1992)
1.7×10^{-7} M	10.4 (pcH)	Low	3.8	$K_2U_2O_7$ (undersaturation)	Yamazaki et al. (1992)

Table 8-4 Results of Ligand Sensitivity FMT Calculations for Microbial Vectors, GWB

Actinide or Organic Ligand	No Organic Ligands	Organic Ligands Equivalent to CRA Concentrations	CRA Concentrations of Organic Ligands Plus Microbially Produced Acetate and Lactate	10 Times CRA Concentrations of Organic Ligands Plus Microbially Produced Acetate and Lactate Concentrations
Actinide(III)	2.26×10^{-7}	3.07×10^{-7}	3.07×10^{-7}	8.98×10^{-7}
Actinide(IV)	1.19×10^{-8}	1.19×10^{-8}	1.18×10^{-8}	1.15×10^{-8}
Actinide(V)	2.36×10^{-7}	1.02×10^{-6}	1.02×10^{-6}	7.62×10^{-6}
Total Acetate	0	5.37×10^{-3}	8.39×10^{-3}	8.23×10^{-2}

Total Citrate	0	4.07×10^{-4}	4.07×10^{-4}	4.00×10^{-3}
Total EDTA	0	4.12×10^{-6}	4.12×10^{-6}	4.04×10^{-5}
Total Lactate	0	0	5.10×10^{-4}	5.01×10^{-3}
Total Oxalate	0	2.30×10^{-2}	2.30×10^{-2}	2.25×10^{-1}
FMT File Name	AP098_FMT_RUN017	AP098_FMT_RUN018	FMT_CRA1V_ORGS_014	FMT_CRA1V_ORGS_018

all concentrations are from Tables 3 and 4 of Brush and Xiong (2004), units of moles/liter (M)

Table 8-5 Results of Ligand Sensitivity FMT Calculations for Microbial Vectors, ERDA-6

Actinide or Organic Ligand	No Organic Ligands	Organic Ligands Equivalent to CRA Concentrations	CRA Concentrations of Organic Ligands Plus Microbially Produced Acetate and Lactate	10 Times CRA Concentrations of Organic Ligands Plus Microbially Produced Acetate and Lactate Concentrations
Actinide(III)	8.67×10^{-8}	1.69×10^{-7}	1.69×10^{-7}	9.168×10^{-7}
Actinide(IV)	2.50×10^{-8}	2.47×10^{-8}	2.46×10^{-8}	2.02×10^{-8}
Actinide(V)	5.38×10^{-7}	5.08×10^{-6}	5.12×10^{-6}	3.62×10^{-5}
Total Acetate	0	5.00×10^{-3}	7.81×10^{-3}	7.72×10^{-2}

Total Citrate	0	3.79×10^{-4}	3.79×10^{-4}	3.75×10^{-3}
Total EDTA	0	3.83×10^{-6}	3.83×10^{-6}	3.79×10^{-5}
Total Lactate	0	0	4.79×10^{-4}	4.70×10^{-3}
Total Oxalate	0	2.14×10^{-2}	2.14×10^{-2}	1.73×10^{-1}
FMT File Name	AP098_FMT_RUN027	AP098_FMT_RUN028	FMT_CRA1V_ORGS_016	FMT_CRA1V_ORGS_020

all concentrations are from Tables 3 and 4 of Brush and Xiong (2004), units of moles/liter (M)

Table 8-6 Uranium(VI) Fractional Speciation Calculated Using Ligand Concentrations from FMT_CRA1V_ORGS_014.OUT and Zero-Ionic-Strength Thermodynamic Data from Wall and Wall (2004) and Choppin et al. (2001)

Aqueous Uranium(VI) Species	Fraction	Combined Fractions	
$UO_2CO_3(aq)$	0.0020	carbonate species	0.996
$UO_2(CO_3)_2^{2-}$	0.209		
$UO_2(CO_3)_3^{4-}$	0.785		
UO_2OH^+	4.17×10^{-5}	hydrolysis species	0.0038
$UO_2(OH)_2(aq)$	0.0037		
$UO_2Acetate^+$	4.73×10^{-8}	ligand species	0.00012
$UO_2Citrate^-$	7.75×10^{-5}		
UO_2EDTA^{2-}	6.46×10^{-6}		
$UO_2Oxalate(aq)$	3.30×10^{-5}		
$UO_2Lactate^+$	6.56×10^{-9}		
UO_2HEDTA^-	8.52×10^{-12}		
UO_2Cl^+	8.19×10^{-8}	chloride species	1.05×10^{-7}
UO_2Cl_2	2.33×10^{-8}		
UO_2SO_4	2.13×10^{-6}	sulfate species	5.12×10^{-6}
$UO_2(SO_4)_2^{2-}$	2.95×10^{-6}		
$UO_2(SO_4)_3^{4-}$	3.24×10^{-8}		

9.0 ACTINIDES INCLUDED IN PA CALCULATIONS

Figure TRU WASTE-5 and Table TRU WASTE-9 indicate that curium-243, curium-244, curium-245 and neptunium-237 are included in the actinide source term for direct brine release. However, DOE stated that neptunium and curium are not transported in PA (US DOE 2004b, Appendix PA Attachment SOTERM Section 4.3 and Attachment SOTERM Section 4.6). Table SOTERM-3 indicates that curium and neptunium were not included in the CRA PA, which seems inconsistent with the reported inclusion of these actinides in direct brine release (US DOE 2004b, Figure TRU WASTE-5 and Table TRU WASTE-9). The actual meaning of the statements regarding neptunium and curium not being transported in PA appears to be that they were not included in Culebra or Salado transport.

DOE stated that radionuclide releases are dominated by plutonium and americium (US DOE 2004b, Appendix TRU WASTE). As an independent verification of this assertion, the Agency evaluated the potential importance of neptunium-237 on PA (US EPA 2005), because of the potential for high neptunium solubilities in the presence of organic ligands (Section 8.5). The results of these calculations indicated that neptunium-237 would not contribute significantly to potential releases, and that its omission from the CRA PA was acceptable. Curium isotopes also form a relatively small fraction of the radionuclide inventory and appear unlikely to contribute significantly to radionuclide releases compared to americium and plutonium (US DOE 2004b, Appendix TRU WASTE Table TRU WASTE-9).

10.0 CULEBRA DOLOMITE DISTRIBUTION COEFFICIENTS

Radionuclides may reach the Culebra member of the Rustler Formation because of brine flow through a borehole that intersects the repository or because of brine flow up the shaft (US DOE 2004b, Section 6.4.6.2.1). Radionuclides introduced into the Culebra may be transported through natural groundwater flow (US DOE 2004b, Section 6.4.6.2). Predictions of transport and release of radionuclides through the Culebra are affected by sorption onto minerals along this potential pathway. Accordingly, DOE developed single-parameter distribution coefficients (K_ds) to express a linear relationship between sorbed and aqueous concentrations of the radionuclides (US DOE 2004b, Section 6.4.6.2.1).

10.1 Culebra Dolomite Distribution Coefficients Used in the CCA PA and PAVT

Distribution coefficients were developed using data from:

- Sorption studies carried out on 'dolomite-rich Culebra rock' by Triay and co-workers (LANL);
- Sorption studies on pure dolomite from Norway using synthetic NaCl solutions by Brady and co-workers (Sandia and LANL); and
- Transport studies using intact core samples of Culebra rock by Lucero and co-workers (Sandia).

Sorption data from these sources were compiled and evaluated by Brush (1996), and these K_d values were used in the CCA PA and in the PAVT (Table 10-1). These values were subsequently updated by Brush and Storz (1996) because of errors in the calculated K_d values. The differences between the K_d values reported by Brush (1996) and by Brush and Storz (1996) resulted from corrections of:

- Errors in the mass of dolomite used to calculate K_d values in the sorption studies by Brady and coworkers; and
- Errors in the density of brine used to calculate K_d values in the experiments by Triay and co-workers (Brush and Storz 1996).

The revised values from Brush and Storz (1996) were not available in time for inclusion in the CCA PA or PAVT; however, Brush and Storz (1996) stated that the relatively small changes in the K_d values were unlikely to significantly impact PA results.

Brush (1996) and Brush and Storz (1996) provided K_d values for actinide elements for both deep (Castile and Salado) brines and Culebra brines. For conservatism, only the ranges of K_ds for the brine having the smaller mean value were used in PA. A uniform distribution was used for all K_d ranges in the CCA PA (Brush 1996, Brush and Storz 1996). Sorption experiments were conducted in the presence of organic ligands, but DOE did not revise the ranges of K_ds to include the potential effects of organic ligands because they assumed that metals present in the waste (such as iron and nickel) would compete with actinides for the organic ligands and would limit the effects of ligands on actinide sorption (Brush 1996; Brush and Storz 1996).

The Agency evaluated the ranges and distributions of K_d values used in the CCA PA (US EPA 1998b). The Agency reviewed and accepted the ranges used in the CCA, but disagreed with the uniform distribution for these ranges. The Agency instead specified a log-uniform distribution for the K_d ranges for use in the PAVT.

10.2 Culebra Distribution Coefficients Used in the CRA

Hansen and Leigh (2003) provide a reconciliation of parameter values between the CCA (PAVT) and the CRA. As shown in Hanson and Leigh (2003), there were no changes in the ranges of K_d values for the radioelements uranium(VI), uranium(IV), plutonium(III), plutonium(IV), thorium(IV), and americium(III) between the CCA and the PAVT. Hansen and Leigh (2003) note the two errors in the procedures used to calculate the matrix K_ds after submission for CCA calculations, and reiterate the conclusion of Brush and Storz (1996) that the influence of the errors is minimal.

Data sheets were reviewed, as well as the references therein, for Parameters 52 to 57 in Appendix PA Attachment PAR, that address the matrix distribution coefficients (K_ds) for uranium(VI), uranium(IV), plutonium(III), plutonium(IV), thorium(IV), and americium(III). Apart from the K_d values themselves (minimum and maximum values), two key pieces of information are provided in each parameter data sheet:

- References containing a discussion of site-specific experimental data; and
- Discussion of the technical basis (laboratory results) for data selection.

The key references for this review have been Brush (1996), Brush and Storz (1996), Wall (2001), and Hansen and Leigh (2003).

In discussing the parameter baseline, including distribution coefficients, Wall (2001) appears to use the Agency's conclusions (US EPA 1998b) to address key technical issues, such as the use of brines with lower pH than expected in the repository, and the effect of organic ligands. Regarding the latter, the Agency agreed at the time of the CCA that the effect of organic ligands on actinide sorption could be ruled out because sufficient concentrations of non-actinide cations would be available to complex with these ligands. However, new thermodynamic data and modeling calculations (Section 8.0) indicate that solubilities of the +III and +V actinides could be affected by organic ligands.

The K_d values measured in brines with organic ligands (Brush and Storz 1996) were re-examined. The reported values for low- and intermediate-concentration organic ligands were judged to be the most applicable to WIPP repository conditions. The ranges of K_d values reported for americium(III) and uranium(VI) in the presence of organic ligands are consistent with the ranges of K_d values used in the CRA PA. However, values on the order of approximately 4 ml/g were observed for thorium(IV) in the presence of organic ligands, whereas the range of values used in PA was 700 to 10,000 ml/g. This reduction in K_d values for thorium(IV) appears to be inconsistent with the results of geochemical modeling, because thorium(IV) does not appear to be significantly complexed by organic ligands (Section 8.5). This inconsistency may be the result of higher carbon dioxide fugacities and lower pH in the experiments than are expected in the WIPP repository.

The data regarding the potential effects of organic ligands on actinide sorption were previously considered by the Agency (US EPA 1998b). At that time, the Agency concluded that the results of the speciation calculations, K_d values reported in the literature, and expected increased adsorption under alkaline conditions indicated that the K_d ranges exclusive of the organic ligands should be sufficiently representative of actinide solid/liquid partitioning for modeling actinide transport in the Culebra. No new sorption data have been presented that challenge that conclusion.

No additional sorption experiments have been carried out since the CCA and PAVT in support of the CRA. Thus, the same laboratory results support the Revised Parameter Baseline (RPB) for the CRA, Brush and Storz (1996) provided corrected K_d values for actinide elements for both deep (Castile and Salado) brines and Culebra brines. For conservatism, only the range of K_ds for the brine having the smaller mean value was used in the RPB. Based on the K_d ranges provided for the PAVT, the changes shown in Table 10-1 are small and all changes result in more conservatism, i.e., small K_d values, which should result in less sorption. The values used in the CRA PA are acceptable because no new experimental sorption data are available, the changes to the K_d ranges are minor and conservative, and these results have been previously reviewed by the Agency (US EPA 1998b).

Table 10-1 Comparison of Matrix K_d Values for the CCA PA and PAVT With CRA PA Matrix K_d Values

Actinide	**Oxidation State Analogue**	**CCA PA and PAVT K_d Range [m^3/kg]** **(Brush 1996)**	**CRA PA K_d Range [m^3/kg]** **(Brush and Storz 1996)**
Americium(III)	Plutonium(V)[1]	0.02 - 0.5	0.02 - 0.4
Plutonium(III)	Plutonium(V)	0.02 - 0.5	0.02 - 0.4
Uranium(IV)	Thorium(IV)	0.9 - 20	0.7 - 10
Neptunium(IV)	Thorium(IV)	0.9 - 20	0.7 - 10
Thorium(IV)	Thorium(IV)	0.9 - 20	0.7 - 10
Plutonium(IV)	Thorium(IV)	0.9 - 20	0.7 - 10
Neptunium(V)	Neptunium(V)	0.001 - 0.2	0.001 - 0.2
Uranium(VI)	Uranium(VI)	0.00003 - 0.03	0.00003 - 0.02

[1] The K_d value for plutonium(V) was used conservatively as a substitute for americium(III) and plutonium(III) K_d values rather than a direct oxidation state analogue.

11.0 CONCLUSIONS AND KEY ISSUES

Information in the CRA has been reviewed to determine whether DOE appropriately included in the CRA PA all new chemistry-related information acquired since the CCA, as required by 40 CFR 194.15(a).

As a result of the Agency's review EPA directed DOE to change many parameters related to chemistry (EPA 2005b, see Docket A-98-49 Item II-B2-25). DOE implemented these changes in a new performance assessment, call the Performance Assessment Baseline Calculation or PABC. EPA reviewed these changes (EPA 2006, see Docket A-98-49 Item II-B1-16) and found that DOE adequately implemented then in the PABC.

DOE adequately accounted for new information related to a number of chemistry issues:

- There have been no documented changes to the FMT geochemical modeling code or conceptual models. The FMT database has been updated to account for new thermodynamic data available for the +III, +IV and +V actinide oxidation states, and adequate documentation of this update has been provided.
- The Salado Formation intergranular brine formulation used for actinide solubility modeling has changed from Brine A to GWB since the PAVT. Although small differences in +III and +V actinide solubilities are observed using the revised Salado brine formulation, the GWB formulation is expected to better represent Salado brine chemistry and the GWB formulation appears to be adequately documented.
- DOE assumed that the brucite-hydromagnesite$_{5424}$ reaction would control carbon dioxide fugacities in PA vectors that included significant microbial degradation of CPR. This assumption regarding the phase likely to control carbon dioxide fugacity is unchanged since the PAVT and is consistent with experimental data developed since the CCA.
- DOE has assumed that increased temperatures will not have a significant impact on actinide solubilities in the WIPP repository. This assumption is appropriate, provided the WIPP inventory does not include heat-source plutonium or wastes with fission product concentrations in excess of the quantities assumed in the CCA.
- Changes to the Culebra distribution coefficient values (K_ds) since the PAVT are acceptable because these changes are relatively small and, because the values have decreased, the K_d values are more conservative than those used in the PAVT.

However, a number of issues required additional documentation and/or new PA calculations:

- EPA directed DOE to assume for the PABC calculations a probability of 1 for significant microbial degradation. This assumption is necessary because of the higher probability of the presence of microbes capable of degrading CPR, the increased probability of nutrients because of the increased phosphate inventory since the CCA, and possible evidence of the long-term viability of microbes in geologic environments.

- Changing the implementation of microbial gas generation rates for the PABC to more closely represent initially rapid gas generation followed by much slower rates resulted in a gas-generation model that is more consistent with the available data regarding likely gas generation in the WIPP repository.

- Because of the increased probability of microbial degradation, all PABC vectors included the assumption that carbon dioxide fugacity is controlled by the brucite-hydromagnesite$_{5424}$ reaction and included microbial colloid transport of actinides.

- DOE carried out sensitivity analyses to determine if uncertainties in organic ligand concentrations, including the possible production of organic ligands by CPR degradation, could significantly affect PA. The results of these calculations indicate that actinide solubilities do not appear to be particularly sensitive to microbially produced lactate or acetate. However, these calculations have indicated that +III and +V actinide solubilities may be sensitive to EDTA and oxalate concentrations, respectively. Therefore, DOE included estimates of organic ligands in the waste inventory for the CRA PA and PABC.

- The actinide solubility uncertainties have been recalculated by DOE using the new FMT thermodynamic database and additional experimental data. Separate uncertainty estimates are now available for the +III, +IV, and +V actinide solubilities, compared to a single uncertainty distribution that was used for all three actinide oxidation states in the CCA PA and the PAVT. These changes are included in the PABC.

- DOE did not consider all potentially relevant information that has been developed since the CCA to determine if the uranium(VI) concentration used in the CRA PA is still defensible. An evaluation of the available data, including the possible effects of carbonate concentrations and ligands on uranium(VI) solubilities in WIPP repository brines, has indicated that a higher uranium(VI) solubility than has previously should been used. EPA directed DOE to use a higher value in the PABC.

- The presence of large quantities of iron-based metals and microbial degradation of CPR will produce reducing conditions over the long term in the WIPP repository. The appropriate actinide oxidation states have been assumed in the CRA PA, including the expected presence of plutonium in the +III and +IV oxidation states within a short time period after repository closure. However, some contradictory data exist that indicate plutonium(V) could persist in the repository for an unspecified period of time. Additional data regarding the factors controlling plutonium(V) reduction to plutonium(III) or plutonium(IV) in WIPP brines would reduce the remaining uncertainty regarding plutonium oxidation states in the repository environment.

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ATTACHMENT A

ANNOTATED VERSION OF THERMODYNAMIC DATABASE
FMT_021120.CHEMDAT

The attached database listing includes the thermodynamic database FMT_021120.CHEMDAT that was used with the FMT code (Version 2.4) to calculate actinide solubilities for the CRA PA. Revisions to the database used for the PAVT (FMT_970407.CHEMDAT) are indicated by shading of those entries; data that were replaced are included within square brackets.

fmt_021120.chemdat

```
'FMT_021120.chemdat'
'ERG update of FMT_970407.chemdat (PAVT db)'

27 214 'nNEW T' 'nACTCOEF' 'nECHO' 'nABCD'
200 1.d-6 1.d-18
'NONE' 298.15 1.d0 1.d0

'Hydrogen' 'Oxygen' 'Sodium' 'Potassium' 'Magnesium' 'Calcium' 'Chlorine' 'Sulfur' 'Carbon' 'PosIon:EL'
   'NegIon:EL' 'Oxalate:EL' 'Boron' 'Bromine' 'Acetate:EL' 'Th(IV)' 'Am(III)' 'Pu(III)' 'Np(V)'
   'ClO4:EL' 'Phosphorus' 'U(IV)' 'Lactate:EL' 'EDTA:EL' 'Citrate:EL' 'Electron:EL' 'Charge:EL'
1.0079 15.9994 22.98977 39.0983 24.305 40.08 35.453 32.06 12.011 0.0 0.0 28.84 10.81 79.904 59.044
    232.0381 243.0 238.029 237.0482 99.4506 30.974 242.0 89.07 888.888 189.1 0.0 0.0

'H2O                          WATER'  2  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -95.6635     HMW84
'Na+                            Na+'  0  0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -105.651     HMW84
'K+                              K+'  0  0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -113.957     HMW84
'Ca++                          Ca++'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -223.30      HMW84
'Mg++                          Mg++'  0  0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  2   1 -183.468     HMW84
'MgOH+                        MgOH+'  1  1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -251.94      HMW84
'H+                              H+'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1  0.          HMW84

'Cl-                            Cl-'  0  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -52.955      HMW84
'SO4=                          SO4='  0  4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1 -300.386     HMW84
'HSO4-                        HSO4-'  1  4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -304.942     HMW84
'OH-                            OH-'  1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -63.435      HMW84
'HCO3-                        HCO3-'  1  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -236.751     HMW84
'CO3=                          CO3='  0  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1 -212.944     HMW84

'CO2(aq)                    CO2(aq)'  0  2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -155.68      HMW84
'CaCO3(aq)                CaCO3(aq)'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -443.5       HMW84
'MgCO3(aq)                MgCO3(aq)'  0  3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -403.155     HMW84

'B(OH)3(aq)              B(OH)3(aq)'  3  3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -390.81      FW86
'B(OH)4-                    B(OH)4-'  4  4 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -465.20      FW86
'B3O3(OH)4-              B3O3(OH)4-'  4  7 0 0 0 0 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -963.77      FW86
'B4O5(OH)4=              B4O5(OH)4='  4  9 0 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1 -1239.10     FW86
'CaB(OH)4+                CaB(OH)4+'  4  4 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -692.30      FW86
'MgB(OH)4+                MgB(OH)4+'  4  4 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1 -651.89      FW86
'Br-                            Br-'  0  0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 -1   1 -999.99      arbitrary
'ClO4-                  perchlorate'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 -1   1 -73.81       CFN950705

'NaOH(aq)      to.titrate.base.only'  1  1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'HCl(aq)       to.titrate.acid.only'  1  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1  500.        arbitrary
'HClO4(aq)     to.titrate.acid.only'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0  0   1  500.        arbitrary
'PosIon                POSITIVE.ION'  0  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1  0.          arbitrary
'NegIon                NEGATIVE.ION'  0  0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  0.          arbitrary
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'PosIon(OH)(aq)      to.titrate.base'  1  1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   1  500.        arbitrary
'HNegIon(aq)         to.titrate.acid'  1  0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   1  500.        arbitrary

'H3PO4(aq)                 H3PO4(aq)'  3  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0   0   1 -460.90       RFF92
'H2PO4-                       H2PO4-'  2  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  -1   1 -455.96       RFF92
'HPO4=                         HPO4='  1  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  -2   1 -439.367      CFN95a
'PO4=-                         PO4=-'  0  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0  -3   1 -410.947      RFF92

'Am+++                         Am+++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   3   1 -241.694      FO76
                                                                                                            [OLD VALUE IN SQUARE BRACKETS]
'AmCO3+                       AmCO3+'  0  3 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   1   1 -473.29 [-472.060]
FK98/Fanghanel et al 1999
'Am(CO3)2-                 Am(CO3)2-'  0  6 0 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  -1   1 -697.52 [-695.880]
FK98/Fanghanel et al 1999
'Am(CO3)3=-               Am(CO3)3=-'  0  9 0 0 0 0 0 0 3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  -3   1 -915.53 [-915.460]
FK98/Fanghanel et al 1999
'AmOH++                       AmOH++'  1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2   1 -319.96 [-315.352]
FK98/Fanghanel et al 1994
'Am(OH)2+                   Am(OH)2+'  2  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   1   1 -396.89 [-392.281]
FK98/Fanghanel et al 1994
'Am(OH)3(aq)             Am(OH)3(aq)'  3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   0   1 -469.53 [-471.603]
FK98/Fanghanel et al 1994
[NEW SPECIES]
'AmCl++  [NEW]                AmCl++'  0  0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   2   1 -295.20       FK98/Konnecke et al
1997
'AmCl2+                       AmCl2+'  0  0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   1   1 -345.90       FK98/Konnecke et al
1997  [NEW]
'Am(CO3)4==-             Am(CO3)4==-'  0 12 0 0 0 0 0 0 4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  -5   1 -1123.40      FK98/Fanghanel et al
1999  [NEW]
'Am(SO4)2-   [NEW]         Am(SO4)2-'  0  8 0 0 0 0 0 2 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0  -1   1 -850.99       FK98
'AmSO4+   [NEW]               AmSO4+'  0  4 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   1   1 -549.56       FK98

'Pu(OH)2+                deactivated'  2  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0   1   1  999.999 DEACTIVATED
'Pu(OH)3(aq)             deactivated'  3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0   0   1  999.999 DEACTIVATED

'Th++++                       Th++++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   4   1 -284.227      FO76
'Th(CO3)5===              Th(CO3)5==='  0 15 0 0 0 0 0 0 5 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0  -6   1 -1411.378     CFN960119/FRSMHC97
'Th(OH)3(CO3)-         Th(OH)3(CO3)-'  3  6 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0  -1   1 -775.627      CFN960119/FRSMHC97
'Th(OH)4(aq)             Th(OH)4(aq)'  4  4 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   1 -622.47 [-622.840]
ERG_Th_memo/RR87
'Th(SO4)2(aq)           Th(SO4)2(aq)'  0  8 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   1 -911.69       FR92
'Th(SO4)3=                 Th(SO4)3='  0 12 0 0 0 0 0 3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0  -2   1 -1214.0       FR92

'U++++                         U++++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0   4   1 -214.19       RFSMMN
'UOH+++                       UOH+++'  1  1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0   3   1 -308.7        RFSMMN
'U(CO3)5===               U(CO3)5==='  0 15 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  -6   1 -1345.393     Rai96
'U(OH)2(CO3)2=         U(OH)2(CO3)2='  2  8 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  -2   1 -863.383      Rai96
'U(OH)4(CO3)2==       U(OH)4(CO3)2=='  4 10 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  -4   1 -998.662      Rai96
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'U(OH)4(aq)           deactivated'  4  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   1  999.999
'U(SO4)2(aq)          deactivated'  0  8 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0  0   1  999.999
'U(SO4)3=             deactivated'  0 12 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 -2   1  999.999

'NpO2+                      NpO2+'  0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0  1   1 -369.105 [-369.109]    FO76
'NpO2CO3-                NpO2CO3-'  0  5 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -1   1 -593.601 [-593.635]    FNK95
'NpO2(CO3)2=-         NpO2(CO3)2=-'  0  8 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -3   1 -809.832 [-809.895]    FNK95
'NpO2(CO3)3==-      NpO2(CO3)3==-'  0 11 0 0 0 0 0 0 3 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -5   1 -1020.214 [-1020.306]   FNK95
'NpO2OH(aq)            NpO2OH(aq)'  1  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0  0   1 -438.730 [-438.738]    FNK95
'NpO2(OH)2-            NpO2(OH)2-'  2  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -1   1 -506.238 [-506.249]    FNK95

'HAc(aq)              AceticAcid'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  0   1 -158.300      SAND99/NBC96
'Ac-                     Acetate-'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 -1   1 -147.347      SAND99/NBC96

'H3Citrate(aq)        CitricAcid'  3  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0  0   1  000.000      SAND99/Mizera
'H2Citrate-           H2Citrate-'  2  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1    7.476 [7.245]     SAND99/Mizera
'HCitrate=              HCitrate='  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -2   1   18.620 [18.3]     SAND99/Mizera
'Citrate=-              Citrate=-'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -3   1   33.410 [33.068]     SAND99/Mizera

'H4EDTA(aq)           H4EDTA(aq)'  4  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0  0   1  000.000      SAND99/Mizera
'H3EDTA-                  H3EDTA-'  3  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -1   1    5.761 [5.360]     SAND99/Mizera
'H2EDTA=                  H2EDTA='  2  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -2   1   12.870 [11.659]     SAND99/Mizera
'HEDTA=-                  HEDTA=-'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -3   1   28.710 [26.700]     SAND99/Mizera
'EDTA==                    EDTA=='  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -4   1   53.050 [52.109]     SAND99/Mizera

'H2Ox(aq)             OxalicAcid'  2  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1    0.000      SAND99/Mizera
'HOx-                  Bioxalate-'  1  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1    3.209 [3.052]      SAND99/Mizera
'Ox=                     Oxalate='  0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2   1   13.017 [12.790]      SAND99/Mizera

'HLactate(aq)         LacticAcid'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  0   1  000.000      SAND99
'Lactate-                Lactate-'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 -1   1    8.798 [9.002]     SAND99

'AmAc++               AmAcetate++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0  2   1 -395.356 [-395.358]    ERG_org_memo
'AmCit(aq)         AmCitrate(aq)'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0  0   1 -228.543 [-228.687]    SAND99
'AmEDTA-                  AmEDTA-'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 -1   1 -232.324 [-232.977]    SAND99
'AmOx+                 AmOxalate+'  0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0  1   1 -242.853 [243.483]
SAND99/Borkowski et al 01
'AmLac++              AmLactate++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0  2   1 -241.436 [-242.339]    SAND99/Moore
et al 99 deemed data insufficient

'ThAc2++             ThAcetate2++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0  2   1 -604.800      Moore et al 1999
[NEW]
'PuCit(aq)            deactivated'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0  0   1  999.999 DEACTIVATED
'NpO2H2EDTA-          NpO2H2EDTA-'  2  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 -1   1 -364.098      SAND99/PBMC98   [NEW]
'PuOx+                deactivated'  0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0  1   1  999.999 DEACTIVATED
'ThLac2++            ThLactate2++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 2 0 0 0  2   1 -292.400      Moore et al 1999
[NEW]
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'ThAc+++                 ThAc+++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0  3   1 -448.525 [-448.639]    SAND99
'ThCit+                   ThCit+'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0  1   1 -285.898 [-285.706]    SAND99/data
of CEX96
'ThEDTA(aq)           ThEDTA(aq)'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0  0   1 -285.419 [-285.817]    ERG_org_memo
'ThOx++              Th(C2O4)++'  0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0  2   1 -297.428 [-297.076]
SAND99/Borkowski et al 01
'ThLac+++               ThLac+++'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0  3   1 -291.152 [-291.182]    SAND99/Moore
et al 99

'UAc+++              deactivated'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0  3   1  999.999 DEACTIVATED
'UCit+               deactivated'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0  1   1  999.999 DEACTIVATED
'UEDTA(aq)           deactivated'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0  0   1  999.999 DEACTIVATED
'ULac+++             deactivated'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0  3   1  999.999 DEACTIVATED
'UOx++               deactivated'  0  0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0  2   1  999.999 DEACTIVATED

'NpO2Ac(aq)           NpO2Ac(aq)'  0  0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0  0   1 -519.615 [-519.809]
ERG_release_memo
'NpO2Cit=          NpO2Citrate='  0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 0 -2   1 -343.747 [-343.066]    SAND99/data
of BPBC99
'NpO2EDTA=-          NpO2EDTA=-'  0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 -3   1 -335.708 [-337.03]    SAND99/PBMC98
'NpO2Ox-          NpO2Oxalate-'  0  2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 -1   1 -365.851 [-366.452]
SAND99/Borkowski et al 01
'NpO2Lac(aq)     NpO2Lactate(aq)'  0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0  0   1 -364.837 [-364.266]    SAND99/Moore
et al 99

'MgAc+                     MgAc+'  0  0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  1   1 -333.378 [-333.346]    ERG_org_memo
'MgCit-                   MgCit-'  0  0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1 -162.261 [-161.979]    ERG_org_memo
'MgEDTA=                 MgEDTA='  0  0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -2   1 -153.734 [-160.325]    ERG_org_memo
'MgOx(aq)               MgOx(aq)'  0  0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -179.185 [-178.880]    ERG_org_memo
'MgLac+                   MgLac+'  0  0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  1   1  999.999     No MgLac data

'CaAc+              (Mg-analog)'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0  1   1 -373.210 [-373.178]    analogy
w/Mg++ (ERG_org_memo)  [NOT DIRECT ANALOGY BUT OK]
'CaCit-             (Mg-analog)'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 -1   1 -202.093 [-201.811]    analogy
w/Mg++ (ERG_org_memo) [NOT DIRECT ANALOGY BUT OK]
'CaEDTA=            (Mg-analog)'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 -2   1 -193.566 [-200.157]    analogy
w/Mg++ (ERG_org_memo) [NOT DIRECT ANALOGY BUT OK]
'CaOx(aq)           (Mg-analog)'  0  0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1 -219.017 [-218.712]    analogy
w/Mg++ (ERG_org_memo) [NOT DIRECT ANALOGY BUT OK]
'CaLac+             (Mg-analog)'  0  0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0  1   1  999.999     No MgLac data
'UnuCat#1+                 UC#1+'  0  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   1  999.999
'NpO2HEDTA=           NpO2HEDTA='  1  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 -2   1 -351.852     SAND99/PBMC98   [NEW]
'UnuAn#2-                  UA#2-'  0  0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuAn#3-                  UA#3-'  0  0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuAn#4-                  UA#4-'  0  0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   1  999.999
'UnuNeu#1(aq)           UN#1(aq)'  0  0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   1  999.999
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'AmOHCO3(c)_______________AmOHCO3(c)'  1  4 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   0   2  -570.34 [-569.980]     Fanghanel et
al. 1999
'Am(OH)3(s)_______________Am(OH)3(s)'  3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   0   2  -495.32 [-492.294]     Konnecke et
al. 1997
'NaAm(CO3)2.6H2O(c)_________________' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0   0   2 -1396.47      RRFFN96
'AmPO4(c)___________________AmPO4(c)'  0  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0   0   2  -709.75      RFF92

'PuOHCO3(c)_______________deactivated'  1  4 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0   0   2   999.999 DEACTIVATED
'Pu(OH)3(s)_______________deactivated'  3  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0   0   2   999.999 DEACTIVATED
'NaPu(CO3)2.6H2O(c)_______deactivated' 12 12 1 0 0 0 0 0 2 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0   0   2   999.999 DEACTIVATED
'PuPO4(c)_________________deactivated'  0  4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 0 0 0 0 0   0   2   999.999 DEACTIVATED

'ThO2(am)_____Hydrous_Thorium_Oxide'  0  2 0  0 0 0 0  0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -451.408      FRM91
'Th(SO4)2.9H2O(s)__________________' 18 17 0  0 0 0 0  2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -1775.90      FR92
'Th(SO4)2.8H2O(s)__________________' 16 16 0  0 0 0 0  2 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -1680.00      FR92
'Th(SO4)2.Na2SO4.6H2O(16C,s)_______' 12 18 2  0 0 0 0  3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -2011.29      FR92
'Th(SO4)2.K2SO4.4H2O(16C,s)________'  8 16 0  2 0 0 0  3 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -1837.57      FR92
'Th(SO4)2.2K2SO4.2H2O(16C,s)_______'  4 18 0  4 0 0 0  4 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0   0   2 -2181.81      FR92
'2[Th(SO4)2.7/2K2SO4(16C,s)]_______'  0 44 0 14 0 0 0 11 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0   0   2 -5581.66 =2[-2790.83] FR92

'UO2(am)________Hydrous_U(IV)_Oxide'  0  2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0   0   2 -399.67       RFSMMN

'NpO2OH(aged)__________NpO2OH(aged)'  1  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   0   2  -454.369 [-454.373]    FNK95/NFRK95
'NpO2OH(amor)__________NpO2OH(amor)'  1  3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   0   2  -452.757 [-452.761]    FNK95/NFRK95
'2[NaNpO2CO3.7/2H2O(s)]____________' 14 17 2 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 0 0   0   2 -2096.116 [-2096.124]    =2*(-
1048.058)  FNK95/NFRK95
'Na3NpO2(CO3)2(s)__Na3NpO2(CO3)2(s)'  0  8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   0   2 -1144.597 [-1144.601]
FNK95/NFRK95
'KNpO2CO3(s)____________KNpO2CO3(s)'  0  5 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   0   2  -727.330     Novak et al. 1997
'K3NpO2(CO3)2(s)____K3NpO2(CO3)2(s)'  0  8 0 3 0 0 0 0 2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0   0   2 -1173.546     Novak et al. 1997

'H2Ox.2H2O(s)_________H2C2O4.2H2O(s)'  6  2 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -191.346 [-191.370]     ERG_ox_memo
'NaHOx.H2O(s)_________NaHC2O4.H2O(s)'  3  1 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -202.253 [-202.245]     ERG_ox_memo
'Na2Ox(s)__________________Na2C2O4(s)'  0  0 2 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -203.823 [-203.651]     ERG_ox_memo
'CO2("solid",DISABLED)______________'  0  2 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2     0.0  [999.999]

'CaSO4______________________Anhydrite'  0  4 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -533.73       HMW84
'NaK3(SO4)2__Aphthitalite/Glaserite'  0  8 1 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -1057.05      HMW84
'CaCl2.6H2O_____________Antarcticite' 12  6 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -893.65       HMW84
'CaCO3______________________Aragonite'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -455.17       HMW84
'K2SO4_______________________Arcanite'  0  4 0 2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -532.39       HMW84
'MgCl2.6H2O_______________Bischofite' 12  6 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -853.1        HMW84
'Na2Mg(SO4)2.4H2O___________Bloedite'  8 12 2 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -1383.6       HMW84
'Mg(OH)2______________________Brucite'  2  2 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -335.4        HMW84
'Na6CO3(SO4)2_______________Burkeite'  0 11 6 0 0 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -1449.4       HMW84
'CaCO3_________________________Calcite'  0  3 0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -455.6        HMW84
'CaCl2.4H2O______CaCl2_Tetrahydrite'  8  4 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -698.7        HMW84
'Ca4Cl2(OH)6.13H2O__CaOxychloride_A' 32 19 0 0 0 4 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   0   2 -2658.45      HMW84
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'Ca2Cl2(OH)2.H2O____CaOxychloride_B'  4  3 0 0 0 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -778.41    HMW84
'KMgCl3.6H2O_____________Carnallite' 12  6 0 1 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1020.3    HMW84
'MgSO4.7H2O________________Epsomite' 14 11 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1157.83   HMW84
'CaNa2(CO3)2.5H2O________Gaylussite' 10 11 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1360.5    HMW84
'Na2Ca(SO4)2_____________Glauberite'  0  8 2 0 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1047.45   HMW84
'CaSO4.2H2O__________________Gypsum'  4  6 0 0 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -725.56    HMW84
'NaCl________________________Halite'  0  0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -154.99    HMW84
'MgSO4.6H2O_____________Hexahydrite' 12 10 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1061.60   HMW84
'KMgClSO4.3H2O______________Kainite'  6  7 0 1 1 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -938.2     HMW84
'KHCO3___________________Kalicinite'  1  3 0 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -350.06    HMW84
'MgSO4.H2O________________Kieserite'  2  5 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -579.80    HMW84
'K2Mg(SO4)2.4H2O____________Leonite'  8 12 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1403.97   HMW84
'Na4Ca(SO4)3.2H2O_______Labile_Salt'  4 14 4 0 0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1751.45   HMW84
'MgCO3____________________Magnesite'  0  3 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -414.45    HMW84
'Mg2Cl(OH)3.4H2O______MgOxychloride' 11  7 0 0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1029.6    HMW84
'KHSO4___________________Mercallite'  1  4 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -417.57    HMW84
'Na2SO4.10H2O____________Mirabilite' 20 14 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1471.15   HMW84
'K8H6(SO4)7________________Misenite'  6 28 0 8 0 0 0 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -3039.24   HMW84
'NaHCO3___________________Nahcolite'  1  3 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -343.33    HMW84
'Na2CO3.10H2O________________Natron' 20 13 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1382.78   HMW84
'MgCO3.3H2O____________Nesquehonite'  6  6 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -695.3     HMW84
'K2Mg(SO4)2.6H2O_Picromerite/Schoen' 12 14 0 2 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1596.1    HMW84
'Na2Ca(CO3)2.2H2O________Pirssonite'  4  8 2 0 0 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1073.1    HMW84
'K2MgCa2(SO4)4.2H2O______Polyhalite'  4 18 0 2 1 2 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2282.5    HMW84
'Ca(OH)2________________Portlandite'  2  2 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -362.12    HMW84
'K2CO3.3/2H2O___Potassium_Carbonate' 3 4.5 0 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -577.37    HMW84
'K8H4(CO3)6.3H2O___K-Sequicarbonate' 10 21 0 8 0 0 0 0 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2555.4    HMW84
'KNaCO3.6H2O_________K-Na-Carbonate' 12  9 1 1 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1006.8    HMW84
'K2NaH(CO3)2.2H2O___Potassium_Trona'  5  8 1 2 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -971.74    HMW84
'K3H(SO4)2__Sesquipotassium_Sulfate'  1  8 0 3 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -950.8     HMW84
'Na3H(SO4)2____Sesquisodium_Sulfate'  1  8 3 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -919.6     HMW84
'Na2CO3.7H2O____Na2CO3-Heptahydrate' 14 10 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1094.95   HMW84
'KCl________________________Sylvite'  0  0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -164.84    HMW84
'K2Ca(SO4)2.H2O___________Syngenite'  2  9 0 2 0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1164.8    HMW84
'Mg2CaCl6.12H2O________Tachyhydrite' 24 12 0 0 2 1 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2015.9    HMW84
'Na2SO4__________________Thenardite'  0  4 2 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -512.35    HMW84
'Na2CO3.H2O___________Thermonatrite'  2  4 2 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -518.8     HMW84
'Na3H(CO3)2.2H2O______________Trona'  5  8 3 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -960.38    HMW84
'Na2B4O7.10H2O________________Borax' 20 17 2 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2224.16   FW86
'B(OH)3____________Borix_Acid_Solid'  3  3 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -390.88    FW86
'KB5O8.4H2O____K-Pentaborate_(30_C)'  8 12 0 1 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1770.26   FW86
'K2B4O7.4H2O___K-Tetraborate_(30_C)'  8 11 0 2 0 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1663.47   FW86
'NaBO2.4H2O_______Sodium_Metaborate'  8  6 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -761.42    FW86
'NaB5O8.5H2O_____Sodium_Pentaborate' 10 13 1 0 0 0 0 0 0 0 0 0 5 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1854.80   FW86
'NaBO2.NaCl.2H2O___Teepleite_(20_C)'  4  4 2 0 0 0 1 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -725.77    FW86
'CaMg(CO3)2________________Dolomite'  0  6 0 0 1 1 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -871.99    HMW84
'Mg5(CO3)4(OH)2.4H2O_HydroMagne5424' 10 18 0 0 5 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -2364.06   R&H73
'Mg4(CO3)3(OH)2.3H2O_HydroMagne4323'  8 14 0 0 4 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  0   2 -1856.104  Lang65
```

```
'H+(solid)_______________to.set.aH+'  1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  1   2  0.0
'OH-/H2O(solid)__________to.set.aH+' -1  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1   2  0.0

'nDG_BYPASS' 0
'PITZACT'
 39 #Cations
 53 #Anions
 26 #Neutrals

  1  .0765     .2644    .0      .00127   Na+ Cl-           HMW84  (beta0, beta1, beta2, cphi) NOTE: HMW gives .2644; P91 gives .2664
  1  .01958   1.113     .0      .00497   Na+ SO4=          HMW84
  1  .0454     .398     .0      .0       Na+ HSO4-         HMW84
  1  .0864     .253     .0      .0044    Na+ OH-           HMW84
  1  .0277     .0411    .0      .0       Na+ HCO3-         HMW84
  1  .0399    1.389     .0      .0044    Na+ CO3=          HM284
  1 -.0427     .089     .0      .0114    Na+ B(OH)4-       FW86
  1 -.056     -.910     .0      .0       Na+ B3O3(OH)4-    FW86
  1 -.11      -.40      .0      .0       Na+ B4O5(OH)4=    FW86
  1  .0        .0       .0      .0       Na+ Br-
  1 -.240      .224     .0      .0284    Na+ Am(CO3)2-     FK98/Fanghanel et al. 1999  [.0           .0     .0     .0]
  1  .125     4.73      .0      .0007    Na+ Am(CO3)3=-    FK98/Fanghanel et al. 1999  [-.256  5.0   .0     .0443]
  1  .0554     .2755    .0     -.00118   Na+ ClO4-         P91
  1  .0        .0       .0      .0       Na+ NpO2(OH)2-    FNK95
  1  .10       .34      .0      .0       Na+ NpO2CO3-      FNK95
  1  .48      4.4       .0      .0       Na+ NpO2(CO3)2=-  FNK95
  1  1.80     22.7      .0      .0       Na+ NpO2(CO3)3==- FNK95
  1 -.0533     .0396    .0      .00795   Na+ H2PO4-        P91
  1 -.0583    1.466     .0      .0294    Na+ HPO4=         P91
  1  .1781    3.851     .0     -.05154   Na+ PO4=-         P91
  1  .12       .0       .0      .0       Na+ Th(SO4)3=     FR92
  1  .0        .0       .0      .0       Na+ Th(OH)3(CO3)-
  1  1.31    30.        .0      .0       Na+ Th(CO3)5===    FRSMHC97
  1 -0.2448    .29      .0      .068     Na+ HOx-          SAND99/Mizera
  1 -0.2176   1.74      .0      .122     Na+ Ox=           SAND99/Mizera
  1  0.1426    .22      .0     -.00629   Na+ Ac-           SAND99/NBC96
  1 -0.0563    .29      .0      .047     Na+ Lac-          SAND99/Moore et al 99
  1 -0.1296    .29      .0      .013     Na+ H2Cit-        SAND99/Mizera
  1 -0.0989   1.74      .0      .027     Na+ HCit=         SAND99/Mizera
  1  0.0887   5.22      .0      .047     Na+ Cit=-         SAND99/Mizera
  1 -0.2345    .29      .0      .059     Na+ H3EDTA-       SAND99/Mizera
  1 -0.1262   1.74      .0      .054     Na+ H2EDTA=       SAND99/Mizera
  1  0.5458   5.22      .0    -0.048     Na+ HEDTA=-       SAND99/Mizera
  1  1.016   11.6       .0      .001     Na+ EDTA==        SAND99/Mizera
  1 -.2239     .29      .0      .002     Na+ AmEDTA-       SAND99
  1 -.4226    1.75      .0      .142     Na+ NpO2Cit=      SAND99
  1  .683     5.911     .0      .0       Na+ NpO2EDTA=-    SAND99/PBMC98
  1 -.5418     .29      .0      .095     Na+ NpO2Ox-       SAND99/Borkowski et al 01
  1  .41     17.25      .0      .0       Na+ U(OH)4(CO3)2==  Rai96
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```
1 1.31     30.0        .0      .0      Na+ U(CO3)5===       Rai96
1  .0        .0        .0      .0      Na+ U(SO4)3=
1 2.022    19.22       .0    -.305     Na+ Am(CO3)4==-     FK98/Fanghanel et al. 1999
1 -.354     0.40       .0     .051     Na+ Am(SO4)2-       FK98
1 -.8285    .2575      .0     .256     Na+ NpO2H2EDTA-     PBMC98   [NEW]
1  .1742     .29       .0    -.06923   Na+ CaCit-          analogy w/Mg   (ERG_org_memo)
1  .2134    1.74       .0     .00869   Na+ CaEDTA=         analogy w/Mg   (ERG_org_memo)
1  .0        .0        .0      .0      Na+ UnuAn#2-
1  .0        .0        .0      .0      Na+ UnuAn#3-
1  .0        .0        .0      .0      Na+ UnuAn#4-
1  .0        .0        .0      .0      Na+ U(OH)2(CO3)2=
1  .1742     .29       .0    -.06923   Na+ MgCit-            ERG_org_memo
1  .2134    1.74       .0     .00869   Na+ MgEDTA=           ERG_org_memo
1  .4733   -1.504      .0      .0      Na+ NpO2HEDTA=        PBMC98

1  .04835    .2122     .0    -.00084   K+ Cl-              HMW84
1  .04995    .7793     .0      .0      K+ SO4=             HMW84
1 -.0003     .1735     .0      .0      K+ HSO4-            HMW84
1  .1298     .320      .0     .0041    K+ OH-              HMW84
1  .0296    -.013      .0    -.008     K+ HCO3-            HMW84
1  .1488    1.43       .0    -.0015    K+ CO3=             HMW84
1  .035      .14       .0      .0      K+ B(OH)4-          FW86
1 -.13       .0        .0      .0      K+ B3O3(OH)4-       FW86
1 -.022      .0        .0      .0      K+ B4O5(OH)4=       FW86
1  .0        .0        .0      .0      K+ Br-
1 -.240      .224      .0     .0284    K+ Am(CO3)2-        analogy w/ Na (FK98)
1  .125     4.73       .0     .0007    K+ Am(CO3)3=-       analogy w/ Na (FK98)
1  .0        .0        .0      .0      K+ ClO4-
1  .0        .0        .0      .0      K+ NpO2(OH)2-       Novak et al. 1997 (made analogy w/Na+)
1  .10       .34       .0      .0      K+ NpO2CO3-         Novak et al. 1997 (made analogy w/Na+)
1  .48      4.4        .0      .0      K+ NpO2(CO3)2=-     Novak et al. 1997 (made analogy w/Na+)
1 2.34     22.7     -96.     -.22      K+ NpO2(CO3)3==-    Novak et al. 1997 (calculated from K+ data)
1 -.0678   -.1042      .0      .0      K+ H2PO4-           P91
1  .0248   1.274       .0     .0164    K+ HPO4=            P91
1  .3729   3.972       .0    -.08680   K+ PO4=-            P91
1  .90       .0        .0      .0      K+ Th(SO4)3=        FR92
1  .0        .0        .0      .0      K+ Th(OH)3(CO3)-
1 1.31     30.         .0      .0      K+ Th(CO3)5===      analogy w/ Na (FRSMHC97)
1 -0.2448    .29       .0     .068     K+ HOx-             analogy w/ Na (SAND99/Mizera)
1 -0.2176   1.74       .0     .122     K+ Ox=              analogy w/ Na (SAND99/Mizera)
1  .1587     .3251     .0    -.0066    K+ Ac-              P91
1 -0.0563    .29       .0     .047     K+ Lac-             analogy w/ Na (SAND99/Moore et al 99)
1 -0.1296    .29       .0     .013     K+ H2Cit-           analogy w/ Na (SAND99/Mizera)
1 -0.0989   1.74       .0     .027     K+ HCit=            analogy w/ Na (SAND99/Mizera)
1  0.0887   5.22       .0     .047     K+ Cit=-            analogy w/ Na (SAND99/Mizera)
1 -0.2345    .29       .0     .059     K+ H3EDTA-          analogy w/ Na (SAND99/Mizera)
1 -0.1262   1.74       .0     .054     K+ H2EDTA=          analogy w/ Na (SAND99/Mizera)
1  0.5458   5.22       .0   -0.048     K+ HEDTA=-          analogy w/ Na (SAND99/Mizera)
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```
1  1.016    11.6        .0      .001     K+ EDTA==          analogy w/ Na (SAND99/Mizera)
1 -.2239      .29       .0      .002     K+ AmEDTA-         analogy w/ Na (SAND99)
1 -.4226     1.75       .0      .142     K+ NpO2Cit=        analogy w/ Na (SAND99)
1  .683     5.911       .0      .0       K+ NpO2EDTA=-      analogy w/ Na (SAND99/PBMC98)
1 -.5418      .29       .0      .095     K+ NpO2Ox-         analogy w/ Na (SAND99/Borkowski et al 01)
1  .41      17.25       .0      .0       K+ U(OH)4(CO3)2== analogy w/ Na (Rai96)
1 1.31      30.0        .0      .0       K+ U(CO3)5===      analogy w/ Na, analogy w/Th (FRSMHC97)
1  .0         .0        .0      .0       K+ U(SO4)3=
1 2.022     19.22       .0     -.305     K+ Am(CO3)4==-     analogy w/ Na (FK98)   [NEW]
1 -.354      0.40       .0      .051     K+ Am(SO4)2-       analogy w/ Na (FK98)   [NEW]
1 -.8285     .2575      .0      .256     K+ NpO2H2EDTA-     analogy w/ Na (PBMC98) [NEW]
1  .1742      .29       .0     -.06923   K+ CaCit-          analogy w/ Na, analogy w/ Mg  (ERG_org_memo)
1  .2134     1.74       .0      .00869   K+ CaEDTA=         analogy w/ Na, analogy w/ Mg  (ERG_org_memo)
1  .0         .0        .0      .0       K+ UnuAn#2-
1  .0         .0        .0      .0       K+ UnuAn#3-
1  .0         .0        .0      .0       K+ UnuAn#4-
1  .0         .0        .0      .0       K+ U(OH)2(CO3)2=
1  .1742      .29       .0     -.06923   K+ MgCit-            analogy w/ Na (ERG_org_memo)
1  .2134     1.74       .0      .00869   K+ MgEDTA=           analogy w/ Na (ERG_org_memo)
1  .4733    -1.504      .0      .0       K+ NpO2HEDTA=        analogy w/ Na (PBMC98)  [NEW]

1  .3159      1.614     .0     -.00034   Ca++ Cl-           HMW84
2  .20        3.1973 -54.24     .0       Ca++ SO4=          HMW84
1  .2145      2.53      .0      .0       Ca++ HSO4-         HMW84
1 -.1747      -.2303  -5.72     .0       Ca++ OH-           HMW84
1  .4         2.977     .0      .0       Ca++ HCO3-         HMW84
2  .0          .0       .0      .0       Ca++ CO3=          HMW84
1  .0          .0       .0      .0       Ca++ B(OH)4-       FW86
1  .0          .0       .0      .0       Ca++ B3O3(OH)4-    FW86
2  .0          .0       .0      .0       Ca++ B4O5(OH)4=    FW86
1  .0          .0       .0      .0       Ca++ Br-
1  .0          .0       .0      .0       Ca++ Am(CO3)2-
3  .0          .0       .0      .0       Ca++ Am(CO3)3=-
1  .4511      1.756     .0     -.00500   Ca++ ClO4-         P91
1  .0          .0       .0      .0       Ca++ NpO2(OH)2-
1  .10        .34       .0      .0       Ca++ NpO2CO3-       by analogy w/ Mg++ (Al Mahamid et al. 1998)
3  .48       4.4        .0      .0       Ca++ NpO2(CO3)2=-   by analogy w/ Mg++ (Al Mahamid et al. 1998)
3  2.07      22.7     -48.     -.11      Ca++ NpO2(CO3)3==-  by analogy w/ Mg++ (Al Mahamid et al. 1998)
1  .0          .0       .0      .0       Ca++ H2PO4-
2  .0          .0       .0      .0       Ca++ HPO4=
3  .0          .0       .0      .0       Ca++ PO4=-
2  .0          .0       .0      .0       Ca++ Th(SO4)3=
1  .0          .0       .0      .0       Ca++ Th(OH)3(CO3)-
3  .0          .0       .0      .0       Ca++ Th(CO3)5===
1  .0          .0       .0      .0       Ca++ HOx-
2  .0          .0       .0      .0       Ca++ Ox=
1  .0          .0       .0      .0       Ca++ Ac-
1  .0          .0       .0      .0       Ca++ Lac-
```

```
1  .0         .0       .0     .0       Ca++ H2Cit-
2  .0         .0       .0     .0       Ca++ HCit=
3  .0         .0       .0     .0       Ca++ Cit=-
3  .0         .0       .0     .0       Ca++ H3EDTA-
3  .0         .0       .0     .0       Ca++ H2EDTA=
3  .0         .0       .0     .0       Ca++ HEDTA=-
3  .0         .0       .0     .0       Ca++ EDTA==
3  .0         .0       .0     .0       Ca++ AmEDTA-
2  .0         .0       .0     .0       Ca++ NpO2Cit=
3  .0         .0       .0     .0       Ca++ NpO2EDTA==-
1  .0         .0       .0     .0       Ca++ NpO2Ox-
3  .0         .0       .0     .0       Ca++ U(OH)4(CO3)2==
3  .0         .0       .0     .0       Ca++ U(CO3)5===
2  .0         .0       .0     .0       Ca++ U(SO4)3=
3  .0         .0       .0     .0       Ca++ Am(CO3)4==-   [NEW]
1  .0         .0       .0     .0       Ca++ Am(SO4)2-     [NEW]
1  .0         .0       .0     .0       Ca++ NpO2H2EDTA-   [NEW]
1  .0         .0       .0     .0       Ca++ CaCit-
3  .0         .0       .0     .0       Ca++ CaEDTA=
3  .0         .0       .0     .0       Ca++ UnuAn#2-
1  .0         .0       .0     .0       Ca++ UnuAn#3-
3  .0         .0       .0     .0       Ca++ UnuAn#4-
2  .0         .0       .0     .0       Ca++ U(OH)2(CO3)2=
1  .0         .0       .0     .0       Ca++ MgCit-
2  .0         .0       .0     .0       Ca++ MgEDTA=
2  .0         .0       .0     .0       Ca++ NpO2HEDTA=   [NEW]

1  .35235   1.6815     .0     .00519   Mg++ Cl-           HMW84
2  .2210    3.343   -37.23    .025     Mg++ SO4=          HMW84
1  .4746    1.729      .0     .0       Mg++ HSO4-         HMW84
1  .0         .0       .0     .0       Mg++ OH-           HMW84
1  .329      .6072     .0     .0       Mg++ HCO3-         HMW84
2  .0         .0       .0     .0       Mg++ CO3=          HMW84
1  .0         .0       .0     .0       Mg++ B(OH)4-       FW86
1  .0         .0       .0     .0       Mg++ B3O3(OH)4-    FW86
2  .0         .0       .0     .0       Mg++ B4O5(OH)4=    FW86
1  .0         .0       .0     .0       Mg++ Br-
1  .0         .0       .0     .0       Mg++ Am(CO3)2-
3  .0         .0       .0     .0       Mg++ Am(CO3)3=-
1  .4961    2.008      .0     .009578  Mg++ ClO4-           P91
1  .0         .0       .0     .0       Mg++ NpO2(OH)2-
1  .10       .34       .0     .0       Mg++ NpO2CO3-        Al Mahamid et al. 1998  (made analogy w/ Na)
3  .48      4.4        .0     .0       Mg++ NpO2(CO3)2=-    Al Mahamid et al. 1998  (made analogy w/ Na)
3  2.07     22.7     -48.    -.11      Mg++ NpO2(CO3)3==-   Al Mahamid et al. 1998  (averaged Na and K values)
1  .0         .0       .0     .0       Mg++ H2PO4-
2  .0         .0       .0     .0       Mg++ HPO4=
3  .0         .0       .0     .0       Mg++ PO4=-
2  .0         .0       .0     .0       Mg++ Th(SO4)3=
```

```
1  .0        .0       .0     .0       Mg++ Th(OH)3(CO3)-
3  .0        .0       .0     .0       Mg++ Th(CO3)5===
1  .0        .0       .0     .0       Mg++ HOx-
2  .0        .0       .0     .0       Mg++ Ox=
1  .0        .0       .0     .0       Mg++ Ac-
1  .0        .0       .0     .0       Mg++ Lac-
1  .0        .0       .0     .0       Mg++ H2Cit-
2  .0        .0       .0     .0       Mg++ HCit=
3  .0        .0       .0     .0       Mg++ Cit=-
3  .0        .0       .0     .0       Mg++ H3EDTA-
3  .0        .0       .0     .0       Mg++ H2EDTA=
3  .0        .0       .0     .0       Mg++ HEDTA=-
3  .0        .0       .0     .0       Mg++ EDTA==
3  .0        .0       .0     .0       Mg++ AmEDTA-
2  .0        .0       .0     .0       Mg++ NpO2Cit=
3  .0        .0       .0     .0       Mg++ NpO2EDTA==-
1  .0        .0       .0     .0       Mg++ NpO2Ox-
3  .0        .0       .0     .0       Mg++ U(OH)4(CO3)2==
3  .0        .0       .0     .0       Mg++ U(CO3)5===
2  .0        .0       .0     .0       Mg++ U(SO4)3=
3  .0        .0       .0     .0       Mg++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       Mg++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       Mg++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       Mg++ CaCit-
3  .0        .0       .0     .0       Mg++ CaEDTA=
3  .0        .0       .0     .0       Mg++ UnuAn#2-
1  .0        .0       .0     .0       Mg++ UnuAn#3-
2  .0        .0       .0     .0       Mg++ UnuAn#4-
2  .0        .0       .0     .0       Mg++ U(OH)2(CO3)2=
1  .0        .0       .0     .0       Mg++ MgCit-
2  .0        .0       .0     .0       Mg++ MgEDTA=
2  .0        .0       .0     .0       Mg++ NpO2HEDTA=   [NEW]

1 -.10      1.658     .0     .0       MgOH+ Cl-          HMW84
1  .0        .0       .0     .0       MgOH+ SO4=         HMW84
1  .0        .0       .0     .0       MgOH+ HSO4-        HMW84
1  .0        .0       .0     .0       MgOH+ OH-          HMW84
1  .0        .0       .0     .0       MgOH+ HCO3-        HMW84
1  .0        .0       .0     .0       MgOH+ CO3=         HMW84
1  .0        .0       .0     .0       MgOH+ B(OH)4-
1  .0        .0       .0     .0       MgOH+ B3O3(OH)4-
1  .0        .0       .0     .0       MgOH+ B4O5(OH)4=
1  .0        .0       .0     .0       MgOH+ Br-
1  .0        .0       .0     .0       MgOH+ Am(CO3)2-
1  .0        .0       .0     .0       MgOH+ Am(CO3)3=-
1  .0        .0       .0     .0       MgOH+ ClO4-
1  .0        .0       .0     .0       MgOH+ NpO2(OH)2-
1  .0        .0       .0     .0       MgOH+ NpO2CO3-
```

```
1   .0         .0        .0      .0        MgOH+ NpO2(CO3)2=-
1   .0         .0        .0      .0        MgOH+ NpO2(CO3)3==-
1   .0         .0        .0      .0        MgOH+ H2PO4-
1   .0         .0        .0      .0        MgOH+ HPO4=
1   .0         .0        .0      .0        MgOH+ PO4=-
1   .0         .0        .0      .0        MgOH+ Th(SO4)3=
1   .0         .0        .0      .0        MgOH+ Th(OH)3(CO3)-
1   .0         .0        .0      .0        MgOH+ Th(CO3)5===
1   .0         .0        .0      .0        MgOH+ HOx-
1   .0         .0        .0      .0        MgOH+ Ox=
1   .0         .0        .0      .0        MgOH+ Ac-
1   .0         .0        .0      .0        MgOH+ Lac-
1   .0         .0        .0      .0        MgOH+ H2Cit-
1   .0         .0        .0      .0        MgOH+ HCit=
1   .0         .0        .0      .0        MgOH+ Cit=-
1   .0         .0        .0      .0        MgOH+ H3EDTA-
1   .0         .0        .0      .0        MgOH+ H2EDTA=
1   .0         .0        .0      .0        MgOH+ HEDTA=-
1   .0         .0        .0      .0        MgOH+ EDTA==
1   .0         .0        .0      .0        MgOH+ AmEDTA-
1   .0         .0        .0      .0        MgOH+ NpO2Cit=
1   .0         .0        .0      .0        MgOH+ NpO2EDTA==-
1   .0         .0        .0      .0        MgOH+ NpO2Ox-
1   .0         .0        .0      .0        MgOH+ U(OH)4(CO3)2==
1   .0         .0        .0      .0        MgOH+ U(CO3)5===
1   .0         .0        .0      .0        MgOH+ U(SO4)3=
1   .0         .0        .0      .0        MgOH+ Am(CO3)4==-   [NEW]
1   .0         .0        .0      .0        MgOH+ Am(SO4)2-     [NEW]
1   .0         .0        .0      .0        MgOH+ NpO2H2EDTA-   [NEW]
1   .0         .0        .0      .0        MgOH+ CaCit-
1   .0         .0        .0      .0        MgOH+ CaEDTA=
1   .0         .0        .0      .0        MgOH+ UnuAn#2-
1   .0         .0        .0      .0        MgOH+ UnuAn#3-
1   .0         .0        .0      .0        MgOH+ UnuAn#4-
1   .0         .0        .0      .0        MgOH+ U(OH)2(CO3)2=
1   .0         .0        .0      .0        MgOH+ MgCit-
1   .0         .0        .0      .0        MgOH+ MgEDTA=
1   .0         .0        .0      .0        MgOH+ NpO2HEDTA=    [NEW]

1   .1775      .2945     .0      .0008     H+  Cl-             HMW84
1   .0298      .0        .0      .0438     H+  SO4=            HMW84
1   .2065      .5556     .0      .0        H+  HSO4-           HMW84
1   .0         .0        .0      .0        H+  OH-             HMW84
1   .0         .0        .0      .0        H+  HCO3-           HMW84
1   .0         .0        .0      .0        H+  CO3=            HMW84
1   .0         .0        .0      .0        H+  B(OH)4-         FW86
1   .0         .0        .0      .0        H+  B3O3(OH)4-      FW86
1   .0         .0        .0      .0        H+  B4O5(OH)4=      FW86
```

```
1  .0        .0      .0     .0        H+ Br-
1  .0        .0      .0     .0        H+ Am(CO3)2-
1  .0        .0      .0     .0        H+ Am(CO3)3=-
1  .1747     .2931   .0     .00819    H+ ClO4-           P91
1  .0        .0      .0     .0        H+ NpO2(OH)2-
1  .0        .0      .0     .0        H+ NpO2CO3-
1  .0        .0      .0     .0        H+ NpO2(CO3)2=-
1  .0        .0      .0     .0        H+ NpO2(CO3)3==-
1  .0        .0      .0     .0        H+ H2PO4-
1  .0        .0      .0     .0        H+ HPO4=
1  .0        .0      .0     .0        H+ PO4=-
1  .84       .0      .0     .0        H+ Th(SO4)3=       FR92
1  .0        .0      .0     .0        H+ Th(OH)3(CO3)-
1  .0        .0      .0     .0        H+ Th(CO3)5===
1  .0        .0      .0     .0        H+ HOx-
1  .0        .0      .0     .0        H+ Ox=
1  .0        .0      .0     .0        H+ Ac-             NBC96/Mesmer et al. 89
1  .0        .0      .0     .0        H+ Lac-
1  .0        .0      .0     .0        H+ H2Cit-
1  .0        .0      .0     .0        H+ HCit=
1  .0        .0      .0     .0        H+ Cit=-
1  .0        .0      .0     .0        H+ H3EDTA-
1  .0        .0      .0     .0        H+ H2EDTA=
1  .0        .0      .0     .0        H+ HEDTA=-
1  .0        .0      .0     .0        H+ EDTA==
1  .0        .0      .0     .0        H+ AmEDTA-
1  .0        .0      .0     .0        H+ NpO2Cit=
1  .0        .0      .0     .0        H+ NpO2EDTA==-
1  .0        .0      .0     .0        H+ NpO2Ox-
1  .0        .0      .0     .0        H+ U(OH)4(CO3)2==
1  .0        .0      .0     .0        H+ U(CO3)5===
1  .0        .0      .0     .0        H+ U(SO4)3=
1  .0        .0      .0     .0        H+ Am(CO3)4==-   [NEW]
1  .0        .0      .0     .0        H+ Am(SO4)2-     [NEW]
1  .0        .0      .0     .0        H+ NpO2H2EDTA-   [NEW]
1  .0        .0      .0     .0        H+ CaCit-
1  .0        .0      .0     .0        H+ CaEDTA=
1  .0        .0      .0     .0        H+ UnuAn#2-
1  .0        .0      .0     .0        H+ UnuAn#3-
1  .0        .0      .0     .0        H+ UnuAn#4-
1  .0        .0      .0     .0        H+ U(OH)2(CO3)2=
1  .0        .0      .0     .0        H+ MgCit-
1  .0        .0      .0     .0        H+ MgEDTA=
1  .0        .0      .0     .0        H+ NpO2HEDTA=   [NEW]

1  .16       .0      .0     .0        MgB(OH)4+ Cl-      FW86
1  .0        .0      .0     .0        MgB(OH)4+ SO4=
1  .0        .0      .0     .0        MgB(OH)4+ HSO4-
```

```
1  .0         .0        .0      .0        MgB(OH)4+ OH-
1  .0         .0        .0      .0        MgB(OH)4+ HCO3-
1  .0         .0        .0      .0        MgB(OH)4+ CO3=
1  .0         .0        .0      .0        MgB(OH)4+ B(OH)4-
1  .0         .0        .0      .0        MgB(OH)4+ B3O3(OH)4-
1  .0         .0        .0      .0        MgB(OH)4+ B4O5(OH)4=
1  .0         .0        .0      .0        MgB(OH)4+ Br-
1  .0         .0        .0      .0        MgB(OH)4+ Am(CO3)2-
1  .0         .0        .0      .0        MgB(OH)4+ Am(CO3)3=-
1  .0         .0        .0      .0        MgB(OH)4+ ClO4-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2(OH)2-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2CO3-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2(CO3)2=-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2(CO3)3==-
1  .0         .0        .0      .0        MgB(OH)4+ H2PO4-
1  .0         .0        .0      .0        MgB(OH)4+ HPO4=
1  .0         .0        .0      .0        MgB(OH)4+ PO4=-
1  .0         .0        .0      .0        MgB(OH)4+ Th(SO4)3=
1  .0         .0        .0      .0        MgB(OH)4+ Th(OH)3(CO3)-
1  .0         .0        .0      .0        MgB(OH)4+ Th(CO3)5===
1  .0         .0        .0      .0        MgB(OH)4+ HOx-
1  .0         .0        .0      .0        MgB(OH)4+ Ox=
1  .0         .0        .0      .0        MgB(OH)4+ Ac-
1  .0         .0        .0      .0        MgB(OH)4+ Lac-
1  .0         .0        .0      .0        MgB(OH)4+ H2Cit-
1  .0         .0        .0      .0        MgB(OH)4+ HCit=
1  .0         .0        .0      .0        MgB(OH)4+ Cit=-
1  .0         .0        .0      .0        MgB(OH)4+ H3EDTA-
1  .0         .0        .0      .0        MgB(OH)4+ H2EDTA=
1  .0         .0        .0      .0        MgB(OH)4+ HEDTA=-
1  .0         .0        .0      .0        MgB(OH)4+ EDTA==
1  .0         .0        .0      .0        MgB(OH)4+ AmEDTA-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2Cit=
1  .0         .0        .0      .0        MgB(OH)4+ NpO2EDTA==-
1  .0         .0        .0      .0        MgB(OH)4+ NpO2Ox-
1  .0         .0        .0      .0        MgB(OH)4+ U(OH)4(CO3)2==
1  .0         .0        .0      .0        MgB(OH)4+ U(CO3)5===
1  .0         .0        .0      .0        MgB(OH)4+ U(SO4)3=
1  .0         .0        .0      .0        MgB(OH)4+ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0        MgB(OH)4+ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0        MgB(OH)4+ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0        MgB(OH)4+ CaCit-
1  .0         .0        .0      .0        MgB(OH)4+ CaEDTA=
1  .0         .0        .0      .0        MgB(OH)4+ UnuAn#2-
1  .0         .0        .0      .0        MgB(OH)4+ UnuAn#3-
1  .0         .0        .0      .0        MgB(OH)4+ UnuAn#4-
1  .0         .0        .0      .0        MgB(OH)4+ U(OH)2(CO3)2=
1  .0         .0        .0      .0        MgB(OH)4+ MgCit-
```

```
1  .0      .0      .0     .0      MgB(OH)4+ MgEDTA=
1  .0      .0      .0     .0      MgB(OH)4+ NpO2HEDTA=   [NEW]

1  .12     .0      .0     .0      CaB(OH)4+ Cl-      FW86
1  .0      .0      .0     .0      CaB(OH)4+ SO4=
1  .0      .0      .0     .0      CaB(OH)4+ HSO4-
1  .0      .0      .0     .0      CaB(OH)4+ OH-
1  .0      .0      .0     .0      CaB(OH)4+ HCO3-
1  .0      .0      .0     .0      CaB(OH)4+ CO3=
1  .0      .0      .0     .0      CaB(OH)4+ B(OH)4-
1  .0      .0      .0     .0      CaB(OH)4+ B3O3(OH)4-
1  .0      .0      .0     .0      CaB(OH)4+ B4O5(OH)4=
1  .0      .0      .0     .0      CaB(OH)4+ Br-
1  .0      .0      .0     .0      CaB(OH)4+ Am(CO3)2-
1  .0      .0      .0     .0      CaB(OH)4+ Am(CO3)3=-
1  .0      .0      .0     .0      CaB(OH)4+ ClO4-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2(OH)2-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2CO3-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2(CO3)2=-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2(CO3)3==-
1  .0      .0      .0     .0      CaB(OH)4+ H2PO4-
1  .0      .0      .0     .0      CaB(OH)4+ HPO4=
1  .0      .0      .0     .0      CaB(OH)4+ PO4=-
1  .0      .0      .0     .0      CaB(OH)4+ Th(SO4)3=
1  .0      .0      .0     .0      CaB(OH)4+ Th(OH)3(CO3)-
1  .0      .0      .0     .0      CaB(OH)4+ Th(CO3)5===
1  .0      .0      .0     .0      CaB(OH)4+ HOx-
1  .0      .0      .0     .0      CaB(OH)4+ Ox=
1  .0      .0      .0     .0      CaB(OH)4+ Ac-
1  .0      .0      .0     .0      CaB(OH)4+ Lac-
1  .0      .0      .0     .0      CaB(OH)4+ H2Cit-
1  .0      .0      .0     .0      CaB(OH)4+ HCit=
1  .0      .0      .0     .0      CaB(OH)4+ Cit=-
1  .0      .0      .0     .0      CaB(OH)4+ H3EDTA-
1  .0      .0      .0     .0      CaB(OH)4+ H2EDTA=
1  .0      .0      .0     .0      CaB(OH)4+ HEDTA=-
1  .0      .0      .0     .0      CaB(OH)4+ EDTA==
1  .0      .0      .0     .0      CaB(OH)4+ AmEDTA-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2Cit=
1  .0      .0      .0     .0      CaB(OH)4+ NpO2EDTA==-
1  .0      .0      .0     .0      CaB(OH)4+ NpO2Ox-
1  .0      .0      .0     .0      CaB(OH)4+ U(OH)4(CO3)2==
1  .0      .0      .0     .0      CaB(OH)4+ U(CO3)5===
1  .0      .0      .0     .0      CaB(OH)4+ U(SO4)3=
1  .0      .0      .0     .0      CaB(OH)4+ Am(CO3)4==-   [NEW]
1  .0      .0      .0     .0      CaB(OH)4+ Am(SO4)2-     [NEW]
1  .0      .0      .0     .0      CaB(OH)4+ NpO2H2EDTA-   [NEW]
1  .0      .0      .0     .0      CaB(OH)4+ CaCit-
```

```
1  .0        .0       .0      .0      CaB(OH)4+ CaEDTA=
1  .0        .0       .0      .0      CaB(OH)4+ UnuAn#2-
1  .0        .0       .0      .0      CaB(OH)4+ UnuAn#3-
1  .0        .0       .0      .0      CaB(OH)4+ UnuAn#4-
1  .0        .0       .0      .0      CaB(OH)4+ U(OH)2(CO3)2=
1  .0        .0       .0      .0      CaB(OH)4+ MgCit-
1  .0        .0       .0      .0      CaB(OH)4+ MgEDTA=
1  .0        .0       .0      .0      CaB(OH)4+ NpO2HEDTA=  [NEW]

1  .5856    5.6       .0   -0.0166    Am+++ Cl-          FK98/Konnecke et al. 1997
3 1.792    15.04      .0     .600     Am+++ SO4=         FK98
1  .0        .0       .0      .0      Am+++ HSO4-
1  .0        .0       .0      .0      Am+++ OH-
1  .0        .0       .0      .0      Am+++ HCO3-
3  .0        .0       .0      .0      Am+++ CO3=
1  .0        .0       .0      .0      Am+++ B(OH)4-
1  .0        .0       .0      .0      Am+++ B3O3(OH)4-
3  .0        .0       .0      .0      Am+++ B4O5(OH)4=
1  .0        .0       .0      .0      Am+++ Br-
1  .0        .0       .0      .0      Am+++ Am(CO3)2-
3  .0        .0       .0      .0      Am+++ Am(CO3)3=-
1  .80      5.35      .0   -0.0048    Am+++ ClO4-         FRF90
1  .0        .0       .0      .0      Am+++ NpO2(OH)2-
1  .0        .0       .0      .0      Am+++ NpO2CO3-
3  .0        .0       .0      .0      Am+++ NpO2(CO3)2=-
3  .0        .0       .0      .0      Am+++ NpO2(CO3)3==-
1  .0        .0    -92.9      .0      Am+++ H2PO4-        RFF95 (from Nd-H2PO4 value)
3  .0        .0       .0      .0      Am+++ HPO4=
3  .0        .0       .0      .0      Am+++ PO4=-
3  .0        .0       .0      .0      Am+++ Th(SO4)3=
1  .0        .0       .0      .0      Am+++ Th(OH)3(CO3)-
3  .0        .0       .0      .0      Am+++ Th(CO3)5===
1  .0        .0       .0      .0      Am+++ HOx-
3  .0        .0       .0      .0      Am+++ Ox=
1  .0        .0       .0      .0      Am+++ Ac-
1  .0        .0       .0      .0      Am+++ Lac-
1  .0        .0       .0      .0      Am+++ H2Cit-
3  .0        .0       .0      .0      Am+++ HCit=
3  .0        .0       .0      .0      Am+++ Cit=-
3  .0        .0       .0      .0      Am+++ H3EDTA-
3  .0        .0       .0      .0      Am+++ H2EDTA=
3  .0        .0       .0      .0      Am+++ HEDTA=-
3  .0        .0       .0      .0      Am+++ EDTA==
3  .0        .0       .0      .0      Am+++ AmEDTA-
3  .0        .0       .0      .0      Am+++ NpO2Cit=
3  .0        .0       .0      .0      Am+++ NpO2EDTA==-
1  .0        .0       .0      .0      Am+++ NpO2Ox-
3  .0        .0       .0      .0      Am+++ U(OH)4(CO3)2==
```

```
3  .0         .0        .0      .0        Am+++ U(CO3)5===
3  .0         .0        .0      .0        Am+++ U(SO4)3=
3  .0         .0        .0      .0        Am+++ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0        Am+++ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0        Am+++ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0        Am+++ CaCit-
3  .0         .0        .0      .0        Am+++ CaEDTA=
3  .0         .0        .0      .0        Am+++ UnuAn#2-
1  .0         .0        .0      .0        Am+++ UnuAn#3-
3  .0         .0        .0      .0        Am+++ UnuAn#4-
3  .0         .0        .0      .0        Am+++ U(OH)2(CO3)2=
1  .0         .0        .0      .0        Am+++ MgCit-
3  .0         .0        .0      .0        Am+++ MgEDTA=
3  .0         .0        .0      .0        Am+++ NpO2HEDTA=   [NEW]

1 -.072       .403      .0      .0388     AmCO3+ Cl-       FK98/Fanghanel et al. 1999
1  .0         .0        .0      .0        AmCO3+ SO4=
1  .0         .0        .0      .0        AmCO3+ HSO4-
1  .0         .0        .0      .0        AmCO3+ OH-
1  .0         .0        .0      .0        AmCO3+ HCO3-
1  .0         .0        .0      .0        AmCO3+ CO3=
1  .0         .0        .0      .0        AmCO3+ B(OH)4-
1  .0         .0        .0      .0        AmCO3+ B3O3(OH)4-
1  .0         .0        .0      .0        AmCO3+ B4O5(OH)4=
1  .0         .0        .0      .0        AmCO3+ Br-
1  .0         .0        .0      .0        AmCO3+ Am(CO3)2-
1  .0         .0        .0      .0        AmCO3+ Am(CO3)3=-
1  .0         .0        .0      .0        AmCO3+ ClO4-
1  .0         .0        .0      .0        AmCO3+ NpO2(OH)2-
1  .0         .0        .0      .0        AmCO3+ NpO2CO3-
1  .0         .0        .0      .0        AmCO3+ NpO2(CO3)2=-
1  .0         .0        .0      .0        AmCO3+ NpO2(CO3)3==-
1  .0         .0        .0      .0        AmCO3+ H2PO4-
1  .0         .0        .0      .0        AmCO3+ HPO4=
1  .0         .0        .0      .0        AmCO3+ PO4=-
1  .0         .0        .0      .0        AmCO3+ Th(SO4)3=
1  .0         .0        .0      .0        AmCO3+ Th(OH)3(CO3)-
1  .0         .0        .0      .0        AmCO3+ Th(CO3)5===
1  .0         .0        .0      .0        AmCO3+ HOx-
1  .0         .0        .0      .0        AmCO3+ Ox=
1  .0         .0        .0      .0        AmCO3+ Ac-
1  .0         .0        .0      .0        AmCO3+ Lac-
1  .0         .0        .0      .0        AmCO3+ H2Cit-
1  .0         .0        .0      .0        AmCO3+ HCit=
1  .0         .0        .0      .0        AmCO3+ Cit=-
1  .0         .0        .0      .0        AmCO3+ H3EDTA-
1  .0         .0        .0      .0        AmCO3+ H2EDTA=
1  .0         .0        .0      .0        AmCO3+ HEDTA=-
```

```
1  .0         .0        .0      .0        AmCO3+ EDTA==
1  .0         .0        .0      .0        AmCO3+ AmEDTA-
1  .0         .0        .0      .0        AmCO3+ NpO2Cit=
1  .0         .0        .0      .0        AmCO3+ NpO2EDTA==-
1  .0         .0        .0      .0        AmCO3+ NpO2Ox-
1  .0         .0        .0      .0        AmCO3+ U(OH)4(CO3)2==
1  .0         .0        .0      .0        AmCO3+ U(CO3)5===
1  .0         .0        .0      .0        AmCO3+ U(SO4)3=
1  .0         .0        .0      .0        AmCO3+ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0        AmCO3+ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0        AmCO3+ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0        AmCO3+ CaCit-
1  .0         .0        .0      .0        AmCO3+ CaEDTA=
1  .0         .0        .0      .0        AmCO3+ UnuAn#2-
1  .0         .0        .0      .0        AmCO3+ UnuAn#3-
1  .0         .0        .0      .0        AmCO3+ UnuAn#4-
1  .0         .0        .0      .0        AmCO3+ U(OH)2(CO3)2=
1  .0         .0        .0      .0        AmCO3+ MgCit-
1  .0         .0        .0      .0        AmCO3+ MgEDTA=
1  .0         .0        .0      .0        AmCO3+ NpO2HEDTA=   [NEW]

1  1.092   13.7      -160.   -.112        Th++++ Cl-          Roy92
3  1.56       .0        .0      .0        Th++++ SO4=         FR92
1  1.44       .0        .0      .0        Th++++ HSO4-        FR92
1  .0         .0        .0      .0        Th++++ OH-
1  .0         .0        .0      .0        Th++++ HCO3-
3  .0         .0        .0      .0        Th++++ CO3=
1  .0         .0        .0      .0        Th++++ B(OH)4-
1  .0         .0        .0      .0        Th++++ B3O3(OH)4-
3  .0         .0        .0      .0        Th++++ B4O5(OH)4=
1  .0         .0        .0      .0        Th++++ Br-
1  .0         .0        .0      .0        Th++++ Am(CO3)2-
3  .0         .0        .0      .0        Th++++ Am(CO3)3=-
1  1.19    27.3         .0   -.057        Th++++ ClO4-       CFN960119
1  .0         .0        .0      .0        Th++++ NpO2(OH)2-
1  .0         .0        .0      .0        Th++++ NpO2CO3-
3  .0         .0        .0      .0        Th++++ NpO2(CO3)2=-
3  .0         .0        .0      .0        Th++++ NpO2(CO3)3==-
1  .0         .0        .0      .0        Th++++ H2PO4-
3  .0         .0        .0      .0        Th++++ HPO4=
3  .0         .0        .0      .0        Th++++ PO4=-
3  .0         .0        .0      .0        Th++++ Th(SO4)3=
1  .0         .0        .0      .0        Th++++ Th(OH)3(CO3)-
3  .0         .0        .0      .0        Th++++ Th(CO3)5===
1  .0         .0        .0      .0        Th++++ HOx-
3  .0         .0        .0      .0        Th++++ Ox=
1  .0         .0        .0      .0        Th++++ Ac-
1  .0         .0        .0      .0        Th++++ Lac-
```

```
  1  .0         .0        .0      .0        Th++++ H2Cit-
  3  .0         .0        .0      .0        Th++++ HCit=
  3  .0         .0        .0      .0        Th++++ Cit=-
  3  .0         .0        .0      .0        Th++++ H3EDTA-
  3  .0         .0        .0      .0        Th++++ H2EDTA=
  3  .0         .0        .0      .0        Th++++ HEDTA=-
  3  .0         .0        .0      .0        Th++++ EDTA==
  3  .0         .0        .0      .0        Th++++ AmEDTA-
  3  .0         .0        .0      .0        Th++++ NpO2Cit=
  3  .0         .0        .0      .0        Th++++ NpO2EDTA==-
  1  .0         .0        .0      .0        Th++++ NpO2Ox-
  3  .0         .0        .0      .0        Th++++ U(OH)4(CO3)2==
  3  .0         .0        .0      .0        Th++++ U(CO3)5===
  3  .0         .0        .0      .0        Th++++ U(SO4)3=
  3  .0         .0        .0      .0        Th++++ Am(CO3)4==-   [NEW]
  1  .0         .0        .0      .0        Th++++ Am(SO4)2-     [NEW]
  1  .0         .0        .0      .0        Th++++ NpO2H2EDTA-   [NEW]
  1  .0         .0        .0      .0        Th++++ CaCit-
  3  .0         .0        .0      .0        Th++++ CaEDTA=
  3  .0         .0        .0      .0        Th++++ UnuAn#2-
  1  .0         .0        .0      .0        Th++++ UnuAn#3-
  3  .0         .0        .0      .0        Th++++ UnuAn#4-
  3  .0         .0        .0      .0        Th++++ U(OH)2(CO3)2=
  1  .0         .0        .0      .0        Th++++ MgCit-
  3  .0         .0        .0      .0        Th++++ MgEDTA=
  3  .0         .0        .0      .0        Th++++ NpO2HEDTA=   [NEW]
[ALL AmCl++ INTERACTIONS NEW]
  1  .593     3.15        .0  -0.006        AmCl++ Cl-           FK98/Konnecke et al. 1997
  2  .0         .0        .0      .0        AmCl++ SO4=
  1  .0         .0        .0      .0        AmCl++ HSO4-
  1  .0         .0        .0      .0        AmCl++ OH-
  1  .0         .0        .0      .0        AmCl++ HCO3-
  2  .0         .0        .0      .0        AmCl++ CO3=
  1  .0         .0        .0      .0        AmCl++ B(OH)4-
  1  .0         .0        .0      .0        AmCl++ B3O3(OH)4-
  2  .0         .0        .0      .0        AmCl++ B4O5(OH)4=
  1  .0         .0        .0      .0        AmCl++ Br-
  1  .0         .0        .0      .0        AmCl++ Am(CO3)2-
  3  .0         .0        .0      .0        AmCl++ Am(CO3)3=-
  1  .0         .0        .0      .0        AmCl++ ClO4-
  1  .0         .0        .0      .0        AmCl++ NpO2(OH)2-
  1  .0         .0        .0      .0        AmCl++ NpO2CO3-
  3  .0         .0        .0      .0        AmCl++ NpO2(CO3)2=-
  3  .0         .0        .0      .0        AmCl++ NpO2(CO3)3==-
  1  .0         .0        .0      .0        AmCl++ H2PO4-
  2  .0         .0        .0      .0        AmCl++ HPO4=
  3  .0         .0        .0      .0        AmCl++ PO4=-
  2  .0         .0        .0      .0        AmCl++ Th(SO4)3=
```

```
 1  .0         .0       .0     .0        AmCl++ Th(OH)3(CO3)-
 3  .0         .0       .0     .0        AmCl++ Th(CO3)5===
 1  .0         .0       .0     .0        AmCl++ HOx-
 2  .0         .0       .0     .0        AmCl++ Ox=
 1  .0         .0       .0     .0        AmCl++ Ac-
 1  .0         .0       .0     .0        AmCl++ Lac-
 1  .0         .0       .0     .0        AmCl++ H2Cit-
 2  .0         .0       .0     .0        AmCl++ HCit=
 3  .0         .0       .0     .0        AmCl++ Cit=-
 1  .0         .0       .0     .0        AmCl++ H3EDTA-
 2  .0         .0       .0     .0        AmCl++ H2EDTA=
 3  .0         .0       .0     .0        AmCl++ HEDTA=-
 3  .0         .0       .0     .0        AmCl++ EDTA==
 1  .0         .0       .0     .0        AmCl++ NpO2H2EDTA-
 2  .0         .0       .0     .0        AmCl++ NpO2Cit=
 3  .0         .0       .0     .0        AmCl++ NpO2EDTA==-
 1  .0         .0       .0     .0        AmCl++ NpO2Ox-
 3  .0         .0       .0     .0        AmCl++ U(OH)4(CO3)2==
 3  .0         .0       .0     .0        AmCl++ U(CO3)5===
 2  .0         .0       .0     .0        AmCl++ U(SO4)3=
 3  .0         .0       .0     .0        AmCl++ Am(CO3)4==-
 1  .0         .0       .0     .0        AmCl++ Am(SO4)2-
 1  .0         .0       .0     .0        AmCl++ NpO2H2EDTA-
 1  .0         .0       .0     .0        AmCl++ CaCit-
 2  .0         .0       .0     .0        AmCl++ CaEDTA=
 1  .0         .0       .0     .0        AmCl++ UnuAn#2-
 1  .0         .0       .0     .0        AmCl++ UnuAn#3-
 1  .0         .0       .0     .0        AmCl++ UnuAn#4-
 2  .0         .0       .0     .0        AmCl++ U(OH)2(CO3)2=
 1  .0         .0       .0     .0        AmCl++ MgCit-
 2  .0         .0       .0     .0        AmCl++ MgEDTA=
 2  .0         .0       .0     .0        AmCl++ NpO2HEDTA=

 1  .1415      .281     .0     .0        NpO2+ Cl-                NFRK95
 1  .0         .0       .0     .0        NpO2+ SO4=
 1  .0         .0       .0     .0        NpO2+ HSO4-
 1  .0         .0       .0     .0        NpO2+ OH-
 1  .0         .0       .0     .0        NpO2+ HCO3-
 1  .0         .0       .0     .0        NpO2+ CO3=
 1  .0         .0       .0     .0        NpO2+ B(OH)4-
 1  .0         .0       .0     .0        NpO2+ B3O3(OH)4-
 1  .0         .0       .0     .0        NpO2+ B4O5(OH)4=
 1  .0         .0       .0     .0        NpO2+ Br-
 1  .0         .0       .0     .0        NpO2+ Am(CO3)2-
 1  .0         .0       .0     .0        NpO2+ Am(CO3)3=-
 1  .257       .180     .0     .0081     NpO2+ ClO4-              NFRK95
 1  .0         .0       .0     .0        NpO2+ NpO2(OH)2-
 1  .0         .0       .0     .0        NpO2+ NpO2CO3-
```

```
1  .0        .0       .0     .0       NpO2+ NpO2(CO3)2=-
1  .0        .0       .0     .0       NpO2+ NpO2(CO3)3==-
1  .0        .0       .0     .0       NpO2+ H2PO4-
1  .0        .0       .0     .0       NpO2+ HPO4=
1  .0        .0       .0     .0       NpO2+ PO4=-
1  .0        .0       .0     .0       NpO2+ Th(SO4)3=
1  .0        .0       .0     .0       NpO2+ Th(OH)3(CO3)-
1  .0        .0       .0     .0       NpO2+ Th(CO3)5===
1  .0        .0       .0     .0       NpO2+ HOx-
1  .0        .0       .0     .0       NpO2+ Ox=
1  .0        .0       .0     .0       NpO2+ Ac-
1  .0        .0       .0     .0       NpO2+ Lac-
1  .0        .0       .0     .0       NpO2+ H2Cit-
1  .0        .0       .0     .0       NpO2+ HCit=
1  .0        .0       .0     .0       NpO2+ Cit=-
1  .0        .0       .0     .0       NpO2+ H3EDTA-
1  .0        .0       .0     .0       NpO2+ H2EDTA=
1  .0        .0       .0     .0       NpO2+ HEDTA=-
1  .0        .0       .0     .0       NpO2+ EDTA==
1  .0        .0       .0     .0       NpO2+ AmEDTA-
1  .0        .0       .0     .0       NpO2+ NpO2Cit=
1  .0        .0       .0     .0       NpO2+ NpO2EDTA==-
1  .0        .0       .0     .0       NpO2+ NpO2Ox-
1  .0        .0       .0     .0       NpO2+ U(OH)4(CO3)2==
1  .0        .0       .0     .0       NpO2+ U(CO3)5===
1  .0        .0       .0     .0       NpO2+ U(SO4)3=
1  .0        .0       .0     .0       NpO2+ Am(CO3)4==-  [NEW]
1  .0        .0       .0     .0       NpO2+ Am(SO4)2-    [NEW]
1  .0        .0       .0     .0       NpO2+ NpO2H2EDTA-  [NEW]
1  .0        .0       .0     .0       NpO2+ CaCit-
1  .0        .0       .0     .0       NpO2+ CaEDTA=
1  .0        .0       .0     .0       NpO2+ UnuAn#2-
1  .0        .0       .0     .0       NpO2+ UnuAn#3-
1  .0        .0       .0     .0       NpO2+ UnuAn#4-
1  .0        .0       .0     .0       NpO2+ U(OH)2(CO3)2=
1  .0        .0       .0     .0       NpO2+ MgCit-
1  .0        .0       .0     .0       NpO2+ MgEDTA=
1  .0        .0       .0     .0       NpO2+ NpO2HEDTA=  [NEW]

1 1.644    15.5       .0     .1       U++++ Cl-         RFSMMN  (values really are different from Th++++ values)
3  .0        .0       .0     .0       U++++ SO4=
1  .0        .0       .0     .0       U++++ HSO4-
1  .0        .0       .0     .0       U++++ OH-
1  .0        .0       .0     .0       U++++ HCO3-
3  .0        .0       .0     .0       U++++ CO3=
1  .0        .0       .0     .0       U++++ B(OH)4-
1  .0        .0       .0     .0       U++++ B3O3(OH)4-
3  .0        .0       .0     .0       U++++ B4O5(OH)4=
```

```
1  .0        .0       .0     .0      U++++ Br-
1  .0        .0       .0     .0      U++++ Am(CO3)2-
3  .0        .0       .0     .0      U++++ Am(CO3)3=-
1  .0        .0       .0     .0      U++++ ClO4-
1  .0        .0       .0     .0      U++++ NpO2(OH)2-
1  .0        .0       .0     .0      U++++ NpO2CO3-
3  .0        .0       .0     .0      U++++ NpO2(CO3)2=-
3  .0        .0       .0     .0      U++++ NpO2(CO3)3==-
1  .0        .0       .0     .0      U++++ H2PO4-
3  .0        .0       .0     .0      U++++ HPO4=
3  .0        .0       .0     .0      U++++ PO4=-
3  .0        .0       .0     .0      U++++ Th(SO4)3=
1  .0        .0       .0     .0      U++++ Th(OH)3(CO3)-
3  .0        .0       .0     .0      U++++ Th(CO3)5===
1  .0        .0       .0     .0      U++++ HOx-
3  .0        .0       .0     .0      U++++ Ox=
1  .0        .0       .0     .0      U++++ Ac-
1  .0        .0       .0     .0      U++++ Lac-
1  .0        .0       .0     .0      U++++ H2Cit-
3  .0        .0       .0     .0      U++++ HCit=
3  .0        .0       .0     .0      U++++ Cit=-
3  .0        .0       .0     .0      U++++ H3EDTA-
3  .0        .0       .0     .0      U++++ H2EDTA=
3  .0        .0       .0     .0      U++++ HEDTA=-
3  .0        .0       .0     .0      U++++ EDTA==
3  .0        .0       .0     .0      U++++ AmEDTA-
3  .0        .0       .0     .0      U++++ NpO2Cit=
3  .0        .0       .0     .0      U++++ NpO2EDTA==-
1  .0        .0       .0     .0      U++++ NpO2Ox-
3  .0        .0       .0     .0      U++++ U(OH)4(CO3)2==
3  .0        .0       .0     .0      U++++ U(CO3)5===
3  .0        .0       .0     .0      U++++ U(SO4)3=
3  .0        .0       .0     .0      U++++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0      U++++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0      U++++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0      U++++ CaCit-
3  .0        .0       .0     .0      U++++ CaEDTA=
3  .0        .0       .0     .0      U++++ UnuAn#2-
1  .0        .0       .0     .0      U++++ UnuAn#3-
3  .0        .0       .0     .0      U++++ UnuAn#4-
3  .0        .0       .0     .0      U++++ U(OH)2(CO3)2=
1  .0        .0       .0     .0      U++++ MgCit-
3  .0        .0       .0     .0      U++++ MgEDTA=
3  .0        .0       .0     .0      U++++ NpO2HEDTA=   [NEW]

1 1.0     7.856       .0     .0      UOH+++ Cl-          RFSMMN
3  .0        .0       .0     .0      UOH+++ SO4=
1  .0        .0       .0     .0      UOH+++ HSO4-
```

```
1  .0         .0        .0      .0       UOH+++ OH-
1  .0         .0        .0      .0       UOH+++ HCO3-
3  .0         .0        .0      .0       UOH+++ CO3=
1  .0         .0        .0      .0       UOH+++ B(OH)4-
1  .0         .0        .0      .0       UOH+++ B3O3(OH)4-
3  .0         .0        .0      .0       UOH+++ B4O5(OH)4=
1  .0         .0        .0      .0       UOH+++ Br-
1  .0         .0        .0      .0       UOH+++ Am(CO3)2-
3  .0         .0        .0      .0       UOH+++ Am(CO3)3=-
1  .0         .0        .0      .0       UOH+++ ClO4-
1  .0         .0        .0      .0       UOH+++ NpO2(OH)2-
1  .0         .0        .0      .0       UOH+++ NpO2CO3-
3  .0         .0        .0      .0       UOH+++ NpO2(CO3)2=-
3  .0         .0        .0      .0       UOH+++ NpO2(CO3)3==-
1  .0         .0        .0      .0       UOH+++ H2PO4-
3  .0         .0        .0      .0       UOH+++ HPO4=
3  .0         .0        .0      .0       UOH+++ PO4=-
3  .0         .0        .0      .0       UOH+++ Th(SO4)3=
1  .0         .0        .0      .0       UOH+++ Th(OH)3(CO3)-
3  .0         .0        .0      .0       UOH+++ Th(CO3)5===
1  .0         .0        .0      .0       UOH+++ HOx-
3  .0         .0        .0      .0       UOH+++ Ox=
1  .0         .0        .0      .0       UOH+++ Ac-
1  .0         .0        .0      .0       UOH+++ Lac-
1  .0         .0        .0      .0       UOH+++ H2Cit-
3  .0         .0        .0      .0       UOH+++ HCit=
3  .0         .0        .0      .0       UOH+++ Cit=-
3  .0         .0        .0      .0       UOH+++ H3EDTA-
3  .0         .0        .0      .0       UOH+++ H2EDTA=
3  .0         .0        .0      .0       UOH+++ HEDTA=-
3  .0         .0        .0      .0       UOH+++ EDTA==
3  .0         .0        .0      .0       UOH+++ AmEDTA-
3  .0         .0        .0      .0       UOH+++ NpO2Cit=
3  .0         .0        .0      .0       UOH+++ NpO2EDTA==-
1  .0         .0        .0      .0       UOH+++ NpO2Ox-
3  .0         .0        .0      .0       UOH+++ U(OH)4(CO3)2==
3  .0         .0        .0      .0       UOH+++ U(CO3)5===
3  .0         .0        .0      .0       UOH+++ U(SO4)3=
3  .0         .0        .0      .0       UOH+++ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0       UOH+++ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0       UOH+++ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0       UOH+++ CaCit-
3  .0         .0        .0      .0       UOH+++ CaEDTA=
3  .0         .0        .0      .0       UOH+++ UnuAn#2-
1  .0         .0        .0      .0       UOH+++ UnuAn#3-
3  .0         .0        .0      .0       UOH+++ UnuAn#4-
3  .0         .0        .0      .0       UOH+++ U(OH)2(CO3)2=
1  .0         .0        .0      .0       UOH+++ MgCit-
```

```
3  .0        .0       .0     .0       UOH+++ MgEDTA=
3  .0        .0       .0     .0       UOH+++ NpO2HEDTA=   [NEW]

1  1.061     5.22     .0     .109     UAc+++ Cl-             analogy w/ Th (SAND99)
3  .0        .0       .0     .0       UAc+++ SO4=
1  .0        .0       .0     .0       UAc+++ HSO4-
1  .0        .0       .0     .0       UAc+++ OH-
1  .0        .0       .0     .0       UAc+++ HCO3-
3  .0        .0       .0     .0       UAc+++ CO3=
1  .0        .0       .0     .0       UAc+++ B(OH)4-
1  .0        .0       .0     .0       UAc+++ B3O3(OH)4-
3  .0        .0       .0     .0       UAc+++ B4O5(OH)4=
1  .0        .0       .0     .0       UAc+++ Br-
1  .0        .0       .0     .0       UAc+++ Am(CO3)2-
3  .0        .0       .0     .0       UAc+++ Am(CO3)3=-
1  .0        .0       .0     .0       UAc+++ ClO4-
1  .0        .0       .0     .0       UAc+++ NpO2(OH)2-
1  .0        .0       .0     .0       UAc+++ NpO2CO3-
3  .0        .0       .0     .0       UAc+++ NpO2(CO3)2=-
3  .0        .0       .0     .0       UAc+++ NpO2(CO3)3==-
1  .0        .0       .0     .0       UAc+++ H2PO4-
3  .0        .0       .0     .0       UAc+++ HPO4=
3  .0        .0       .0     .0       UAc+++ PO4=-
3  .0        .0       .0     .0       UAc+++ Th(SO4)3=
1  .0        .0       .0     .0       UAc+++ Th(OH)3(CO3)-
3  .0        .0       .0     .0       UAc+++ Th(CO3)5===
1  .0        .0       .0     .0       UAc+++ HOx-
1  .0        .0       .0     .0       UAc+++ Ox=
1  .0        .0       .0     .0       UAc+++ Ac-
1  .0        .0       .0     .0       UAc+++ Lac-
1  .0        .0       .0     .0       UAc+++ H2Cit-
3  .0        .0       .0     .0       UAc+++ HCit=
3  .0        .0       .0     .0       UAc+++ Cit=-
3  .0        .0       .0     .0       UAc+++ H3EDTA-
3  .0        .0       .0     .0       UAc+++ H2EDTA=
3  .0        .0       .0     .0       UAc+++ HEDTA=-
3  .0        .0       .0     .0       UAc+++ EDTA==
3  .0        .0       .0     .0       UAc+++ AmEDTA-
3  .0        .0       .0     .0       UAc+++ NpO2Cit=
3  .0        .0       .0     .0       UAc+++ NpO2EDTA==-
1  .0        .0       .0     .0       UAc+++ NpO2Ox-
3  .0        .0       .0     .0       UAc+++ U(OH)4(CO3)2==
3  .0        .0       .0     .0       UAc+++ U(CO3)5===
3  .0        .0       .0     .0       UAc+++ U(SO4)3=
3  .0        .0       .0     .0       UAc+++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       UAc+++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       UAc+++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       UAc+++ CaCit-
```

```
3  .0         .0        .0      .0       UAc+++ CaEDTA=
3  .0         .0        .0      .0       UAc+++ UnuAn#2-
1  .0         .0        .0      .0       UAc+++ UnuAn#3-
3  .0         .0        .0      .0       UAc+++ UnuAn#4-
3  .0         .0        .0      .0       UAc+++ U(OH)2(CO3)2=
1  .0         .0        .0      .0       UAc+++ MgCit-
3  .0         .0        .0      .0       UAc+++ MgEDTA=
3  .0         .0        .0      .0       UAc+++ NpO2HEDTA=   [NEW]

1 -.343      1.74       .0      .5       ThOx++ Cl-              SAND99/Borkowski et al 01
2  .0         .0        .0      .0       ThOx++ SO4=
1  .0         .0        .0      .0       ThOx++ HSO4-
1  .0         .0        .0      .0       ThOx++ OH-
1  .0         .0        .0      .0       ThOx++ HCO3-
2  .0         .0        .0      .0       ThOx++ CO3=
1  .0         .0        .0      .0       ThOx++ B(OH)4-
1  .0         .0        .0      .0       ThOx++ B3O3(OH)4-
2  .0         .0        .0      .0       ThOx++ B4O5(OH)4=
1  .0         .0        .0      .0       ThOx++ Br-
1  .0         .0        .0      .0       ThOx++ Am(CO3)2-
3  .0         .0        .0      .0       ThOx++ Am(CO3)3=-
1  .0         .0        .0      .0       ThOx++ ClO4-
1  .0         .0        .0      .0       ThOx++ NpO2(OH)2-
1  .0         .0        .0      .0       ThOx++ NpO2CO3-
3  .0         .0        .0      .0       ThOx++ NpO2(CO3)2=-
3  .0         .0        .0      .0       ThOx++ NpO2(CO3)3==-
1  .0         .0        .0      .0       ThOx++ H2PO4-
2  .0         .0        .0      .0       ThOx++ HPO4=
3  .0         .0        .0      .0       ThOx++ PO4=-
2  .0         .0        .0      .0       ThOx++ Th(SO4)3=
1  .0         .0        .0      .0       ThOx++ Th(OH)3(CO3)-
3  .0         .0        .0      .0       ThOx++ Th(CO3)5===
1  .0         .0        .0      .0       ThOx++ HOx-
2  .0         .0        .0      .0       ThOx++ Ox=
1  .0         .0        .0      .0       ThOx++ Ac-
1  .0         .0        .0      .0       ThOx++ Lac-
1  .0         .0        .0      .0       ThOx++ H2Cit-
2  .0         .0        .0      .0       ThOx++ HCit=
3  .0         .0        .0      .0       ThOx++ Cit=-
3  .0         .0        .0      .0       ThOx++ H3EDTA-
3  .0         .0        .0      .0       ThOx++ H2EDTA=
3  .0         .0        .0      .0       ThOx++ HEDTA=-
3  .0         .0        .0      .0       ThOx++ EDTA==
3  .0         .0        .0      .0       ThOx++ AmEDTA-
2  .0         .0        .0      .0       ThOx++ NpO2Cit=
3  .0         .0        .0      .0       ThOx++ NpO2EDTA==-
1  .0         .0        .0      .0       ThOx++ NpO2Ox-
3  .0         .0        .0      .0       ThOx++ U(OH)4(CO3)2==
```

```
3  .0          .0         .0      .0         ThOx++ U(CO3)5===
2  .0          .0         .0      .0         ThOx++ U(SO4)3=
3  .0          .0         .0      .0         ThOx++ Am(CO3)4==-   [NEW]
1  .0          .0         .0      .0         ThOx++ Am(SO4)2-     [NEW]
1  .0          .0         .0      .0         ThOx++ NpO2H2EDTA-   [NEW]
1  .0          .0         .0      .0         ThOx++ CaCit-
2  .0          .0         .0      .0         ThOx++ CaEDTA=
1  .0          .0         .0      .0         ThOx++ UnuAn#2-
1  .0          .0         .0      .0         ThOx++ UnuAn#3-
1  .0          .0         .0      .0         ThOx++ UnuAn#4-
2  .0          .0         .0      .0         ThOx++ U(OH)2(CO3)2=
1  .0          .0         .0      .0         ThOx++ MgCit-
2  .0          .0         .0      .0         ThOx++ MgEDTA=
2  .0          .0         .0      .0         ThOx++ NpO2HEDTA=   [NEW]

1  .3088     1.74         .0    -.132        AmAc++ Cl-      ERG_org_memo
2  .0          .0         .0      .0         AmAc++ SO4=
1  .0          .0         .0      .0         AmAc++ HSO4-
1  .0          .0         .0      .0         AmAc++ OH-
1  .0          .0         .0      .0         AmAc++ HCO3-
2  .0          .0         .0      .0         AmAc++ CO3=
1  .0          .0         .0      .0         AmAc++ B(OH)4-
1  .0          .0         .0      .0         AmAc++ B3O3(OH)4-
2  .0          .0         .0      .0         AmAc++ B4O5(OH)4=
1  .0          .0         .0      .0         AmAc++ Br-
1  .0          .0         .0      .0         AmAc++ Am(CO3)2-
3  .0          .0         .0      .0         AmAc++ Am(CO3)3=-
1  .0          .0         .0      .0         AmAc++ ClO4-
1  .0          .0         .0      .0         AmAc++ NpO2(OH)2-
1  .0          .0         .0      .0         AmAc++ NpO2CO3-
3  .0          .0         .0      .0         AmAc++ NpO2(CO3)2=-
3  .0          .0         .0      .0         AmAc++ NpO2(CO3)3==-
1  .0          .0         .0      .0         AmAc++ H2PO4-
2  .0          .0         .0      .0         AmAc++ HPO4=
3  .0          .0         .0      .0         AmAc++ PO4=-
2  .0          .0         .0      .0         AmAc++ Th(SO4)3=
1  .0          .0         .0      .0         AmAc++ Th(OH)3(CO3)-
3  .0          .0         .0      .0         AmAc++ Th(CO3)5===
1  .0          .0         .0      .0         AmAc++ HOx-
2  .0          .0         .0      .0         AmAc++ Ox=
1  .0          .0         .0      .0         AmAc++ Ac-
1  .0          .0         .0      .0         AmAc++ Lac-
1  .0          .0         .0      .0         AmAc++ H2Cit-
2  .0          .0         .0      .0         AmAc++ HCit=
3  .0          .0         .0      .0         AmAc++ Cit=-
3  .0          .0         .0      .0         AmAc++ H3EDTA-
3  .0          .0         .0      .0         AmAc++ H2EDTA=
3  .0          .0         .0      .0         AmAc++ HEDTA=-
```

```
3  .0        .0       .0     .0      AmAc++ EDTA==
3  .0        .0       .0     .0      AmAc++ AmEDTA-
2  .0        .0       .0     .0      AmAc++ NpO2Cit=
3  .0        .0       .0     .0      AmAc++ NpO2EDTA==-
1  .0        .0       .0     .0      AmAc++ NpO2Ox-
3  .0        .0       .0     .0      AmAc++ U(OH)4(CO3)2==
3  .0        .0       .0     .0      AmAc++ U(CO3)5===
2  .0        .0       .0     .0      AmAc++ U(SO4)3=
3  .0        .0       .0     .0      AmAc++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0      AmAc++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0      AmAc++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0      AmAc++ CaCit-
2  .0        .0       .0     .0      AmAc++ CaEDTA=
1  .0        .0       .0     .0      AmAc++ UnuAn#2-
1  .0        .0       .0     .0      AmAc++ UnuAn#3-
1  .0        .0       .0     .0      AmAc++ UnuAn#4-
2  .0        .0       .0     .0      AmAc++ U(OH)2(CO3)2=
1  .0        .0       .0     .0      AmAc++ MgCit-
2  .0        .0       .0     .0      AmAc++ MgEDTA=
2  .0        .0       .0     .0      AmAc++ NpO2HEDTA=   [NEW]

1 0.8397    1.74      .0   -0.332    AmLac++ Cl-             SAND99/Moore et al 1999
2  .0        .0       .0     .0      AmLac++ SO4=
1  .0        .0       .0     .0      AmLac++ HSO4-
1  .0        .0       .0     .0      AmLac++ OH-
1  .0        .0       .0     .0      AmLac++ HCO3-
2  .0        .0       .0     .0      AmLac++ CO3=
1  .0        .0       .0     .0      AmLac++ B(OH)4-
1  .0        .0       .0     .0      AmLac++ B3O3(OH)4-
2  .0        .0       .0     .0      AmLac++ B4O5(OH)4=
1  .0        .0       .0     .0      AmLac++ Br-
1  .0        .0       .0     .0      AmLac++ Am(CO3)2-
3  .0        .0       .0     .0      AmLac++ Am(CO3)3=-
1  .0        .0       .0     .0      AmLac++ ClO4-
1  .0        .0       .0     .0      AmLac++ NpO2(OH)2-
1  .0        .0       .0     .0      AmLac++ NpO2CO3-
3  .0        .0       .0     .0      AmLac++ NpO2(CO3)2=-
3  .0        .0       .0     .0      AmLac++ NpO2(CO3)3==-
1  .0        .0       .0     .0      AmLac++ H2PO4-
2  .0        .0       .0     .0      AmLac++ HPO4=
3  .0        .0       .0     .0      AmLac++ PO4=-
2  .0        .0       .0     .0      AmLac++ Th(SO4)3=
1  .0        .0       .0     .0      AmLac++ Th(OH)3(CO3)-
3  .0        .0       .0     .0      AmLac++ Th(CO3)5===
1  .0        .0       .0     .0      AmLac++ HOx-
2  .0        .0       .0     .0      AmLac++ Ox=
1  .0        .0       .0     .0      AmLac++ Ac-
1  .0        .0       .0     .0      AmLac++ Lac-
```

```
1  .0        .0       .0     .0       AmLac++ H2Cit-
2  .0        .0       .0     .0       AmLac++ HCit=
3  .0        .0       .0     .0       AmLac++ Cit=-
3  .0        .0       .0     .0       AmLac++ H3EDTA-
3  .0        .0       .0     .0       AmLac++ H2EDTA=
3  .0        .0       .0     .0       AmLac++ HEDTA=-
3  .0        .0       .0     .0       AmLac++ EDTA==
3  .0        .0       .0     .0       AmLac++ AmEDTA-
2  .0        .0       .0     .0       AmLac++ NpO2Cit=
3  .0        .0       .0     .0       AmLac++ NpO2EDTA==-
1  .0        .0       .0     .0       AmLac++ NpO2Ox-
3  .0        .0       .0     .0       AmLac++ U(OH)4(CO3)2==
3  .0        .0       .0     .0       AmLac++ U(CO3)5===
2  .0        .0       .0     .0       AmLac++ U(SO4)3=
3  .0        .0       .0     .0       AmLac++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       AmLac++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       AmLac++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       AmLac++ CaCit-
2  .0        .0       .0     .0       AmLac++ CaEDTA=
1  .0        .0       .0     .0       AmLac++ UnuAn#2-
1  .0        .0       .0     .0       AmLac++ UnuAn#3-
1  .0        .0       .0     .0       AmLac++ UnuAn#4-
2  .0        .0       .0     .0       AmLac++ U(OH)2(CO3)2=
1  .0        .0       .0     .0       AmLac++ MgCit-
2  .0        .0       .0     .0       AmLac++ MgEDTA=
2  .0        .0       .0     .0       AmLac++ NpO2HEDTA=   [NEW]

1 -.9374     .29      .0     .248     AmOx+ Cl-            SAND99/Borkowski et al 01
1  .0        .0       .0     .0       AmOx+ SO4=
1  .0        .0       .0     .0       AmOx+ HSO4-
1  .0        .0       .0     .0       AmOx+ OH-
1  .0        .0       .0     .0       AmOx+ HCO3-
1  .0        .0       .0     .0       AmOx+ CO3=
1  .0        .0       .0     .0       AmOx+ B(OH)4-
1  .0        .0       .0     .0       AmOx+ B3O3(OH)4-
2  .0        .0       .0     .0       AmOx+ B4O5(OH)4=
1  .0        .0       .0     .0       AmOx+ Br-
1  .0        .0       .0     .0       AmOx+ Am(CO3)2-
1  .0        .0       .0     .0       AmOx+ Am(CO3)3=-
1  .0        .0       .0     .0       AmOx+ ClO4-
1  .0        .0       .0     .0       AmOx+ NpO2(OH)2-
1  .0        .0       .0     .0       AmOx+ NpO2CO3-
1  .0        .0       .0     .0       AmOx+ NpO2(CO3)2=-
1  .0        .0       .0     .0       AmOx+ NpO2(CO3)3==-
1  .0        .0       .0     .0       AmOx+ H2PO4-
1  .0        .0       .0     .0       AmOx+ HPO4=
1  .0        .0       .0     .0       AmOx+ PO4=-
1  .0        .0       .0     .0       AmOx+ Th(SO4)3=
```

```
1  .0          .0         .0       .0        AmOx+ Th(OH)3(CO3)-
1  .0          .0         .0       .0        AmOx+ Th(CO3)5===
1  .0          .0         .0       .0        AmOx+ HOx-
1  .0          .0         .0       .0        AmOx+ Ox=
1  .0          .0         .0       .0        AmOx+ Ac-
1  .0          .0         .0       .0        AmOx+ Lac-
1  .0          .0         .0       .0        AmOx+ H2Cit-
1  .0          .0         .0       .0        AmOx+ HCit=
1  .0          .0         .0       .0        AmOx+ Cit=-
1  .0          .0         .0       .0        AmOx+ H3EDTA-
1  .0          .0         .0       .0        AmOx+ H2EDTA=
1  .0          .0         .0       .0        AmOx+ HEDTA=-
1  .0          .0         .0       .0        AmOx+ EDTA==
1  .0          .0         .0       .0        AmOx+ AmEDTA-
1  .0          .0         .0       .0        AmOx+ NpO2Cit=
1  .0          .0         .0       .0        AmOx+ NpO2EDTA==-
1  .0          .0         .0       .0        AmOx+ NpO2Ox-
1  .0          .0         .0       .0        AmOx+ U(OH)4(CO3)2==
1  .0          .0         .0       .0        AmOx+ U(CO3)5===
1  .0          .0         .0       .0        AmOx+ U(SO4)3=
1  .0          .0         .0       .0        AmOx+ Am(CO3)4==-   [NEW]
1  .0          .0         .0       .0        AmOx+ Am(SO4)2-     [NEW]
1  .0          .0         .0       .0        AmOx+ NpO2H2EDTA-   [NEW]
1  .0          .0         .0       .0        AmOx+ CaCit-
1  .0          .0         .0       .0        AmOx+ CaEDTA=
1  .0          .0         .0       .0        AmOx+ UnuAn#2-
1  .0          .0         .0       .0        AmOx+ UnuAn#3-
1  .0          .0         .0       .0        AmOx+ UnuAn#4-
1  .0          .0         .0       .0        AmOx+ U(OH)2(CO3)2=
1  .0          .0         .0       .0        AmOx+ MgCit-
1  .0          .0         .0       .0        AmOx+ MgEDTA=
1  .0          .0         .0       .0        AmOx+ NpO2HEDTA=   [NEW]

1 -.7467       .29        .0       .319      UCit+ Cl-            analogy w/ Th (SAND99)
1  .0          .0         .0       .0        UCit+ SO4=
1  .0          .0         .0       .0        UCit+ HSO4-
1  .0          .0         .0       .0        UCit+ OH-
1  .0          .0         .0       .0        UCit+ HCO3-
1  .0          .0         .0       .0        UCit+ CO3=
1  .0          .0         .0       .0        UCit+ B(OH)4-
1  .0          .0         .0       .0        UCit+ B3O3(OH)4-
1  .0          .0         .0       .0        UCit+ B4O5(OH)4=
1  .0          .0         .0       .0        UCit+ Br-
1  .0          .0         .0       .0        UCit+ Am(CO3)2-
1  .0          .0         .0       .0        UCit+ Am(CO3)3=-
1  .0          .0         .0       .0        UCit+ ClO4-
1  .0          .0         .0       .0        UCit+ NpO2(OH)2-
1  .0          .0         .0       .0        UCit+ NpO2CO3-
```

```
1  .0         .0        .0      .0        UCit+ NpO2(CO3)2=-
1  .0         .0        .0      .0        UCit+ NpO2(CO3)3==-
1  .0         .0        .0      .0        UCit+ H2PO4-
1  .0         .0        .0      .0        UCit+ HPO4=
1  .0         .0        .0      .0        UCit+ PO4=-
1  .0         .0        .0      .0        UCit+ Th(SO4)3=
1  .0         .0        .0      .0        UCit+ Th(OH)3(CO3)-
1  .0         .0        .0      .0        UCit+ Th(CO3)5===
1  .0         .0        .0      .0        UCit+ HOx-
1  .0         .0        .0      .0        UCit+ Ox=
1  .0         .0        .0      .0        UCit+ Ac-
1  .0         .0        .0      .0        UCit+ Lac-
1  .0         .0        .0      .0        UCit+ H2Cit-
1  .0         .0        .0      .0        UCit+ HCit=
1  .0         .0        .0      .0        UCit+ Cit=-
1  .0         .0        .0      .0        UCit+ H3EDTA-
1  .0         .0        .0      .0        UCit+ H2EDTA=
1  .0         .0        .0      .0        UCit+ HEDTA=-
1  .0         .0        .0      .0        UCit+ EDTA==
1  .0         .0        .0      .0        UCit+ AmEDTA-
1  .0         .0        .0      .0        UCit+ NpO2Cit=
1  .0         .0        .0      .0        UCit+ NpO2EDTA==-
1  .0         .0        .0      .0        UCit+ NpO2Ox-
1  .0         .0        .0      .0        UCit+ U(OH)4(CO3)2==
1  .0         .0        .0      .0        UCit+ U(CO3)5===
1  .0         .0        .0      .0        UCit+ U(SO4)3=
1  .0         .0        .0      .0        UCit+ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0        UCit+ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0        UCit+ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0        UCit+ CaCit-
1  .0         .0        .0      .0        UCit+ CaEDTA=
1  .0         .0        .0      .0        UCit+ UnuAn#2-
1  .0         .0        .0      .0        UCit+ UnuAn#3-
1  .0         .0        .0      .0        UCit+ UnuAn#4-
1  .0         .0        .0      .0        UCit+ U(OH)2(CO3)2=
1  .0         .0        .0      .0        UCit+ MgCit-
1  .0         .0        .0      .0        UCit+ MgEDTA=
1  .0         .0        .0      .0        UCit+ NpO2HEDTA=   [NEW]

1  .6677     5.22       .0     .341       ULac+++ Cl-        analogy w/ Th (SAND99/Moore et al 1999)
3  .0         .0        .0      .0        ULac+++ SO4=
1  .0         .0        .0      .0        ULac+++ HSO4-
1  .0         .0        .0      .0        ULac+++ OH-
1  .0         .0        .0      .0        ULac+++ HCO3-
3  .0         .0        .0      .0        ULac+++ CO3=
1  .0         .0        .0      .0        ULac+++ B(OH)4-
1  .0         .0        .0      .0        ULac+++ B3O3(OH)4-
3  .0         .0        .0      .0        ULac+++ B4O5(OH)4=
```

```
1  .0        .0       .0     .0       ULac+++ Br-
1  .0        .0       .0     .0       ULac+++ Am(CO3)2-
3  .0        .0       .0     .0       ULac+++ Am(CO3)3=-
1  .0        .0       .0     .0       ULac+++ ClO4-
1  .0        .0       .0     .0       ULac+++ NpO2(OH)2-
1  .0        .0       .0     .0       ULac+++ NpO2CO3-
3  .0        .0       .0     .0       ULac+++ NpO2(CO3)2=-
3  .0        .0       .0     .0       ULac+++ NpO2(CO3)3==-
1  .0        .0       .0     .0       ULac+++ H2PO4-
3  .0        .0       .0     .0       ULac+++ HPO4=
3  .0        .0       .0     .0       ULac+++ PO4=-
3  .0        .0       .0     .0       ULac+++ Th(SO4)3=
1  .0        .0       .0     .0       ULac+++ Th(OH)3(CO3)-
3  .0        .0       .0     .0       ULac+++ Th(CO3)5===
1  .0        .0       .0     .0       ULac+++ HOx-
3  .0        .0       .0     .0       ULac+++ Ox=
1  .0        .0       .0     .0       ULac+++ Ac-
1  .0        .0       .0     .0       ULac+++ Lac-
1  .0        .0       .0     .0       ULac+++ H2Cit-
3  .0        .0       .0     .0       ULac+++ HCit=
3  .0        .0       .0     .0       ULac+++ Cit=-
3  .0        .0       .0     .0       ULac+++ H3EDTA-
3  .0        .0       .0     .0       ULac+++ H2EDTA=
3  .0        .0       .0     .0       ULac+++ HEDTA=-
3  .0        .0       .0     .0       ULac+++ EDTA==
3  .0        .0       .0     .0       ULac+++ AmEDTA-
3  .0        .0       .0     .0       ULac+++ NpO2Cit=
3  .0        .0       .0     .0       ULac+++ NpO2EDTA==-
1  .0        .0       .0     .0       ULac+++ NpO2Ox-
3  .0        .0       .0     .0       ULac+++ U(OH)4(CO3)2==
3  .0        .0       .0     .0       ULac+++ U(CO3)5===
3  .0        .0       .0     .0       ULac+++ U(SO4)3=
3  .0        .0       .0     .0       ULac+++ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       ULac+++ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       ULac+++ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       ULac+++ CaCit-
3  .0        .0       .0     .0       ULac+++ CaEDTA=
1  .0        .0       .0     .0       ULac+++ UnuAn#2-
1  .0        .0       .0     .0       ULac+++ UnuAn#3-
1  .0        .0       .0     .0       ULac+++ UnuAn#4-
3  .0        .0       .0     .0       ULac+++ U(OH)2(CO3)2=
1  .0        .0       .0     .0       ULac+++ MgCit-
3  .0        .0       .0     .0       ULac+++ MgEDTA=
3  .0        .0       .0     .0       ULac+++ NpO2HEDTA=   [NEW]

1 -.343      1.74     .0     .5       UOx++ Cl-          analogy w/Th (SAND99/Borkowski et al 01)
2  .0        .0       .0     .0       UOx++ SO4=
1  .0        .0       .0     .0       UOx++ HSO4-
```

```
1  .0         .0        .0      .0       UOx++ OH-
1  .0         .0        .0      .0       UOx++ HCO3-
2  .0         .0        .0      .0       UOx++ CO3=
1  .0         .0        .0      .0       UOx++ B(OH)4-
1  .0         .0        .0      .0       UOx++ B3O3(OH)4-
2  .0         .0        .0      .0       UOx++ B4O5(OH)4=
1  .0         .0        .0      .0       UOx++ Br-
1  .0         .0        .0      .0       UOx++ Am(CO3)2-
3  .0         .0        .0      .0       UOx++ Am(CO3)3=-
1  .0         .0        .0      .0       UOx++ ClO4-
1  .0         .0        .0      .0       UOx++ NpO2(OH)2-
1  .0         .0        .0      .0       UOx++ NpO2CO3-
3  .0         .0        .0      .0       UOx++ NpO2(CO3)2=-
3  .0         .0        .0      .0       UOx++ NpO2(CO3)3==-
1  .0         .0        .0      .0       UOx++ H2PO4-
2  .0         .0        .0      .0       UOx++ HPO4=
3  .0         .0        .0      .0       UOx++ PO4=-
2  .0         .0        .0      .0       UOx++ Th(SO4)3=
1  .0         .0        .0      .0       UOx++ Th(OH)3(CO3)-
3  .0         .0        .0      .0       UOx++ Th(CO3)5===
1  .0         .0        .0      .0       UOx++ HOx-
2  .0         .0        .0      .0       UOx++ Ox=
1  .0         .0        .0      .0       UOx++ Ac-
1  .0         .0        .0      .0       UOx++ Lac-
1  .0         .0        .0      .0       UOx++ H2Cit-
2  .0         .0        .0      .0       UOx++ HCit=
3  .0         .0        .0      .0       UOx++ Cit=-
3  .0         .0        .0      .0       UOx++ H3EDTA-
3  .0         .0        .0      .0       UOx++ H2EDTA=
3  .0         .0        .0      .0       UOx++ HEDTA=-
3  .0         .0        .0      .0       UOx++ EDTA==
3  .0         .0        .0      .0       UOx++ AmEDTA-
3  .0         .0        .0      .0       UOx++ NpO2Cit=
3  .0         .0        .0      .0       UOx++ NpO2EDTA==-
1  .0         .0        .0      .0       UOx++ NpO2Ox-
3  .0         .0        .0      .0       UOx++ U(OH)4(CO3)2==
3  .0         .0        .0      .0       UOx++ U(CO3)5===
2  .0         .0        .0      .0       UOx++ U(SO4)3=
3  .0         .0        .0      .0       UOx++ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0       UOx++ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0       UOx++ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0       UOx++ CaCit-
2  .0         .0        .0      .0       UOx++ CaEDTA=
1  .0         .0        .0      .0       UOx++ UnuAn#2-
1  .0         .0        .0      .0       UOx++ UnuAn#3-
1  .0         .0        .0      .0       UOx++ UnuAn#4-
2  .0         .0        .0      .0       UOx++ U(OH)2(CO3)2=
1  .0         .0        .0      .0       UOx++ MgCit-
```

```
2  .0         .0        .0      .0       UOx++ MgEDTA=
2  .0         .0        .0      .0       UOx++ NpO2HEDTA=   [NEW]

1  1.061      5.22      .0      .109     ThAc+++ Cl-            SAND99
3  .0         .0        .0      .0       ThAc+++ SO4=
1  .0         .0        .0      .0       ThAc+++ HSO4-
1  .0         .0        .0      .0       ThAc+++ OH-
1  .0         .0        .0      .0       ThAc+++ HCO3-
3  .0         .0        .0      .0       ThAc+++ CO3=
1  .0         .0        .0      .0       ThAc+++ B(OH)4-
1  .0         .0        .0      .0       ThAc+++ B3O3(OH)4-
3  .0         .0        .0      .0       ThAc+++ B4O5(OH)4=
1  .0         .0        .0      .0       ThAc+++ Br-
1  .0         .0        .0      .0       ThAc+++ Am(CO3)2-
3  .0         .0        .0      .0       ThAc+++ Am(CO3)3=-
1  .0         .0        .0      .0       ThAc+++ ClO4-
1  .0         .0        .0      .0       ThAc+++ NpO2(OH)2-
1  .0         .0        .0      .0       ThAc+++ NpO2CO3-
3  .0         .0        .0      .0       ThAc+++ NpO2(CO3)2=-
3  .0         .0        .0      .0       ThAc+++ NpO2(CO3)3==-
1  .0         .0        .0      .0       ThAc+++ H2PO4-
3  .0         .0        .0      .0       ThAc+++ HPO4=
3  .0         .0        .0      .0       ThAc+++ PO4=-
3  .0         .0        .0      .0       ThAc+++ Th(SO4)3=
1  .0         .0        .0      .0       ThAc+++ Th(OH)3(CO3)-
3  .0         .0        .0      .0       ThAc+++ Th(CO3)5===
1  .0         .0        .0      .0       ThAc+++ HOx-
3  .0         .0        .0      .0       ThAc+++ Ox=
1  .0         .0        .0      .0       ThAc+++ Ac-
1  .0         .0        .0      .0       ThAc+++ Lac-
1  .0         .0        .0      .0       ThAc+++ H2Cit-
3  .0         .0        .0      .0       ThAc+++ HCit=
3  .0         .0        .0      .0       ThAc+++ Cit=-
3  .0         .0        .0      .0       ThAc+++ H3EDTA-
3  .0         .0        .0      .0       ThAc+++ H2EDTA=
3  .0         .0        .0      .0       ThAc+++ HEDTA=-
3  .0         .0        .0      .0       ThAc+++ EDTA==
3  .0         .0        .0      .0       ThAc+++ AmEDTA-
3  .0         .0        .0      .0       ThAc+++ NpO2Cit=
3  .0         .0        .0      .0       ThAc+++ NpO2EDTA==-
1  .0         .0        .0      .0       ThAc+++ NpO2Ox-
3  .0         .0        .0      .0       ThAc+++ U(OH)4(CO3)2==
3  .0         .0        .0      .0       ThAc+++ U(CO3)5===
3  .0         .0        .0      .0       ThAc+++ U(SO4)3=
3  .0         .0        .0      .0       ThAc+++ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0       ThAc+++ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0       ThAc+++ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0       ThAc+++ CaCit-
```

```
3  .0         .0        .0      .0        ThAc+++ CaEDTA=
1  .0         .0        .0      .0        ThAc+++ UnuAn#2-
1  .0         .0        .0      .0        ThAc+++ UnuAn#3-
1  .0         .0        .0      .0        ThAc+++ UnuAn#4-
3  .0         .0        .0      .0        ThAc+++ U(OH)2(CO3)2=
1  .0         .0        .0      .0        ThAc+++ MgCit-
3  .0         .0        .0      .0        ThAc+++ MgEDTA=
3  .0         .0        .0      .0        ThAc+++ NpO2HEDTA=   [NEW]

1 -.7467      .29       .0      .319      ThCit+ Cl-           SAND99
1  .0         .0        .0      .0        ThCit+ SO4=
1  .0         .0        .0      .0        ThCit+ HSO4-
1  .0         .0        .0      .0        ThCit+ OH-
1  .0         .0        .0      .0        ThCit+ HCO3-
1  .0         .0        .0      .0        ThCit+ CO3=
1  .0         .0        .0      .0        ThCit+ B(OH)4-
1  .0         .0        .0      .0        ThCit+ B3O3(OH)4-
1  .0         .0        .0      .0        ThCit+ B4O5(OH)4=
1  .0         .0        .0      .0        ThCit+ Br-
1  .0         .0        .0      .0        ThCit+ Am(CO3)2-
1  .0         .0        .0      .0        ThCit+ Am(CO3)3=-
1  .0         .0        .0      .0        ThCit+ ClO4-
1  .0         .0        .0      .0        ThCit+ NpO2(OH)2-
1  .0         .0        .0      .0        ThCit+ NpO2CO3-
1  .0         .0        .0      .0        ThCit+ NpO2(CO3)2=-
1  .0         .0        .0      .0        ThCit+ NpO2(CO3)3==-
1  .0         .0        .0      .0        ThCit+ H2PO4-
1  .0         .0        .0      .0        ThCit+ HPO4=
1  .0         .0        .0      .0        ThCit+ PO4=-
1  .0         .0        .0      .0        ThCit+ Th(SO4)3=
1  .0         .0        .0      .0        ThCit+ Th(OH)3(CO3)-
1  .0         .0        .0      .0        ThCit+ Th(CO3)5===
1  .0         .0        .0      .0        ThCit+ HOx-
1  .0         .0        .0      .0        ThCit+ Ox=
1  .0         .0        .0      .0        ThCit+ Ac-
1  .0         .0        .0      .0        ThCit+ Lac-
1  .0         .0        .0      .0        ThCit+ H2Cit-
1  .0         .0        .0      .0        ThCit+ HCit=
1  .0         .0        .0      .0        ThCit+ Cit=-
1  .0         .0        .0      .0        ThCit+ H3EDTA-
1  .0         .0        .0      .0        ThCit+ H2EDTA=
1  .0         .0        .0      .0        ThCit+ HEDTA=-
1  .0         .0        .0      .0        ThCit+ EDTA==
1  .0         .0        .0      .0        ThCit+ AmEDTA-
1  .0         .0        .0      .0        ThCit+ NpO2Cit=
1  .0         .0        .0      .0        ThCit+ NpO2EDTA==-
1  .0         .0        .0      .0        ThCit+ NpO2Ox-
1  .0         .0        .0      .0        ThCit+ U(OH)4(CO3)2==
```

```
1  .0        .0       .0     .0       ThCit+ U(CO3)5===
1  .0        .0       .0     .0       ThCit+ U(SO4)3=
1  .0        .0       .0     .0       ThCit+ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       ThCit+ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       ThCit+ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       ThCit+ CaCit-
1  .0        .0       .0     .0       ThCit+ CaEDTA=
1  .0        .0       .0     .0       ThCit+ UnuAn#2-
1  .0        .0       .0     .0       ThCit+ UnuAn#3-
1  .0        .0       .0     .0       ThCit+ UnuAn#4-
1  .0        .0       .0     .0       ThCit+ U(OH)2(CO3)2=
1  .0        .0       .0     .0       ThCit+ MgCit-
1  .0        .0       .0     .0       ThCit+ MgEDTA=
1  .0        .0       .0     .0       ThCit+ NpO2HEDTA=   [NEW]

1  .6677     5.22     .0     .341     ThLac+++ Cl-          SAND99/Moore et al 99
3  .0        .0       .0     .0       ThLac+++ SO4=
1  .0        .0       .0     .0       ThLac+++ HSO4-
1  .0        .0       .0     .0       ThLac+++ OH-
1  .0        .0       .0     .0       ThLac+++ HCO3-
3  .0        .0       .0     .0       ThLac+++ CO3=
1  .0        .0       .0     .0       ThLac+++ B(OH)4-
1  .0        .0       .0     .0       ThLac+++ B3O3(OH)4-
3  .0        .0       .0     .0       ThLac+++ B4O5(OH)4=
1  .0        .0       .0     .0       ThLac+++ Br-
1  .0        .0       .0     .0       ThLac+++ Am(CO3)2-
3  .0        .0       .0     .0       ThLac+++ Am(CO3)3=-
1  .0        .0       .0     .0       ThLac+++ ClO4-
1  .0        .0       .0     .0       ThLac+++ NpO2(OH)2-
1  .0        .0       .0     .0       ThLac+++ NpO2CO3-
3  .0        .0       .0     .0       ThLac+++ NpO2(CO3)2=-
3  .0        .0       .0     .0       ThLac+++ NpO2(CO3)3==-
1  .0        .0       .0     .0       ThLac+++ H2PO4-
3  .0        .0       .0     .0       ThLac+++ HPO4=
3  .0        .0       .0     .0       ThLac+++ PO4=-
3  .0        .0       .0     .0       ThLac+++ Th(SO4)3=
1  .0        .0       .0     .0       ThLac+++ Th(OH)3(CO3)-
3  .0        .0       .0     .0       ThLac+++ Th(CO3)5===
1  .0        .0       .0     .0       ThLac+++ HOx-
3  .0        .0       .0     .0       ThLac+++ Ox=
1  .0        .0       .0     .0       ThLac+++ Ac-
1  .0        .0       .0     .0       ThLac+++ Lac-
1  .0        .0       .0     .0       ThLac+++ H2Cit-
3  .0        .0       .0     .0       ThLac+++ HCit=
3  .0        .0       .0     .0       ThLac+++ Cit=-
3  .0        .0       .0     .0       ThLac+++ H3EDTA-
3  .0        .0       .0     .0       ThLac+++ H2EDTA=
3  .0        .0       .0     .0       ThLac+++ HEDTA=-
```

```
3  .0          .0        .0      .0        ThLac+++ EDTA==
3  .0          .0        .0      .0        ThLac+++ AmEDTA-
3  .0          .0        .0      .0        ThLac+++ NpO2Cit=
3  .0          .0        .0      .0        ThLac+++ NpO2EDTA==-
1  .0          .0        .0      .0        ThLac+++ NpO2Ox-
3  .0          .0        .0      .0        ThLac+++ U(OH)4(CO3)2==
3  .0          .0        .0      .0        ThLac+++ U(CO3)5===
3  .0          .0        .0      .0        ThLac+++ U(SO4)3=
3  .0          .0        .0      .0        ThLac+++ Am(CO3)4==-   [NEW]
1  .0          .0        .0      .0        ThLac+++ Am(SO4)2-     [NEW]
1  .0          .0        .0      .0        ThLac+++ NpO2H2EDTA-   [NEW]
1  .0          .0        .0      .0        ThLac+++ CaCit-
3  .0          .0        .0      .0        ThLac+++ CaEDTA=
1  .0          .0        .0      .0        ThLac+++ UnuAn#2-
1  .0          .0        .0      .0        ThLac+++ UnuAn#3-
1  .0          .0        .0      .0        ThLac+++ UnuAn#4-
3  .0          .0        .0      .0        ThLac+++ U(OH)2(CO3)2=
1  .0          .0        .0      .0        ThLac+++ MgCit-
3  .0          .0        .0      .0        ThLac+++ MgEDTA=
3  .0          .0        .0      .0        ThLac+++ NpO2HEDTA=   [NEW]

1 -0.055      1.6        .0      0.050     AmOH++ Cl-    FK98/Konnecke et al. 1997
2  .0          .0        .0      .0        AmOH++ SO4=
1  .0          .0        .0      .0        AmOH++ HSO4-
1  .0          .0        .0      .0        AmOH++ OH-
1  .0          .0        .0      .0        AmOH++ HCO3-
2  .0          .0        .0      .0        AmOH++ CO3=
1  .0          .0        .0      .0        AmOH++ B(OH)4-
1  .0          .0        .0      .0        AmOH++ B3O3(OH)4-
2  .0          .0        .0      .0        AmOH++ B4O5(OH)4=
1  .0          .0        .0      .0        AmOH++ Br-
1  .0          .0        .0      .0        AmOH++ Am(CO3)2-
3  .0          .0        .0      .0        AmOH++ Am(CO3)3=-
1  .0          .0        .0      .0        AmOH++ ClO4-
1  .0          .0        .0      .0        AmOH++ NpO2(OH)2-
1  .0          .0        .0      .0        AmOH++ NpO2CO3-
3  .0          .0        .0      .0        AmOH++ NpO2(CO3)2=-
3  .0          .0        .0      .0        AmOH++ NpO2(CO3)3==-
1  .0          .0        .0      .0        AmOH++ H2PO4-
2  .0          .0        .0      .0        AmOH++ HPO4=
3  .0          .0        .0      .0        AmOH++ PO4=-
2  .0          .0        .0      .0        AmOH++ Th(SO4)3=
1  .0          .0        .0      .0        AmOH++ Th(OH)3(CO3)-
3  .0          .0        .0      .0        AmOH++ Th(CO3)5===
1  .0          .0        .0      .0        AmOH++ HOx-
2  .0          .0        .0      .0        AmOH++ Ox=
1  .0          .0        .0      .0        AmOH++ Ac-
1  .0          .0        .0      .0        AmOH++ Lac-
```

```
1  .0         .0        .0      .0        AmOH++ H2Cit-
2  .0         .0        .0      .0        AmOH++ HCit=
3  .0         .0        .0      .0        AmOH++ Cit=-
3  .0         .0        .0      .0        AmOH++ H3EDTA-
3  .0         .0        .0      .0        AmOH++ H2EDTA=
3  .0         .0        .0      .0        AmOH++ HEDTA=-
3  .0         .0        .0      .0        AmOH++ EDTA==
3  .0         .0        .0      .0        AmOH++ AmEDTA-
3  .0         .0        .0      .0        AmOH++ NpO2Cit=
3  .0         .0        .0      .0        AmOH++ NpO2EDTA==-
1  .0         .0        .0      .0        AmOH++ NpO2Ox-
3  .0         .0        .0      .0        AmOH++ U(OH)4(CO3)2==
3  .0         .0        .0      .0        AmOH++ U(CO3)5===
2  .0         .0        .0      .0        AmOH++ U(SO4)3=
3  .0         .0        .0      .0        AmOH++ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0        AmOH++ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0        AmOH++ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0        AmOH++ CaCit-
2  .0         .0        .0      .0        AmOH++ CaEDTA=
1  .0         .0        .0      .0        AmOH++ UnuAn#2-
1  .0         .0        .0      .0        AmOH++ UnuAn#3-
1  .0         .0        .0      .0        AmOH++ UnuAn#4-
2  .0         .0        .0      .0        AmOH++ U(OH)2(CO3)2=
1  .0         .0        .0      .0        AmOH++ MgCit-
2  .0         .0        .0      .0        AmOH++ MgEDTA=
2  .0         .0        .0      .0        AmOH++ NpO2HEDTA=   [NEW]

1 -0.616     -0.45      .0     .050       Am(OH)2+ Cl-    FK98/Konnecke et al. 1997
1  .0         .0        .0      .0        Am(OH)2+ SO4=
1  .0         .0        .0      .0        Am(OH)2+ HSO4-
1  .0         .0        .0      .0        Am(OH)2+ OH-
1  .0         .0        .0      .0        Am(OH)2+ HCO3-
1  .0         .0        .0      .0        Am(OH)2+ CO3=
1  .0         .0        .0      .0        Am(OH)2+ B(OH)4-
1  .0         .0        .0      .0        Am(OH)2+ B3O3(OH)4-
1  .0         .0        .0      .0        Am(OH)2+ B4O5(OH)4=
1  .0         .0        .0      .0        Am(OH)2+ Br-
1  .0         .0        .0      .0        Am(OH)2+ Am(CO3)2-
1  .0         .0        .0      .0        Am(OH)2+ Am(CO3)3=-
1  .0         .0        .0      .0        Am(OH)2+ ClO4-
1  .0         .0        .0      .0        Am(OH)2+ NpO2(OH)2-
1  .0         .0        .0      .0        Am(OH)2+ NpO2CO3-
1  .0         .0        .0      .0        Am(OH)2+ NpO2(CO3)2=-
1  .0         .0        .0      .0        Am(OH)2+ NpO2(CO3)3==-
1  .0         .0        .0      .0        Am(OH)2+ H2PO4-
1  .0         .0        .0      .0        Am(OH)2+ HPO4=
1  .0         .0        .0      .0        Am(OH)2+ PO4=-
1  .0         .0        .0      .0        Am(OH)2+ Th(SO4)3=
```

```
1  .0      .0     .0    .0      Am(OH)2+ Th(OH)3(CO3)-
1  .0      .0     .0    .0      Am(OH)2+ Th(CO3)5===
1  .0      .0     .0    .0      Am(OH)2+ HOx-
1  .0      .0     .0    .0      Am(OH)2+ Ox=
1  .0      .0     .0    .0      Am(OH)2+ Ac-
1  .0      .0     .0    .0      Am(OH)2+ Lac-
1  .0      .0     .0    .0      Am(OH)2+ H2Cit-
1  .0      .0     .0    .0      Am(OH)2+ HCit=
1  .0      .0     .0    .0      Am(OH)2+ Cit=-
1  .0      .0     .0    .0      Am(OH)2+ H3EDTA-
1  .0      .0     .0    .0      Am(OH)2+ H2EDTA=
1  .0      .0     .0    .0      Am(OH)2+ HEDTA=-
1  .0      .0     .0    .0      Am(OH)2+ EDTA==
1  .0      .0     .0    .0      Am(OH)2+ AmEDTA-
1  .0      .0     .0    .0      Am(OH)2+ NpO2Cit=
1  .0      .0     .0    .0      Am(OH)2+ NpO2EDTA==-
1  .0      .0     .0    .0      Am(OH)2+ NpO2Ox-
1  .0      .0     .0    .0      Am(OH)2+ U(OH)4(CO3)2==
1  .0      .0     .0    .0      Am(OH)2+ U(CO3)5===
1  .0      .0     .0    .0      Am(OH)2+ U(SO4)3=
1  .0      .0     .0    .0      Am(OH)2+ Am(CO3)4==-   [NEW]
1  .0      .0     .0    .0      Am(OH)2+ Am(SO4)2-     [NEW]
1  .0      .0     .0    .0      Am(OH)2+ NpO2H2EDTA-   [NEW]
1  .0      .0     .0    .0      Am(OH)2+ CaCit-
1  .0      .0     .0    .0      Am(OH)2+ CaEDTA=
1  .0      .0     .0    .0      Am(OH)2+ UnuAn#2-
1  .0      .0     .0    .0      Am(OH)2+ UnuAn#3-
1  .0      .0     .0    .0      Am(OH)2+ UnuAn#4-
1  .0      .0     .0    .0      Am(OH)2+ U(OH)2(CO3)2=
1  .0      .0     .0    .0      Am(OH)2+ MgCit-
1  .0      .0     .0    .0      Am(OH)2+ MgEDTA=
1  .0      .0     .0    .0      Am(OH)2+ NpO2HEDTA=   [NEW]

[AmCl2+ INTERACTIONS ADDED]
1  .516    1.75   .0    .010    AmCl2+ Cl-       FK98/Konnecke et al. 1997
1  .0      .0     .0    .0      AmCl2+ SO4=
1  .0      .0     .0    .0      AmCl2+ HSO4-
1  .0      .0     .0    .0      AmCl2+ OH-
1  .0      .0     .0    .0      AmCl2+ HCO3-
1  .0      .0     .0    .0      AmCl2+ CO3=
1  .0      .0     .0    .0      AmCl2+ B(OH)4-
1  .0      .0     .0    .0      AmCl2+ B3O3(OH)4-
1  .0      .0     .0    .0      AmCl2+ B4O5(OH)4=
1  .0      .0     .0    .0      AmCl2+ Br-
1  .0      .0     .0    .0      AmCl2+ Am(CO3)2-
1  .0      .0     .0    .0      AmCl2+ Am(CO3)3=-
1  .0      .0     .0    .0      AmCl2+ ClO4-
1  .0      .0     .0    .0      AmCl2+ NpO2(OH)2-
```

```
  1  .0          .0        .0      .0        AmCl2+ NpO2CO3-
  1  .0          .0        .0      .0        AmCl2+ NpO2(CO3)2=-
  1  .0          .0        .0      .0        AmCl2+ NpO2(CO3)3==-
  1  .0          .0        .0      .0        AmCl2+ H2PO4-
  1  .0          .0        .0      .0        AmCl2+ HPO4=
  1  .0          .0        .0      .0        AmCl2+ PO4=-
  1  .0          .0        .0      .0        AmCl2+ Th(SO4)3=
  1  .0          .0        .0      .0        AmCl2+ Th(OH)3(CO3)-
  1  .0          .0        .0      .0        AmCl2+ Th(CO3)5===
  1  .0          .0        .0      .0        AmCl2+ HOx-
  1  .0          .0        .0      .0        AmCl2+ Ox=
  1  .0          .0        .0      .0        AmCl2+ Ac-
  1  .0          .0        .0      .0        AmCl2+ Lac-
  1  .0          .0        .0      .0        AmCl2+ H2Cit-
  1  .0          .0        .0      .0        AmCl2+ HCit=
  1  .0          .0        .0      .0        AmCl2+ Cit=-
  1  .0          .0        .0      .0        AmCl2+ H3EDTA-
  1  .0          .0        .0      .0        AmCl2+ H2EDTA=
  1  .0          .0        .0      .0        AmCl2+ HEDTA=-
  1  .0          .0        .0      .0        AmCl2+ EDTA==
  1  .0          .0        .0      .0        AmCl2+ AmEDTA-
  1  .0          .0        .0      .0        AmCl2+ NpO2Cit=
  1  .0          .0        .0      .0        AmCl2+ NpO2EDTA==-
  1  .0          .0        .0      .0        AmCl2+ NpO2Ox-
  1  .0          .0        .0      .0        AmCl2+ U(OH)4(CO3)2==
  1  .0          .0        .0      .0        AmCl2+ U(CO3)5===
  1  .0          .0        .0      .0        AmCl2+ U(SO4)3=
  1  .0          .0        .0      .0        AmCl2+ Am(CO3)4==-
  1  .0          .0        .0      .0        AmCl2+ Am(SO4)2-
  1  .0          .0        .0      .0        AmCl2+ NpO2H2EDTA-
  1  .0          .0        .0      .0        AmCl2+ CaCit-
  1  .0          .0        .0      .0        AmCl2+ CaEDTA=
  1  .0          .0        .0      .0        AmCl2+ UnuAn#2-
  1  .0          .0        .0      .0        AmCl2+ UnuAn#3-
  1  .0          .0        .0      .0        AmCl2+ UnuAn#4-
  1  .0          .0        .0      .0        AmCl2+ U(OH)2(CO3)2=
  1  .0          .0        .0      .0        AmCl2+ MgCit-
  1  .0          .0        .0      .0        AmCl2+ MgEDTA=
  1  .0          .0        .0      .0        AmCl2+ NpO2HEDTA=

[AmSO4+ INTERACTIONS ADDED]
  1 -0.091     -.39        .0      0.048     AmSO4+ Cl-    FK98
  1  .0          .0        .0      .0        AmSO4+ SO4=
  1  .0          .0        .0      .0        AmSO4+ HSO4-
  1  .0          .0        .0      .0        AmSO4+ OH-
  1  .0          .0        .0      .0        AmSO4+ HCO3-
  1  .0          .0        .0      .0        AmSO4+ CO3=
  1  .0          .0        .0      .0        AmSO4+ B(OH)4-
```

```
  1  .0          .0        .0      .0        AmSO4+ B3O3(OH)4-
  1  .0          .0        .0      .0        AmSO4+ B4O5(OH)4=
  1  .0          .0        .0      .0        AmSO4+ Br-
  1  .0          .0        .0      .0        AmSO4+ Am(CO3)2-
  1  .0          .0        .0      .0        AmSO4+ Am(CO3)3=-
  1  .0          .0        .0      .0        AmSO4+ ClO4-
  1  .0          .0        .0      .0        AmSO4+ NpO2(OH)2-
  1  .0          .0        .0      .0        AmSO4+ NpO2CO3-
  1  .0          .0        .0      .0        AmSO4+ NpO2(CO3)2=-
  1  .0          .0        .0      .0        AmSO4+ NpO2(CO3)3==-
  1  .0          .0        .0      .0        AmSO4+ H2PO4-
  1  .0          .0        .0      .0        AmSO4+ HPO4=
  1  .0          .0        .0      .0        AmSO4+ PO4=-
  1  .0          .0        .0      .0        AmSO4+ Th(SO4)3=
  1  .0          .0        .0      .0        AmSO4+ Th(OH)3(CO3)-
  1  .0          .0        .0      .0        AmSO4+ Th(CO3)5===
  1  .0          .0        .0      .0        AmSO4+ HOx-
  1  .0          .0        .0      .0        AmSO4+ Ox=
  1  .0          .0        .0      .0        AmSO4+ Ac-
  1  .0          .0        .0      .0        AmSO4+ Lac-
  1  .0          .0        .0      .0        AmSO4+ H2Cit-
  1  .0          .0        .0      .0        AmSO4+ HCit=
  1  .0          .0        .0      .0        AmSO4+ Cit=-
  1  .0          .0        .0      .0        AmSO4+ H3EDTA-
  1  .0          .0        .0      .0        AmSO4+ H2EDTA=
  1  .0          .0        .0      .0        AmSO4+ HEDTA=-
  1  .0          .0        .0      .0        AmSO4+ EDTA==
  1  .0          .0        .0      .0        AmSO4+ AmEDTA-
  1  .0          .0        .0      .0        AmSO4+ NpO2Cit=
  1  .0          .0        .0      .0        AmSO4+ NpO2EDTA==-
  1  .0          .0        .0      .0        AmSO4+ NpO2Ox-
  1  .0          .0        .0      .0        AmSO4+ U(OH)4(CO3)2==
  1  .0          .0        .0      .0        AmSO4+ U(CO3)5===
  1  .0          .0        .0      .0        AmSO4+ U(SO4)3=
  1  .0          .0        .0      .0        AmSO4+ Am(CO3)4==-
  1  .0          .0        .0      .0        AmSO4+ Am(SO4)2-
  1  .0          .0        .0      .0        AmSO4+ NpO2H2EDTA-
  1  .0          .0        .0      .0        AmSO4+ CaCit-
  1  .0          .0        .0      .0        AmSO4+ CaEDTA=
  1  .0          .0        .0      .0        AmSO4+ UnuAn#2-
  1  .0          .0        .0      .0        AmSO4+ UnuAn#3-
  1  .0          .0        .0      .0        AmSO4+ UnuAn#4-
  1  .0          .0        .0      .0        AmSO4+ U(OH)2(CO3)2=
  1  .0          .0        .0      .0        AmSO4+ MgCit-
  1  .0          .0        .0      .0        AmSO4+ MgEDTA=
  1  .0          .0        .0      .0        AmSO4+ NpO2HEDTA=

  1 -0.616      -0.45      .0     .050       Pu(OH)2+ Cl-    analogy w/ Am (FK98)
```

```
1   .0          .0        .0      .0         Pu(OH)2+ SO4=
1   .0          .0        .0      .0         Pu(OH)2+ HSO4-
1   .0          .0        .0      .0         Pu(OH)2+ OH-
1   .0          .0        .0      .0         Pu(OH)2+ HCO3-
1   .0          .0        .0      .0         Pu(OH)2+ CO3=
1   .0          .0        .0      .0         Pu(OH)2+ B(OH)4-
1   .0          .0        .0      .0         Pu(OH)2+ B3O3(OH)4-
1   .0          .0        .0      .0         Pu(OH)2+ B4O5(OH)4=
1   .0          .0        .0      .0         Pu(OH)2+ Br-
1   .0          .0        .0      .0         Pu(OH)2+ Am(CO3)2-
1   .0          .0        .0      .0         Pu(OH)2+ Am(CO3)3=-
1   .0          .0        .0      .0         Pu(OH)2+ ClO4-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2(OH)2-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2CO3-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2(CO3)2=-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2(CO3)3==-
1   .0          .0        .0      .0         Pu(OH)2+ H2PO4-
1   .0          .0        .0      .0         Pu(OH)2+ HPO4=
1   .0          .0        .0      .0         Pu(OH)2+ PO4=-
1   .0          .0        .0      .0         Pu(OH)2+ Th(SO4)3=
1   .0          .0        .0      .0         Pu(OH)2+ Th(OH)3(CO3)-
1   .0          .0        .0      .0         Pu(OH)2+ Th(CO3)5===
1   .0          .0        .0      .0         Pu(OH)2+ HOx-
1   .0          .0        .0      .0         Pu(OH)2+ Ox=
1   .0          .0        .0      .0         Pu(OH)2+ Ac-
1   .0          .0        .0      .0         Pu(OH)2+ Lac-
1   .0          .0        .0      .0         Pu(OH)2+ H2Cit-
1   .0          .0        .0      .0         Pu(OH)2+ HCit=
1   .0          .0        .0      .0         Pu(OH)2+ Cit=-
1   .0          .0        .0      .0         Pu(OH)2+ H3EDTA-
1   .0          .0        .0      .0         Pu(OH)2+ H2EDTA=
1   .0          .0        .0      .0         Pu(OH)2+ HEDTA=-
1   .0          .0        .0      .0         Pu(OH)2+ EDTA==
1   .0          .0        .0      .0         Pu(OH)2+ AmEDTA-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2Cit=
1   .0          .0        .0      .0         Pu(OH)2+ NpO2EDTA==-
1   .0          .0        .0      .0         Pu(OH)2+ NpO2Ox-
1   .0          .0        .0      .0         Pu(OH)2+ U(OH)4(CO3)2==
1   .0          .0        .0      .0         Pu(OH)2+ U(CO3)5===
1   .0          .0        .0      .0         Pu(OH)2+ U(SO4)3=
1   .0          .0        .0      .0         Pu(OH)2+ Am(CO3)4==-   [NEW]
1   .0          .0        .0      .0         Pu(OH)2+ Am(SO4)2-     [NEW]
1   .0          .0        .0      .0         Pu(OH)2+ NpO2H2EDTA-   [NEW]
1   .0          .0        .0      .0         Pu(OH)2+ CaCit-
1   .0          .0        .0      .0         Pu(OH)2+ CaEDTA=
1   .0          .0        .0      .0         Pu(OH)2+ UnuAn#2-
1   .0          .0        .0      .0         Pu(OH)2+ UnuAn#3-
1   .0          .0        .0      .0         Pu(OH)2+ UnuAn#4-
```

```
  1  .0         .0        .0      .0       Pu(OH)2+ U(OH)2(CO3)2=
  1  .0         .0        .0      .0       Pu(OH)2+ MgCit-
  1  .0         .0        .0      .0       Pu(OH)2+ MgEDTA=
  1  .0         .0        .0      .0       Pu(OH)2+ NpO2HEDTA=   [NEW]

[ThAc2+ INTERACTIONS ADDED]
  1  .4671     1.74       .0      .143     ThAc2++ Cl-      Moore et al 1999
  2  .0         .0        .0      .0       ThAc2++ SO4=
  1  .0         .0        .0      .0       ThAc2++ HSO4-
  1  .0         .0        .0      .0       ThAc2++ OH-
  1  .0         .0        .0      .0       ThAc2++ HCO3-
  2  .0         .0        .0      .0       ThAc2++ CO3=
  1  .0         .0        .0      .0       ThAc2++ B(OH)4-
  1  .0         .0        .0      .0       ThAc2++ B3O3(OH)4-
  2  .0         .0        .0      .0       ThAc2++ B4O5(OH)4=
  1  .0         .0        .0      .0       ThAc2++ Br-
  1  .0         .0        .0      .0       ThAc2++ Am(CO3)2-
  3  .0         .0        .0      .0       ThAc2++ Am(CO3)3=-
  1  .0         .0        .0      .0       ThAc2++ ClO4-
  1  .0         .0        .0      .0       ThAc2++ NpO2(OH)2-
  1  .0         .0        .0      .0       ThAc2++ NpO2CO3-
  3  .0         .0        .0      .0       ThAc2++ NpO2(CO3)2=-
  3  .0         .0        .0      .0       ThAc2++ NpO2(CO3)3==-
  1  .0         .0        .0      .0       ThAc2++ H2PO4-
  2  .0         .0        .0      .0       ThAc2++ HPO4=
  3  .0         .0        .0      .0       ThAc2++ PO4=-
  2  .0         .0        .0      .0       ThAc2++ Th(SO4)3=
  1  .0         .0        .0      .0       ThAc2++ Th(OH)3(CO3)-
  3  .0         .0        .0      .0       ThAc2++ Th(CO3)5===
  1  .0         .0        .0      .0       ThAc2++ HOx-
  2  .0         .0        .0      .0       ThAc2++ Ox=
  1  .0         .0        .0      .0       ThAc2++ Ac-
  1  .0         .0        .0      .0       ThAc2++ Lac-
  1  .0         .0        .0      .0       ThAc2++ H2Cit-
  2  .0         .0        .0      .0       ThAc2++ HCit=
  3  .0         .0        .0      .0       ThAc2++ Cit=-
  3  .0         .0        .0      .0       ThAc2++ H3EDTA-
  3  .0         .0        .0      .0       ThAc2++ H2EDTA=
  3  .0         .0        .0      .0       ThAc2++ HEDTA=-
  3  .0         .0        .0      .0       ThAc2++ EDTA==
  3  .0         .0        .0      .0       ThAc2++ AmEDTA-
  3  .0         .0        .0      .0       ThAc2++ NpO2Cit=
  3  .0         .0        .0      .0       ThAc2++ NpO2EDTA==-
  1  .0         .0        .0      .0       ThAc2++ NpO2Ox-
  3  .0         .0        .0      .0       ThAc2++ U(OH)4(CO3)2==
  3  .0         .0        .0      .0       ThAc2++ U(CO3)5===
  2  .0         .0        .0      .0       ThAc2++ U(SO4)3=
  3  .0         .0        .0      .0       ThAc2++ Am(CO3)4==-
```

```
  1  .0         .0        .0      .0        ThAc2++ Am(SO4)2-
  1  .0         .0        .0      .0        ThAc2++ NpO2H2EDTA-
  1  .0         .0        .0      .0        ThAc2++ CaCit-
  3  .0         .0        .0      .0        ThAc2++ CaEDTA=
  1  .0         .0        .0      .0        ThAc2++ UnuAn#2-
  1  .0         .0        .0      .0        ThAc2++ UnuAn#3-
  1  .0         .0        .0      .0        ThAc2++ UnuAn#4-
  2  .0         .0        .0      .0        ThAc2++ U(OH)2(CO3)2=
  1  .0         .0        .0      .0        ThAc2++ MgCit-
  2  .0         .0        .0      .0        ThAc2++ MgEDTA=
  2  .0         .0        .0      .0        ThAc2++ NpO2HEDTA=

  1 -.9374      .29       .0      .248      PuOx+ Cl-         analogy w/ Am (SAND99/Borkowski et al 01)
  1  .0         .0        .0      .0        PuOx+ SO4=
  1  .0         .0        .0      .0        PuOx+ HSO4-
  1  .0         .0        .0      .0        PuOx+ OH-
  1  .0         .0        .0      .0        PuOx+ HCO3-
  1  .0         .0        .0      .0        PuOx+ CO3=
  1  .0         .0        .0      .0        PuOx+ B(OH)4-
  1  .0         .0        .0      .0        PuOx+ B3O3(OH)4-
  1  .0         .0        .0      .0        PuOx+ B4O5(OH)4=
  1  .0         .0        .0      .0        PuOx+ Br-
  1  .0         .0        .0      .0        PuOx+ Am(CO3)2-
  1  .0         .0        .0      .0        PuOx+ Am(CO3)3=-
  1  .0         .0        .0      .0        PuOx+ ClO4-
  1  .0         .0        .0      .0        PuOx+ NpO2(OH)2-
  1  .0         .0        .0      .0        PuOx+ NpO2CO3-
  1  .0         .0        .0      .0        PuOx+ NpO2(CO3)2=-
  1  .0         .0        .0      .0        PuOx+ NpO2(CO3)3==-
  1  .0         .0        .0      .0        PuOx+ H2PO4-
  1  .0         .0        .0      .0        PuOx+ HPO4=
  1  .0         .0        .0      .0        PuOx+ PO4=-
  1  .0         .0        .0      .0        PuOx+ Th(SO4)3=
  1  .0         .0        .0      .0        PuOx+ Th(OH)3(CO3)-
  1  .0         .0        .0      .0        PuOx+ Th(CO3)5===
  1  .0         .0        .0      .0        PuOx+ HOx-
  1  .0         .0        .0      .0        PuOx+ Ox=
  1  .0         .0        .0      .0        PuOx+ Ac-
  1  .0         .0        .0      .0        PuOx+ Lac-
  1  .0         .0        .0      .0        PuOx+ H2Cit-
  1  .0         .0        .0      .0        PuOx+ HCit=
  1  .0         .0        .0      .0        PuOx+ Cit=-
  1  .0         .0        .0      .0        PuOx+ H3EDTA-
  1  .0         .0        .0      .0        PuOx+ H2EDTA=
  1  .0         .0        .0      .0        PuOx+ HEDTA=-
  1  .0         .0        .0      .0        PuOx+ EDTA==
  1  .0         .0        .0      .0        PuOx+ AmEDTA-
  1  .0         .0        .0      .0        PuOx+ NpO2Cit=
```

```
 1  .0        .0       .0     .0        PuOx+ NpO2EDTA==-
 1  .0        .0       .0     .0        PuOx+ NpO2Ox-
 1  .0        .0       .0     .0        PuOx+ U(OH)4(CO3)2==
 1  .0        .0       .0     .0        PuOx+ U(CO3)5===
 1  .0        .0       .0     .0        PuOx+ U(SO4)3=
 1  .0        .0       .0     .0        PuOx+ Am(CO3)4==-  [NEW]
 1  .0        .0       .0     .0        PuOx+ Am(SO4)2-    [NEW]
 1  .0        .0       .0     .0        PuOx+ NpO2H2EDTA-  [NEW]
 1  .0        .0       .0     .0        PuOx+ CaCit-
 1  .0        .0       .0     .0        PuOx+ CaEDTA=
 1  .0        .0       .0     .0        PuOx+ UnuAn#2-
 1  .0        .0       .0     .0        PuOx+ UnuAn#3-
 1  .0        .0       .0     .0        PuOx+ UnuAn#4-
 1  .0        .0       .0     .0        PuOx+ U(OH)2(CO3)2=
 1  .0        .0       .0     .0        PuOx+ MgCit-
 1  .0        .0       .0     .0        PuOx+ MgEDTA=
 1  .0        .0       .0     .0        PuOx+ NpO2HEDTA=  [NEW]

[ThLac2++ INTERACTIONS ADDED]
 1  .5058    1.74      .0    0.225      ThLac2++ Cl-       Moore et al 1999
 2  .0        .0       .0     .0        ThLac2++ SO4=
 1  .0        .0       .0     .0        ThLac2++ HSO4-
 1  .0        .0       .0     .0        ThLac2++ OH-
 1  .0        .0       .0     .0        ThLac2++ HCO3-
 2  .0        .0       .0     .0        ThLac2++ CO3=
 1  .0        .0       .0     .0        ThLac2++ B(OH)4-
 1  .0        .0       .0     .0        ThLac2++ B3O3(OH)4-
 2  .0        .0       .0     .0        ThLac2++ B4O5(OH)4=
 1  .0        .0       .0     .0        ThLac2++ Br-
 1  .0        .0       .0     .0        ThLac2++ Am(CO3)2-
 3  .0        .0       .0     .0        ThLac2++ Am(CO3)3=-
 1  .0        .0       .0     .0        ThLac2++ ClO4-
 1  .0        .0       .0     .0        ThLac2++ NpO2(OH)2-
 1  .0        .0       .0     .0        ThLac2++ NpO2CO3-
 3  .0        .0       .0     .0        ThLac2++ NpO2(CO3)2=-
 3  .0        .0       .0     .0        ThLac2++ NpO2(CO3)3==-
 1  .0        .0       .0     .0        ThLac2++ H2PO4-
 2  .0        .0       .0     .0        ThLac2++ HPO4=
 3  .0        .0       .0     .0        ThLac2++ PO4=-
 2  .0        .0       .0     .0        ThLac2++ Th(SO4)3=
 1  .0        .0       .0     .0        ThLac2++ Th(OH)3(CO3)-
 3  .0        .0       .0     .0        ThLac2++ Th(CO3)5===
 1  .0        .0       .0     .0        ThLac2++ HOx-
 2  .0        .0       .0     .0        ThLac2++ Ox=
 1  .0        .0       .0     .0        ThLac2++ Ac-
 1  .0        .0       .0     .0        ThLac2++ Lac-
 1  .0        .0       .0     .0        ThLac2++ H2Cit-
 2  .0        .0       .0     .0        ThLac2++ HCit=
```

```
  3  .0         .0        .0      .0        ThLac2++ Cit=-
  1  .0         .0        .0      .0        ThLac2++ H3EDTA-
  2  .0         .0        .0      .0        ThLac2++ H2EDTA=
  3  .0         .0        .0      .0        ThLac2++ HEDTA=-
  3  .0         .0        .0      .0        ThLac2++ EDTA==
  1  .0         .0        .0      .0        ThLac2++ AmEDTA-
  2  .0         .0        .0      .0        ThLac2++ NpO2Cit=
  3  .0         .0        .0      .0        ThLac2++ NpO2EDTA==-
  1  .0         .0        .0      .0        ThLac2++ NpO2Ox-
  3  .0         .0        .0      .0        ThLac2++ U(OH)4(CO3)2==
  3  .0         .0        .0      .0        ThLac2++ U(CO3)5===
  2  .0         .0        .0      .0        ThLac2++ U(SO4)3=
  3  .0         .0        .0      .0        ThLac2++ Am(CO3)4==-
  1  .0         .0        .0      .0        ThLac2++ Am(SO4)2-
  1  .0         .0        .0      .0        ThLac2++ NpO2H2EDTA-
  1  .0         .0        .0      .0        ThLac2++ CaCit-
  2  .0         .0        .0      .0        ThLac2++ CaEDTA=
  1  .0         .0        .0      .0        ThLac2++ UnuAn#2-
  1  .0         .0        .0      .0        ThLac2++ UnuAn#3-
  1  .0         .0        .0      .0        ThLac2++ UnuAn#4-
  2  .0         .0        .0      .0        ThLac2++ U(OH)2(CO3)2=
  1  .0         .0        .0      .0        ThLac2++ MgCit-
  2  .0         .0        .0      .0        ThLac2++ MgEDTA=
  2  .0         .0        .0      .0        ThLac2++ NpO2HEDTA=

  1 -.0833      .29       .0      .0987     CaAc+ Cl-           analogy w/Mg (ERG_org_memo)
  1  .0         .0        .0      .0        CaAc+ SO4=
  1  .0         .0        .0      .0        CaAc+ HSO4-
  1  .0         .0        .0      .0        CaAc+ OH-
  1  .0         .0        .0      .0        CaAc+ HCO3-
  1  .0         .0        .0      .0        CaAc+ CO3=
  1  .0         .0        .0      .0        CaAc+ B(OH)4-
  1  .0         .0        .0      .0        CaAc+ B3O3(OH)4-
  1  .0         .0        .0      .0        CaAc+ B4O5(OH)4=
  1  .0         .0        .0      .0        CaAc+ Br-
  1  .0         .0        .0      .0        CaAc+ Am(CO3)2-
  1  .0         .0        .0      .0        CaAc+ Am(CO3)3=-
  1  .0         .0        .0      .0        CaAc+ ClO4-
  1  .0         .0        .0      .0        CaAc+ NpO2(OH)2-
  1  .0         .0        .0      .0        CaAc+ NpO2CO3-
  1  .0         .0        .0      .0        CaAc+ NpO2(CO3)2=-
  1  .0         .0        .0      .0        CaAc+ NpO2(CO3)3==-
  1  .0         .0        .0      .0        CaAc+ H2PO4-
  1  .0         .0        .0      .0        CaAc+ HPO4=
  1  .0         .0        .0      .0        CaAc+ PO4=-
  1  .0         .0        .0      .0        CaAc+ Th(SO4)3=
  1  .0         .0        .0      .0        CaAc+ Th(OH)3(CO3)-
  1  .0         .0        .0      .0        CaAc+ Th(CO3)5===
```

```
1  .0        .0        .0      .0        CaAc+ HOx-
1  .0        .0        .0      .0        CaAc+ Ox=
1  .0        .0        .0      .0        CaAc+ Ac-
1  .0        .0        .0      .0        CaAc+ Lac-
1  .0        .0        .0      .0        CaAc+ H2Cit-
1  .0        .0        .0      .0        CaAc+ HCit=
1  .0        .0        .0      .0        CaAc+ Cit=-
1  .0        .0        .0      .0        CaAc+ H3EDTA-
1  .0        .0        .0      .0        CaAc+ H2EDTA=
1  .0        .0        .0      .0        CaAc+ HEDTA=-
1  .0        .0        .0      .0        CaAc+ EDTA==
1  .0        .0        .0      .0        CaAc+ AmEDTA-
1  .0        .0        .0      .0        CaAc+ NpO2Cit=
1  .0        .0        .0      .0        CaAc+ NpO2EDTA==-
1  .0        .0        .0      .0        CaAc+ NpO2Ox-
1  .0        .0        .0      .0        CaAc+ U(OH)4(CO3)2==
1  .0        .0        .0      .0        CaAc+ U(CO3)5===
1  .0        .0        .0      .0        CaAc+ U(SO4)3=
1  .0        .0        .0      .0        CaAc+ Am(CO3)4==-   [NEW]
1  .0        .0        .0      .0        CaAc+ Am(SO4)2-     [NEW]
1  .0        .0        .0      .0        CaAc+ NpO2H2EDTA-   [NEW]
1  .0        .0        .0      .0        CaAc+ CaCit-
1  .0        .0        .0      .0        CaAc+ CaEDTA=
1  .0        .0        .0      .0        CaAc+ UnuAn#2-
1  .0        .0        .0      .0        CaAc+ UnuAn#3-
1  .0        .0        .0      .0        CaAc+ UnuAn#4-
1  .0        .0        .0      .0        CaAc+ U(OH)2(CO3)2=
1  .0        .0        .0      .0        CaAc+ MgCit-
1  .0        .0        .0      .0        CaAc+ MgEDTA=
1  .0        .0        .0      .0        CaAc+ NpO2HEDTA=   [NEW]

1  .0        .0        .0      .0        CaLac+ Cl-
1  .0        .0        .0      .0        CaLac+ SO4=
1  .0        .0        .0      .0        CaLac+ HSO4-
1  .0        .0        .0      .0        CaLac+ OH-
1  .0        .0        .0      .0        CaLac+ HCO3-
1  .0        .0        .0      .0        CaLac+ CO3=
1  .0        .0        .0      .0        CaLac+ B(OH)4-
1  .0        .0        .0      .0        CaLac+ B3O3(OH)4-
1  .0        .0        .0      .0        CaLac+ B4O5(OH)4=
1  .0        .0        .0      .0        CaLac+ Br-
1  .0        .0        .0      .0        CaLac+ Am(CO3)2-
1  .0        .0        .0      .0        CaLac+ Am(CO3)3=-
1  .0        .0        .0      .0        CaLac+ ClO4-
1  .0        .0        .0      .0        CaLac+ NpO2(OH)2-
1  .0        .0        .0      .0        CaLac+ NpO2CO3-
1  .0        .0        .0      .0        CaLac+ NpO2(CO3)2=-
1  .0        .0        .0      .0        CaLac+ NpO2(CO3)3==-
```

```
1  .0        .0       .0     .0       CaLac+ H2PO4-
1  .0        .0       .0     .0       CaLac+ HPO4=
1  .0        .0       .0     .0       CaLac+ PO4=-
1  .0        .0       .0     .0       CaLac+ Th(SO4)3=
1  .0        .0       .0     .0       CaLac+ Th(OH)3(CO3)-
1  .0        .0       .0     .0       CaLac+ Th(CO3)5===
1  .0        .0       .0     .0       CaLac+ HOx-
1  .0        .0       .0     .0       CaLac+ Ox=
1  .0        .0       .0     .0       CaLac+ Ac-
1  .0        .0       .0     .0       CaLac+ Lac-
1  .0        .0       .0     .0       CaLac+ H2Cit-
1  .0        .0       .0     .0       CaLac+ HCit=
1  .0        .0       .0     .0       CaLac+ Cit=-
1  .0        .0       .0     .0       CaLac+ H3EDTA-
1  .0        .0       .0     .0       CaLac+ H2EDTA=
1  .0        .0       .0     .0       CaLac+ HEDTA=-
1  .0        .0       .0     .0       CaLac+ EDTA==
1  .0        .0       .0     .0       CaLac+ AmEDTA-
1  .0        .0       .0     .0       CaLac+ NpO2Cit=
1  .0        .0       .0     .0       CaLac+ NpO2EDTA==-
1  .0        .0       .0     .0       CaLac+ NpO2Ox-
1  .0        .0       .0     .0       CaLac+ U(OH)4(CO3)2==
1  .0        .0       .0     .0       CaLac+ U(CO3)5===
1  .0        .0       .0     .0       CaLac+ U(SO4)3=
1  .0        .0       .0     .0       CaLac+ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       CaLac+ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       CaLac+ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       CaLac+ CaCit-
1  .0        .0       .0     .0       CaLac+ CaEDTA=
1  .0        .0       .0     .0       CaLac+ UnuAn#2-
1  .0        .0       .0     .0       CaLac+ UnuAn#3-
1  .0        .0       .0     .0       CaLac+ UnuAn#4-
1  .0        .0       .0     .0       CaLac+ U(OH)2(CO3)2=
1  .0        .0       .0     .0       CaLac+ MgCit-
1  .0        .0       .0     .0       CaLac+ MgEDTA=
1  .0        .0       .0     .0       CaLac+ NpO2HEDTA=   [NEW]

1 -.0833     .29      .0     .0987    MgAc+ Cl-            ERG_org_memo
1  .0        .0       .0     .0       MgAc+ SO4=
1  .0        .0       .0     .0       MgAc+ HSO4-
1  .0        .0       .0     .0       MgAc+ OH-
1  .0        .0       .0     .0       MgAc+ HCO3-
1  .0        .0       .0     .0       MgAc+ CO3=
1  .0        .0       .0     .0       MgAc+ B(OH)4-
1  .0        .0       .0     .0       MgAc+ B3O3(OH)4-
1  .0        .0       .0     .0       MgAc+ B4O5(OH)4=
1  .0        .0       .0     .0       MgAc+ Br-
1  .0        .0       .0     .0       MgAc+ Am(CO3)2-
```

```
1  .0         .0        .0      .0       MgAc+ Am(CO3)3=-
1  .0         .0        .0      .0       MgAc+ ClO4-
1  .0         .0        .0      .0       MgAc+ NpO2(OH)2-
1  .0         .0        .0      .0       MgAc+ NpO2CO3-
1  .0         .0        .0      .0       MgAc+ NpO2(CO3)2=-
1  .0         .0        .0      .0       MgAc+ NpO2(CO3)3==-
1  .0         .0        .0      .0       MgAc+ H2PO4-
1  .0         .0        .0      .0       MgAc+ HPO4=
1  .0         .0        .0      .0       MgAc+ PO4=-
1  .0         .0        .0      .0       MgAc+ Th(SO4)3=
1  .0         .0        .0      .0       MgAc+ Th(OH)3(CO3)-
1  .0         .0        .0      .0       MgAc+ Th(CO3)5===
1  .0         .0        .0      .0       MgAc+ HOx-
1  .0         .0        .0      .0       MgAc+ Ox=
1  .0         .0        .0      .0       MgAc+ Ac-
1  .0         .0        .0      .0       MgAc+ Lac-
1  .0         .0        .0      .0       MgAc+ H2Cit-
1  .0         .0        .0      .0       MgAc+ HCit=
1  .0         .0        .0      .0       MgAc+ Cit=-
1  .0         .0        .0      .0       MgAc+ H3EDTA-
1  .0         .0        .0      .0       MgAc+ H2EDTA=
1  .0         .0        .0      .0       MgAc+ HEDTA=-
1  .0         .0        .0      .0       MgAc+ EDTA==
1  .0         .0        .0      .0       MgAc+ AmEDTA-
1  .0         .0        .0      .0       MgAc+ NpO2Cit=
1  .0         .0        .0      .0       MgAc+ NpO2EDTA==-
1  .0         .0        .0      .0       MgAc+ NpO2Ox-
1  .0         .0        .0      .0       MgAc+ U(OH)4(CO3)2==
1  .0         .0        .0      .0       MgAc+ U(CO3)5===
1  .0         .0        .0      .0       MgAc+ U(SO4)3=
1  .0         .0        .0      .0       MgAc+ Am(CO3)4==-   [NEW]
1  .0         .0        .0      .0       MgAc+ Am(SO4)2-     [NEW]
1  .0         .0        .0      .0       MgAc+ NpO2H2EDTA-   [NEW]
1  .0         .0        .0      .0       MgAc+ CaCit-
1  .0         .0        .0      .0       MgAc+ CaEDTA=
1  .0         .0        .0      .0       MgAc+ UnuAn#2-
1  .0         .0        .0      .0       MgAc+ UnuAn#3-
1  .0         .0        .0      .0       MgAc+ UnuAn#4-
1  .0         .0        .0      .0       MgAc+ U(OH)2(CO3)2=
1  .0         .0        .0      .0       MgAc+ MgCit-
1  .0         .0        .0      .0       MgAc+ MgEDTA=
1  .0         .0        .0      .0       MgAc+ NpO2HEDTA=   [NEW]

1  .0         .0        .0      .0       MgLac+ Cl-
1  .0         .0        .0      .0       MgLac+ SO4=
1  .0         .0        .0      .0       MgLac+ HSO4-
1  .0         .0        .0      .0       MgLac+ OH-
1  .0         .0        .0      .0       MgLac+ HCO3-
```

```
1  .0         .0        .0       .0        MgLac+ CO3=
1  .0         .0        .0       .0        MgLac+ B(OH)4-
1  .0         .0        .0       .0        MgLac+ B3O3(OH)4-
1  .0         .0        .0       .0        MgLac+ B4O5(OH)4=
1  .0         .0        .0       .0        MgLac+ Br-
1  .0         .0        .0       .0        MgLac+ Am(CO3)2-
1  .0         .0        .0       .0        MgLac+ Am(CO3)3=-
1  .0         .0        .0       .0        MgLac+ ClO4-
1  .0         .0        .0       .0        MgLac+ NpO2(OH)2-
1  .0         .0        .0       .0        MgLac+ NpO2CO3-
1  .0         .0        .0       .0        MgLac+ NpO2(CO3)2=-
1  .0         .0        .0       .0        MgLac+ NpO2(CO3)3==-
1  .0         .0        .0       .0        MgLac+ H2PO4-
1  .0         .0        .0       .0        MgLac+ HPO4=
1  .0         .0        .0       .0        MgLac+ PO4=-
1  .0         .0        .0       .0        MgLac+ Th(SO4)3=
1  .0         .0        .0       .0        MgLac+ Th(OH)3(CO3)-
1  .0         .0        .0       .0        MgLac+ Th(CO3)5===
1  .0         .0        .0       .0        MgLac+ HOx-
1  .0         .0        .0       .0        MgLac+ Ox=
1  .0         .0        .0       .0        MgLac+ Ac-
1  .0         .0        .0       .0        MgLac+ Lac-
1  .0         .0        .0       .0        MgLac+ H2Cit-
1  .0         .0        .0       .0        MgLac+ HCit=
1  .0         .0        .0       .0        MgLac+ Cit=-
1  .0         .0        .0       .0        MgLac+ H3EDTA-
1  .0         .0        .0       .0        MgLac+ H2EDTA=
1  .0         .0        .0       .0        MgLac+ HEDTA=-
1  .0         .0        .0       .0        MgLac+ EDTA==
1  .0         .0        .0       .0        MgLac+ AmEDTA-
1  .0         .0        .0       .0        MgLac+ NpO2Cit=
1  .0         .0        .0       .0        MgLac+ NpO2EDTA==-
1  .0         .0        .0       .0        MgLac+ NpO2Ox-
1  .0         .0        .0       .0        MgLac+ U(OH)4(CO3)2==
1  .0         .0        .0       .0        MgLac+ U(CO3)5===
1  .0         .0        .0       .0        MgLac+ U(SO4)3=
1  .0         .0        .0       .0        MgLac+ Am(CO3)4==-   [NEW]
1  .0         .0        .0       .0        MgLac+ Am(SO4)2-     [NEW]
1  .0         .0        .0       .0        MgLac+ NpO2H2EDTA-   [NEW]
1  .0         .0        .0       .0        MgLac+ CaCit-
1  .0         .0        .0       .0        MgLac+ CaEDTA=
1  .0         .0        .0       .0        MgLac+ UnuAn#2-
1  .0         .0        .0       .0        MgLac+ UnuAn#3-
1  .0         .0        .0       .0        MgLac+ UnuAn#4-
1  .0         .0        .0       .0        MgLac+ U(OH)2(CO3)2=
1  .0         .0        .0       .0        MgLac+ MgCit-
1  .0         .0        .0       .0        MgLac+ MgEDTA=
1  .0         .0        .0       .0        MgLac+ NpO2HEDTA=  [NEW]
```

```
1  .0        .0       .0     .0       UnuCat#1+ Cl-
1  .0        .0       .0     .0       UnuCat#1+ SO4=
1  .0        .0       .0     .0       UnuCat#1+ HSO4-
1  .0        .0       .0     .0       UnuCat#1+ OH-
1  .0        .0       .0     .0       UnuCat#1+ HCO3-
1  .0        .0       .0     .0       UnuCat#1+ CO3=
1  .0        .0       .0     .0       UnuCat#1+ B(OH)4-
1  .0        .0       .0     .0       UnuCat#1+ B3O3(OH)4-
1  .0        .0       .0     .0       UnuCat#1+ B4O5(OH)4=
1  .0        .0       .0     .0       UnuCat#1+ Br-
1  .0        .0       .0     .0       UnuCat#1+ Am(CO3)2-
1  .0        .0       .0     .0       UnuCat#1+ Am(CO3)3=-
1  .0        .0       .0     .0       UnuCat#1+ ClO4-
1  .0        .0       .0     .0       UnuCat#1+ NpO2(OH)2-
1  .0        .0       .0     .0       UnuCat#1+ NpO2CO3-
1  .0        .0       .0     .0       UnuCat#1+ NpO2(CO3)2=-
1  .0        .0       .0     .0       UnuCat#1+ NpO2(CO3)3==-
1  .0        .0       .0     .0       UnuCat#1+ H2PO4-
1  .0        .0       .0     .0       UnuCat#1+ HPO4=
1  .0        .0       .0     .0       UnuCat#1+ PO4=-
1  .0        .0       .0     .0       UnuCat#1+ Th(SO4)3=
1  .0        .0       .0     .0       UnuCat#1+ Th(OH)3(CO3)-
1  .0        .0       .0     .0       UnuCat#1+ Th(CO3)5===
1  .0        .0       .0     .0       UnuCat#1+ HOx-
1  .0        .0       .0     .0       UnuCat#1+ Ox=
1  .0        .0       .0     .0       UnuCat#1+ Ac-
1  .0        .0       .0     .0       UnuCat#1+ Lac-
1  .0        .0       .0     .0       UnuCat#1+ H2Cit-
1  .0        .0       .0     .0       UnuCat#1+ HCit=
1  .0        .0       .0     .0       UnuCat#1+ Cit=-
1  .0        .0       .0     .0       UnuCat#1+ H3EDTA-
1  .0        .0       .0     .0       UnuCat#1+ H2EDTA=
1  .0        .0       .0     .0       UnuCat#1+ HEDTA=-
1  .0        .0       .0     .0       UnuCat#1+ EDTA==
1  .0        .0       .0     .0       UnuCat#1+ AmEDTA-
1  .0        .0       .0     .0       UnuCat#1+ NpO2Cit=
1  .0        .0       .0     .0       UnuCat#1+ NpO2EDTA==-
1  .0        .0       .0     .0       UnuCat#1+ NpO2Ox-
1  .0        .0       .0     .0       UnuCat#1+ U(OH)4(CO3)2==
1  .0        .0       .0     .0       UnuCat#1+ U(CO3)5===
1  .0        .0       .0     .0       UnuCat#1+ U(SO4)3=
1  .0        .0       .0     .0       UnuCat#1+ Am(CO3)4==-   [NEW]
1  .0        .0       .0     .0       UnuCat#1+ Am(SO4)2-     [NEW]
1  .0        .0       .0     .0       UnuCat#1+ NpO2H2EDTA-   [NEW]
1  .0        .0       .0     .0       UnuCat#1+ CaCit-
1  .0        .0       .0     .0       UnuCat#1+ CaEDTA=
1  .0        .0       .0     .0       UnuCat#1+ UnuAn#2-
```

```
  1  .0        .0       .0     .0       UnuCat#1+ UnuAn#3-
  1  .0        .0       .0     .0       UnuCat#1+ UnuAn#4-
  1  .0        .0       .0     .0       UnuCat#1+ U(OH)2(CO3)2=
  1  .0        .0       .0     .0       UnuCat#1+ MgCit-
  1  .0        .0       .0     .0       UnuCat#1+ MgEDTA=
  1  .0        .0       .0     .0       UnuCat#1+ NpO2HEDTA=   [NEW]

 -.012  .07  .07 0 .036 0 0 .1 0 .42 .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Na         1 w/2-39) theta  Th++++
RFSMMN, Am+++ FK98
       .032    0 0 .005 0 0 .1 0 .42  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  K:         2 w/3-39) theta  Th++++,
Am+++ by analogy w/Na+ (RFSMMN, FK98)
            .007 0 .092 0 0 .2 0 .60 -.014  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -.196 0 0 0 0 0 0 0 0 0 0  Ca:       3 w/4-39) theta
Am+++ FK98, Th++++ by analogy w/Mg++ (RFSMMN)
                 0 .10  0 0 .2 0 .60 -.014  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -.196 0 0 0 0 0 0 0 0 0 0  Mg:       4 w/5-39) theta
Th++++ RFSMMN, Am by analogy w/Ca++ (FK98)
                      0 0 0 0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgOH:     5 w/6-39) theta
                        0 0 0 0 .60 .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H :       6 w/7-39) theta  Roy92

      0 0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgB(OH)4: 7 w/8-39) theta
        0 0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaB(OH)4: 8 w/9-39) theta
          0   0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am+++:    9 w/10-39) theta
              0  0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmCO3+:  10 w/11-39) theta
                 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th++++:  11 w/12-39) theta
                      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmCl++:  12 w/13-39) theta  replaces Pu+++
                        0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2+:   13 w/14-39) theta
                          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U++++:   14 w/15-39) theta
                            0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UOH+++:  15 w/16-39) theta
                              0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UAc+++:  16 w/17-39) theta
                                0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThOx++   17 w/18-39) theta
                                  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmAc++   18 w/19-39) theta
                                    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmLac++  19 w/20-39) theta
                                      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmOx+    20 w/21-39) theta
                                        0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UCit+    21 w/22-39) theta
                                          0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ULac+++  22 w/23-39) theta
                                            0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UOx++    23 w/24-39) theta
                                              0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThAc+++  24 w/25-39) theta
                                                0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThCit+   25 w/26-39) theta
                                                  0 0 0 0 0 0 0 0 0 0 0 0 0  ThLac+++ 26 w/27-39) theta
                                                    0 0 0 0 0 0 0 0 0 0 0 0  AmOH++   27 w/28-39) theta
                                                      0 0 0 0 0 0 0 0 0 0 0  Am(OH)2+ 28 w/29-39) theta
                                                        0 0 0 0 0 0 0 0 0 0  AmCl2+   29 w/30-39) theta replaces PuCO3+
                                                          0 0 0 0 0 0 0 0 0  AmSO4+   30 w/31-39) theta replaces PuOH++
                                                            0 0 0 0 0 0 0 0  Pu(OH)2+ 31 w/32-39) theta
                                                              0 0 0 0 0 0 0  ThAc2++    32 w/33-39)theta replaces PuAc++
                                                                0 0 0 0 0 0  PuOx+    33 w/34-39) theta
                                                                  0 0 0 0 0  ThLac2++ 34 w/35-39)theta replaces PuLac++
                                                                    0 0 0 0  CaAc+    35 w/36-39) theta
                                                                      0 0 0  CaLac+   36 w/37-39) theta
```

```
                                                                        0 0  MgAc+    37 w/38-39) theta
                                                                          0  MgLac+   38 w/39-39) theta

.02 -.006 -.05  .03 -.02 -.065  .12  .074 0 0 0     0 -.24 -.21 -.26 -.26 .1 0 0  0 0 1.8 0 0 -.09 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                    0 0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 Cl, Th
FR99, Np FNK95
        0 -.013 .01  .02 -.012  .10   .12 0 0 0     0    0    0    0    0  0 0 0  0 0   0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                    0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 SO4
              0   0    0     0    0     0 0 0 0     0    0    0    0    0  0 0 0  0 0   0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                    0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 HSO4
                  0  .10     0    0     0 0 0 0 -.032    0    0    0    0  0 0 0  0 0   0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                    0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 OH
                    -.04     0 -.10 -.087 0 0 0  .095    0    0    0    0  0 0 0  0 0   0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0
                                                                                    0 0 0 0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 HCO3

      0 0 0 0 0 0 .21 0 0 0  -1.9 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 CO3, Np
Novak et al 1997
        0 0 0 0 0   0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B(OH)4
          0 0 0 0   0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B3O3(OH)4
            0 0 0   0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 B4O5(OH)4
              0 0   0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Br
                0   0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(CO3)2-
                    0 0 0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Am(CO3)3=-
                      0 0 0     0 0 0 0 0 0  5.5   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ClO4-, Th
FRSMHC97
                        0 0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2(OH)2-
                          0     0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC-
                                0 0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC2=-
                                  0 0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpC3==-
                                    0 0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2PO4-
                                      0 0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HPO4=
                                        0 0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 PO4=-
                                          0    0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(SO4)=
                                               0   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(OH)3CO3-
                                                   0 0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Th(CO3)5===
                                                     0 0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HOx-
                                                       0 0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ox=
                                                         0    0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Ac-
                                                              0     0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Lac-
                                                                    0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2Cit-
                                                                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HCit=
                                                                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 Cit=-
                                                                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H3EDTA-
                                                                       0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H2EDTA=
                                                                         0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 HEDTA=-
                                                                           0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 EDTA==
                                                                             0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 AmEDTA-
                                                                               0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2Cit=
```

```
                                                                                 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2EDTA==-
                                                                                   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 NpO2Ox-
                                                                                     0 0 0 0 0 0 0 0 0 0 0 0 0 0 U(OH)3CO3-
                                                                                       0 0 0 0 0 0 0 0 0 0 0 0 0 U(CO3)5===
                                                                                         0 0 0 0 0 0 0 0 0 0 0 0 U(SO4)3=
                                                                                           0 0 0 0 0 0 0 0 0 0 0 Am(CO3)4==-
                                                                                             0 0 0 0 0 0 0 0 0 0 Am(SO4)2-
                                                                                               0 0 0 0 0 0 0 0 0 NpO2H2EDTA-
                                                                                                 0 0 0 0 0 0 0 0 CaCit-
                                                                                                   0 0 0 0 0 0 0 CaEDTA=
                                                                                                     0 0 0 0 0 0 UnuAn#2-
                                                                                                       0 0 0 0 0 UnuAn#3-
                                                                                                         0 0 0 0 UnuAn#4-
                                                                                                           0 0 0 U(OH)2(CO3)2=
                                                                                                             0 0 MgCit-
                                                                                                               0 MgEDTA=

 -.0018 -.010     .0 0 -.003 .003 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-K+:anions psi
  -.007 -.055     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Ca++:
  -.012 -.015     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Mg++:
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-MgOH+:
  -.004    .0 -.0129 0   .0   .0 0 0 0 0 0 0 -.016 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-H+:
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-MgB(OH)4+
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-CaB(OH)4+
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Am+++
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmCO3+
    .21    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Th++++ RFSMMN
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmCl++
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-NpO2++
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-U++++
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-UOH+++
     .0    .0     .0 0   .0   .0 0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-UAc+++
```

```
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThOx++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmAc++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmLac++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmOx+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-UCit+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ULac+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-UOx++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThAc+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThCit+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThLac+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmOH++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Am(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmCl2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-AmSO4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-Pu(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThAc2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-PuOx+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-ThLac2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-CaAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-CaLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-MgAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-MgLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Na+-UnuCat#1+
```

```
 -.025      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Ca:
 -.022  -.048      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Mg:
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-MgOH:
 -.011   .197 -.0265 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-H :
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-MgB(OH)4+
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-CaB(OH)4+
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Am+++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmCO3+
    .21     .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Th++++ analogy w/Na+ (RFSMMN)
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmCl++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-NpO2++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-U++++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-UOH+++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-UAc+++
    .0      .0      .0 0    0    0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThOx++
    .0      .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmAc++
    .0      .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmLac++
    .0      .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmOx+
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-UCit+
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ULac+++
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-UOx++
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThAc+++
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThCit+
     .0     .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThLac+++
```

```
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmOH++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Am(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmCl2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-AmSO4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-Pu(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThAc2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-PuOx+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-ThLac2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-CaAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-CaLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-MgAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-MgLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
K+-UnuCat#1+

  -.012  .024      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Mg:
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-MgOH:
  -.015     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-H  :
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-MgB(OH)4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Ca++B(OH)4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Am+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmCO3+
    .21     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Th++++, analogy w/Mg++ (RFSMMN)
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmCl++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-NpO2++
```

```
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-U++++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-UOH+++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-UAc+++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThOx++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmAc++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmLac++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmOx+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-UCit+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ULac+++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-UOx++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThAc+++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThCit+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThLac+++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmOH++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Am(OH)2+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmCl2+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-AmSO4+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-Pu(OH)2+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThAc2++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-PuOx+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-ThLac2++
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-CaAc+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca++-CaLac+
    .0     .0      .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca+-MgAc+
```

```
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca+-MgLac+
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Ca+-UnuCat#1+

   .028    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-MgOH:
  -.011    .0 -.0178 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-H :
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-MgB(OH)4+
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-CaB(OH)4+
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-Am+++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmCO3+
    .21    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-Th++++ RSFMMN
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmCl++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-NpO2++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-U++++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-UOH+++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-UAc+++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThOx++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmAc++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmLac++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmOx+
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-UCit+
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ULac+++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-UOx++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThAc+++
     .0    .0      .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThCit+
```

```
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThLac+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmOH++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-Am(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmCl2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-AmSO4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-Pu(OH)2+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThAc2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-PuOx+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-ThLac2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-CaAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-CaLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-MgAc+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-MgLac+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Mg++-UnuCat#1+

     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-H  :
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-MgB(OH)4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-CaB(OH)4+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-Am+++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmCO3+
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-Th++++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmCl++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-NpO2++
     .0     .0      .0 0    .0    .0  0 0 0 0 0 0   .0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-U++++
```

```
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-UOH+++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-UAc+++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThOx++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmAc++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmLac++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmOx+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-UCit+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ULac+++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-UOx++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThAc+++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThCit+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThLac+++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmOH++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-Am(OH)2+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmCl2+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-AmSO4+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-Pu(OH)2+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThAc2++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-PuOx+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-ThLac2++
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-CaAc+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-CaLac+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-MgAc+
     .0     .0       .0 0    .0    .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-MgLac+
```

```
     .0    .0     .0 0   .0   .0  0 0 0 0 0 0  .0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgOH+-UnuCat#1+

     .0 0 0 0 0 0 0 0 0 0 0 0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-MgB(OH)4+
     .0 0 0 0 0 0 0 0 0 0 0 0     0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 H+-CaB(OH)4+
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[AmCl++ INTERACTIONS ADDED]
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[AmCl2+ INTERACTIONS ADDED]
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 .0014    .0 -.018 -.004 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- SO4:(vs Cations) psi
 -.006    .0    .0    .0 0 .013 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- HSO4:
 -.006 -.006 -.025    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- OH:
 -.015    .0    .0 -.096 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- HCO3:
 .0085  .004    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- CO3:
-.0073    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- B(OH)4:
 -.024    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- B3O3(OH)4:
  .026    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- B4O5(OH)4:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Br:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Am(CO3)2:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Am(CO3)3: FK98
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- ClO4-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- NpO2(OH)2-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- NpO2CO3-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- NpO2(CO3)2=-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- NpO2(CO3)3==-:
    .0   -.01   .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- H2PO4-: PS76
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- HPO4=:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- PO4=-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Th(SO4)3=:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Th(OH)3CO3-:
   .30   .30    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Th(CO3)5===: FR99, K+ by
analogy w/Na+
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- HOx-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cl- Ox=
```

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  .01029    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  Ac-       NBC96(Na+), K+ NOT by
analogy w/Na+
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  Lac-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  H2Cit=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  HCit=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  Cit=-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  H3EDTA-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  H2EDTA=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  HEDTA=-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  EDTA==
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  AmEDTA-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  NpO2Cit=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  NpO2EDTA==-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  NpO2Ox-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  U(OH)3CO3-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  U(CO3)5===
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  U(SO4)3=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  Am(CO3)4==-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  Am(SO4)2-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  NpO2H2EDTA-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  CaCit-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  CaEDTA=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  UnuAn#2-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  UnuAn#3-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  UnuAn#4-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  U(OH)2(CO3)2=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  MgCit-
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  MgEDTA=
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Cl-  NpO2HEDTA=

 -.0094 -.0677    .0 -.0425 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= HSO4:
  -.009 -.050     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= OH:
  -.005     .0    .0 -.161 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= HCO3:
  -.005 -.009     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= CO3:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= B(OH)4:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= B3O3(OH)4:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= B4O5(OH)4:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= Br:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= Am(CO3)2:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= Am(CO3)3:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= ClO4-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= NpO2(OH)2-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= NpO2CO3-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= NpO2(CO3)2=-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= NpO2(CO3)3==-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= H2PO4-:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= HPO4=:
      .0    .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   SO4= PO4=-:
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  SO4= NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- OH:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HCO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CO3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B(OH)4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B3O3(OH)4:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- B4O5(OH)4:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Br-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(CO3)2-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- ClO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(OH)2-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2(CO3)3==-:
```

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   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2PO4-:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HPO4=:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- PO4=-:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(SO4)3=:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(OH)3CO3-:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Th(CO3)5===:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HOx-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Ox=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Ac-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Lac-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2Cit=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HCit=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Cit=-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H3EDTA-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- H2EDTA=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- HEDTA=-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- EDTA==
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- AmEDTA-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2Cit=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2EDTA==-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2Ox-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(OH)3CO3-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(CO3)5===
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(SO4)3=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(CO3)4==-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- Am(SO4)2-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2H2EDTA-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CaCit-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- CaEDTA=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#2-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#3-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- UnuAn#4-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- U(OH)2(CO3)2=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- MgCit-
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- MgEDTA=
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HSO4- NpO2HEDTA=

   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HCO3:
-.017   -.01     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CO3:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B(OH)4:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B3O3(OH)4:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- B4O5(OH)4:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Br:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(CO3)2:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(CO3)3:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- ClO4-:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(OH)2-:
   .0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2CO3-:
```

```
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(CO3)2=-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2(CO3)3==-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2PO4-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HPO4=:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- PO4=-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(SO4)3=:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(OH)3CO3-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Th(CO3)5===:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HOx-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Ox=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Ac-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Lac-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2Cit=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HCit=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Cit=-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H3EDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- H2EDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- HEDTA=-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- EDTA==
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- AmEDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2Cit=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2EDTA==-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2Ox-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(OH)3CO3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(CO3)5===
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(SO4)3=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(CO3)4==-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- Am(SO4)2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2H2EDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CaCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- CaEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- UnuAn#4-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- U(OH)2(CO3)2=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- MgCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- MgEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  OH- NpO2HEDTA=

   .002 .012    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-CO3:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B(OH)4:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B3O3(OH)4:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-B4O5(OH)4:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Br:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Am(CO3)2:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Am(CO3)3:
 -.010    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-ClO4-:
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(OH)2-:
```

```
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2CO3-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(CO3)2=-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2(CO3)3==-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2PO4-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HPO4=:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-PO4=-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(SO4)3=:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(OH)3CO3-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Th(CO3)5===:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HOx-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Ox=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Ac-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Lac-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2Cit=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HCit=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-Cit=-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H3EDTA-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-H2EDTA=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-HEDTA=-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-EDTA==
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-AmEDTA-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2Cit=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2EDTA==-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-NpO2Ox-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(OH)3CO3-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(CO3)5===
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3-U(SO4)3=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- Am(CO3)4==-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- Am(SO4)2-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- NpO2H2EDTA-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- CaCit-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- CaEDTA=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#2-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#3-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- UnuAn#4-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- U(OH)2(CO3)2=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- MgCit-
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- MgEDTA=
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCO3- NpO2HEDTA=

 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B(OH)4-:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B3O3(OH)4:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= B4O5(OH)4:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Br:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(CO3)2:
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(CO3)3:
-.024   .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= ClO4-:          NFRK95
 .0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(OH)2-:
```

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.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2CO3-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(CO3)2=-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2(CO3)3==-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2PO4-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HPO4=:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= PO4=-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(SO4)3=:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(OH)3CO3-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Th(CO3)5===:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HOx-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Ox=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Ac-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Lac-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2Cit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HCit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Cit=-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H3EDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= H2EDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= HEDTA=-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= EDTA==
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= AmEDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2Cit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2EDTA==-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2Ox-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(OH)3CO3-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(CO3)5===
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(SO4)3=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(CO3)4==-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= Am(SO4)2-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2H2EDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= CaCit-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= CaEDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#2-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#3-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= UnuAn#4-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= U(OH)2(CO3)2=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= MgCit-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= MgEDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO3= NpO2HEDTA=

.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- B3O3(OH)4:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- B4O5(OH)4:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Br:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Am(CO3)2:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- Am(CO3)3:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- ClO4-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2(OH)2-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)4- NpO2CO3-:
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2(CO3)3==-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)4- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- B4O5(OH)4:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- Br:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- Am(CO3)2:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- Am(CO3)3:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- ClO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- NpO2(OH)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- NpO2CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B3O3(OH)4- NpO2(CO3)3==-:
```

```
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2PO4-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HPO4=:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- PO4=-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(SO4)3=:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(OH)3CO3-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Th(CO3)5===:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HOx-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Ox=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Ac-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Lac-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2Cit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HCit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Cit=-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H3EDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- H2EDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- HEDTA=-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- EDTA==
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- AmEDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2Cit=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2EDTA==-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2Ox-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(OH)3CO3-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(CO3)5===
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(SO4)3=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Am(CO3)4==-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- Am(SO4)2-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2H2EDTA-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- CaCit-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- CaEDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#2-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#3-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- UnuAn#4-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- U(OH)2(CO3)2=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- MgCit-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- MgEDTA=
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B3O3(OH)4- NpO2HEDTA=

.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Br:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(CO3)2:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(CO3)3:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= ClO4-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NPO2(OH)2-
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2CO3-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2(CO3)2=-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2(CO3)3==-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2PO4-:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HPO4=:
.0     .0     .0     .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= PO4=-:
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B4O5(OH)4= NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(CO3)2:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(CO3)3:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- ClO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(OH)2-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2(CO3)3==-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HOx-
```

```
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Ox=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Ac-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Lac-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2Cit=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HCit=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Cit=-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H3EDTA-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- H2EDTA=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- HEDTA=-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- EDTA==
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- AmEDTA-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2Cit=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2EDTA==-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2Ox-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- U(OH)3CO3-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- U(CO3)5===
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- U(SO4)3=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(CO3)4==-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- Am(SO4)2-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2H2EDTA-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- CaCit-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- CaEDTA=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- UnuAn#2-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- UnuAn#3-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- UnuAn#4-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- U(OH)2(CO3)2=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- MgCit-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- MgEDTA=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Br- NpO2HEDTA=

.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Am(CO3)3:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- ClO4-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2(OH)2-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2CO3-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2(CO3)2=-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2(CO3)3==-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- H2PO4-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- HPO4=:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- PO4=-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Th(SO4)3=:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Th(OH)3CO3-:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Th(CO3)5===:
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- HOx-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Ox=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Ac-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Lac-
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- H2Cit=
.0    .0    .0    .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- HCit=
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)2- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- ClO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- NpO2(OH)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- NpO2CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- NpO2(CO3)3==-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=- AmEDTA-
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.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  NpO2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  NpO2EDTA==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  NpO2Ox-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  U(OH)3CO3-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  U(CO3)5===
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  U(SO4)3=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  Am(CO3)4==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  Am(SO4)2-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  NpO2H2EDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  CaCit-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  CaEDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  UnuAn#2-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  UnuAn#3-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  UnuAn#4-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  U(OH)2(CO3)2=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  MgCit-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  MgEDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)3=-  NpO2HEDTA=

.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2(OH)2-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2CO3-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2(CO3)2=-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2(CO3)3==-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  H2PO4-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  HPO4=:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  PO4=-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Th(SO4)3=:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Th(OH)3CO3-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Th(CO3)5===:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  HOx-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Ox=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Ac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Lac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  H2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  HCit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Cit=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  H3EDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  H2EDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  HEDTA=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  EDTA==
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  AmEDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2EDTA==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  NpO2Ox-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  U(OH)3CO3-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  U(CO3)5===
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  U(SO4)3=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4-  Am(CO3)4==-
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 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- Am(SO4)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- NpO2H2EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ClO4- NpO2HEDTA=

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2(CO3)2=-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2(CO3)3==-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- H2PO4-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- HPO4=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- PO4=-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Th(SO4)3=:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Th(OH)3CO3-:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Th(CO3)5===:
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- HOx-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Ox=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Ac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Lac-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- H2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- HCit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Cit=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- H3EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- H2EDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- HEDTA=-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- EDTA==
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- AmEDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2Cit=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2EDTA==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2Ox-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Am(CO3)4==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- Am(SO4)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2H2EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- U(OH)2(CO3)2=
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(OH)2- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2(CO3)2=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2(CO3)3==-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2CO3- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2(CO3)3==-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Th(SO4)3=:
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)2=- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2PO4-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HPO4=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- PO4=-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(SO4)3=:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(OH)3CO3-:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- H2EDTA=
```

```
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- HEDTA=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- EDTA==
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- AmEDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2EDTA==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2Ox-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(OH)3CO3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(CO3)5===
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(SO4)3=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Am(CO3)4==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- Am(SO4)2-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2H2EDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- CaCit-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- CaEDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#2-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- UnuAn#4-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- U(OH)2(CO3)2=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- MgCit-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- MgEDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2(CO3)3==- NpO2HEDTA=

.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HPO4=:
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- PO4=-:
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(SO4)3=:
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(OH)3CO3-:
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Th(CO3)5===:
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HOx-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Ox=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Ac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Lac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HCit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Cit=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H3EDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- H2EDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- HEDTA=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- EDTA==
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- AmEDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2EDTA==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2Ox-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(OH)3CO3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(CO3)5===
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- U(SO4)3=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Am(CO3)4==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- Am(SO4)2-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2PO4- NpO2H2EDTA-
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.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- CaCit-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- CaEDTA=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- UnuAn#2-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- UnuAn#3-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- UnuAn#4-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- U(OH)2(CO3)2=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- MgCit-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- MgEDTA=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2PO4- NpO2HEDTA=

.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  PO4=-:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Th(SO4)3=:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Th(OH)3CO3-:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Th(CO3)5===:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  HOx-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Ox=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Ac-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Lac-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  H2Cit=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  HCit=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Cit=-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  H3EDTA-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  H2EDTA=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  HEDTA=-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  EDTA==
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  AmEDTA-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  NpO2Cit=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  NpO2EDTA==-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  NpO2Ox-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  U(OH)3CO3-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  U(CO3)5===
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  U(SO4)3=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Am(CO3)4==-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  Am(SO4)2-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  NpO2H2EDTA-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  CaCit-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  CaEDTA=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  UnuAn#2-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  UnuAn#3-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  UnuAn#4-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  U(OH)2(CO3)2=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  MgCit-
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  MgEDTA=
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HPO4=  NpO2HEDTA=

.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=-  Th(SO4)3=:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=-  Th(OH)3CO3-:
.0      .0      .0      .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PO4=-  Th(CO3)5===:
```

```
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- HOx-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Ox=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Ac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Lac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- H2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- HCit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Cit=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- H3EDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- H2EDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- HEDTA=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- EDTA==
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- AmEDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- NpO2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- NpO2EDTA==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- NpO2Ox-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- U(OH)3CO3-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- U(CO3)5===
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- U(SO4)3=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Am(CO3)4==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- Am(SO4)2-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- NpO2H2EDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- CaCit-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- CaEDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- UnuAn#2-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- UnuAn#3-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- UnuAn#4-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- U(OH)2(CO3)2=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- MgCit-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- MgEDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  PO4=-- NpO2HEDTA=

.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Th(OH)3CO3-:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Th(CO3)5===:
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= HOx-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Ox=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Ac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Lac-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= H2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= HCit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Cit=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= H3EDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= H2EDTA=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= HEDTA=-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= EDTA==
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= AmEDTA-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= NpO2Cit=
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= NpO2EDTA==-
.0     .0     .0     .0 0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= NpO2Ox-
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)3= NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Th(CO3)5===:
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- HOx-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Ox=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Ac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Lac-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)3CO3- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4CO3- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4CO3- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4CO3- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4CO3- NpO2HEDTA=
```

```
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== HOx-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Ox=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Ac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Lac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== H2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== HCit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Cit=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== H3EDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== H2EDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== HEDTA=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== EDTA==
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== AmEDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== NpO2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== NpO2EDTA==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== NpO2Ox-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== U(OH)3CO3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== U(CO3)5===
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== U(SO4)3=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Am(CO3)4==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== Am(SO4)2-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== NpO2H2EDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== CaCit-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== CaEDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== UnuAn#2-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== UnuAn#3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== UnuAn#4-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== U(OH)2(CO3)2=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== MgCit-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== MgEDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(CO3)5=== NpO2HEDTA=

.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- Ox=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- Ac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- Lac-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- H2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- HCit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- Cit=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- H3EDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- H2EDTA=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- HEDTA=-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- EDTA==
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- AmEDTA-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- NpO2Cit=
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- NpO2EDTA==-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- NpO2Ox-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- U(OH)3CO3-
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- U(CO3)5===
.0     .0     .0     .0  0    .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HOx- U(SO4)3=
```

```
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- Am(CO3)4==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- Am(SO4)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- NpO2H2EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HOx- NpO2HEDTA=

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= Ac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= H2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= AmEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= Am(CO3)4==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= Am(SO4)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= NpO2H2EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ox= NpO2HEDTA=

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- Lac-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- H2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- HCit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- Cit=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Ac- H2EDTA=
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Ac- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- H2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- HCit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- Cit=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- H3EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- H2EDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Lac- NpO2HEDTA=
```

```
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- HCit=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- Cit=-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- H3EDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- H2EDTA=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- HEDTA=-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- EDTA==
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- AmEDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- NpO2Cit=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- NpO2EDTA==-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- NpO2Ox-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- U(OH)3CO3-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- U(CO3)5===
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- U(SO4)3=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- Am(CO3)4==-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- Am(SO4)2-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- NpO2H2EDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- CaCit-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- CaEDTA=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- UnuAn#2-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- UnuAn#3-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- UnuAn#4-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- U(OH)2(CO3)2=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- MgCit-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- MgEDTA=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Cit- NpO2HEDTA=

.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= Cit=-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= H3EDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= H2EDTA=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= HEDTA=-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= EDTA==
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= AmEDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= NpO2Cit=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= NpO2EDTA==-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= NpO2Ox-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= U(OH)3CO3-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= U(CO3)5===
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= U(SO4)3=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= Am(CO3)4==-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= Am(SO4)2-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= NpO2H2EDTA-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= CaCit-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= CaEDTA=
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= UnuAn#2-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= UnuAn#3-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= UnuAn#4-
.0       .0       .0       .0 0     .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HCit= U(OH)2(CO3)2=
```

```
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HCit= NpO2HEDTA=

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- H3EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- AmEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- Am(CO3)4==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- Am(SO4)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2H2EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- MgCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- MgEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Cit=- NpO2HEDTA=

.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- H2EDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- HEDTA=-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- EDTA==
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- AmEDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2Cit=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2EDTA==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2Ox-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(OH)3CO3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(CO3)5===
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(SO4)3=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- Am(CO3)4==-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- Am(SO4)2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2H2EDTA-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- CaCit-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- CaEDTA=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#2-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#3-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- UnuAn#4-
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- U(OH)2(CO3)2=
.0   .0   .0   .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- MgCit-
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3EDTA- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= HEDTA=-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2EDTA= NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- EDTA==
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HEDTA=- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== AmEDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2Cit=
```

```
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  EDTA== NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2Cit=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- UnuAn#4-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- U(OH)2(CO3)2=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- MgCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- MgEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmEDTA- NpO2HEDTA=

.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2EDTA==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2Ox-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(OH)3CO3-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(CO3)5===
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(SO4)3=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= Am(CO3)4==-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= Am(SO4)2-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2H2EDTA-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= CaCit-
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= CaEDTA=
.0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#2-
```

```
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Cit= NpO2HEDTA=

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- NpO2Ox-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- Am(CO3)4==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- Am(SO4)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- NpO2H2EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2EDTA=- NpO2HEDTA=

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(OH)3CO3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- Am(CO3)4==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- Am(SO4)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- NpO2H2EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#3-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- UnuAn#4-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- U(OH)2(CO3)2=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- MgCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- MgEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ox- NpO2HEDTA=

 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3-U(CO3)5===
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3-U(SO4)3=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- Am(CO3)4==-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- Am(SO4)2-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- NpO2H2EDTA-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- CaCit-
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- CaEDTA=
 .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#2-
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    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- UnuAn#4-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- U(OH)2(CO3)2=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- MgCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- MgEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)3CO3- NpO2HEDTA=

    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== U(SO4)3=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== Am(CO3)4==-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== Am(SO4)2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== NpO2H2EDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== CaCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== CaEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== UnuAn#4-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== U(OH)2(CO3)2=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== MgCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== MgEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(CO3)5=== NpO2HEDTA=

    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= Am(CO3)4==-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= Am(SO4)2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= NpO2H2EDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= CaCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= CaEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= UnuAn#4-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= U(OH)2(CO3)2=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= MgCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= MgEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)3= NpO2HEDTA=

[Am(CO3)4==- INTERACTIONS ADDED]
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- Am(SO4)2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- NpO2H2EDTA-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- CaCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- CaEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- UnuAn#2-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- UnuAn#3-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- UnuAn#4-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- U(OH)2(CO3)2=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- MgCit-
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- MgEDTA=
    .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(CO3)4==- NpO2HEDTA=

[Am(SO4)2- INTERACTIONS ADDED]
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```
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- NpO2H2EDTA-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- CaCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- CaEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- UnuAn#2-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- UnuAn#3-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Am(SO4)2- NpO2HEDTA=

[NpO2H2EDTA- INTERACTIONS ADDED]
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- CaCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- CaEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- UnuAn#2-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- UnuAn#3-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2H2EDTA- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- CaEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#2-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#3-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCit- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#2-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#3-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaEDTA= NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- UnuAn#3-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#2- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- UnuAn#4-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- U(OH)2(CO3)2=
```

```
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#3- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- U(OH)2(CO3)2=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuAn#4- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= MgCit-
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)2(CO3)2= NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCit- MgEDTA=
     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCit- NpO2HEDTA=

     .0    .0    .0    .0 0   .0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgEDTA= NpO2HEDTA=


  .100 .051  .183 .183 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CO2-Cations      HMW84  lambda
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CaCO3-Cations    HMW84
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   MgCO3-Cations    HMW84
 -.097 -.14    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   B(OH)3-Cations   FW86
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   NpO2OH-Cations
    .0 -.07    .0   .0 .0 .29  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H3PO4-Cations    PS76
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(SO4)2-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H2Ox-Cations     ERG_org_memo
   -.2  -.2    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Am(OH)3(aq)-Cations Na+ FK98, K+
by analogy w Na
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HAc-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   NpO2Ac-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   HLac-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H3Citrate-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   AmCit-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   NpO2Lac-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Th(OH)4-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   U(OH)4-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   U(SO4)2-Cations
   -.2  -.2    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   Pu(OH)3(aq)-Cations analogy w Am
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   PuCit(aq)-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   CaOx(aq)-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   H4EDTA-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   ThEDTA-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   UEDTA-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   MgOx(aq)-Cations
    .0   .0    .0   .0 .0  .0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0   UnuNeu#1-Cations
```

```
 -.005 .097 -.003  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CO2-An
HMW84
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaCO3-An
HMW84
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgCO3-An
HMW84
  .091 .018    .0  0 0 0 0 -.2 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  B(OH)3-An
FW86
  -.19   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2OH-An
FNK95
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0 -.4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H3PO4-An
PS76
   .29   .0   .68  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(SO4)2-
An Roy92
    .0   .0   .0   0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H2Ox-An
ERG_org_memo
   -.2   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Am(OH)3(aq)-An Cl- FK98
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HAc-An
 -.104   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Ac-An
ERG_release_memo(Cl-)
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  HLac-An
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
H3Citrate-An
 -.406   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  AmCit-An
SAND99(Cl-)
  .015   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  NpO2Lac-
An  SAND99/Moore et al 99(Cl-)
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  Th(OH)4-
An
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(OH)4-An
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  U(SO4)2-
An
   -.2   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Pu(OH)3(aq)-An analogy w Am
 -.406   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
PuCit(aq)-An   analogy w/ Am (SAND99(Cl-))
   .0189 .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  CaOx(aq)-
An    analogy w/Mg (ERG_org_memo)
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  H4EDTA-An
   .1111 .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  ThEDTA-An
ERG_org_memo (Cl-)
   .1111 .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UEDTA-An
analogy w/ Th (ERG_org_memo (Cl-))
   .0189 .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  MgOx(aq)-
An   ERG_org_memo (Cl-)
    .0   .0    .0  0 0 0 0  .0 0 0 0 0 0 0 0 0 0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  UnuNeu#1-
An
```

```
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
CO2-C-A
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
(C down
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
A acr
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
CaCO3-Cation-Anion
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MgCO3-Cation-Anion
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0 .046 .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
B(OH)3-Cation-Anion FW86
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
(Cat down, Anions across)
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 -.0102 .0 .0 .0 .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
NpO2OH-C-A
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
H3PO4-Cation-Anion
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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```

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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Th(SO4)2-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
H2Ox-Cation-Anion
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Am(OH)3(aq)-Cation-Anion
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
HAc-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
NpO2Ac-Cation-Anion
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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HLac-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
H3Cit-Cation-Anion
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
AmCit-Cation-Anion
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0   0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
NpO2Lac-Cation-Anion, SAND99/Moore et al 99 (NpO2Lac-Na-Cl = 0)
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Th(OH)4-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
U(OH)4-Cation-Anion
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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  .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
U(SO4)2-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Pu(OH)3(aq)-Cation-Anion
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0    0    0    0    0    0    0    0    0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
PuCit(aq)-Cation-Anion
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0    0    0    0    0    0    0    0    0    0    0   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
CaOx(aq)-Cation-Anion
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
H4EDTA-C-A
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
ThEDTA-C-A
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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UEDTA-C-A
 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0  .0  .0  .0  .0  .0  0  0  0  0  0  0  0  0  0  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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MgOx(aq)-C-A
 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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 .0   .0   .0   .0   .0   .0   0   0   0   0   0   0   0   0   0    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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   2   3   4   5   6   7      Na+       K+        Ca++      Mg++     MgOH+  H+            cation map ELMAP(1,)
  22  21  36  37  50  43      MgB(OH)4+ CaB(OH)4+ Am+++     AmCO3+   Th++++ AmCl++
  64  56  57 101  99  86      NpO2+     U++++     UOH+++    UAc+++   ThOx++ AmAc++
  90  89 102 104 105  96      AmLac++   AmOx+     UCit+     ULac+++  UOx++  ThAc+++
  97 100  40  41  44  47      ThCit+    ThLac+++  AmOH++    Am(OH)2+ AmCl2+ AmSO4+
  48  91  94  95 116 120      Pu(OH)2+  ThAc2++    PuOx+     ThLac2++  CaAc+  CaLac+
 111 115 121                  MgAc+     MgLac+    UnuCat#1+

   8   9  10  11  12  13      Cl-        SO4=          HSO4-          OH-           HCO3-         CO3=        anion map ELMAP(2,)
  18  19  20  23  38  39      B(OH)4-    B3O3(OH)4-    B4O5(OH)4=     Br-           Am(CO3)2-     Am(CO3)3=-
  24  69  65  66  67  33      ClO4-      NpO2(OH)2-    NpO2CO3-       NpO2(CO3)2=-  NpO2(CO3)3==- H2PO4-
  34  35  55  52  51  82      HPO4=      PO4=-         Th(SO4)3=      Th(OH)3(CO3)- Th(CO3)5===   HOx-
  83  71  85  73  74  75      Ox=        Ac-           Lac-           H2Cit-        HCit=         Cit=-
  77  78  79  80  88 107      H3EDTA-    H2EDTA=       HEDTA=-        EDTA==        AmEDTA-      NpO2Cit=
 108 109  60  58  63  45      NpO2EDTA=- NpO2Ox-       U(OH)4(CO3)2== U(CO3)5===    U(SO4)3=      Am(CO3)4==-
  46  93 117 118 123 124      Am(SO4)2- NpO2H2EDTA-       CaCit-          CaEDTA=       UnuAn#2-      UnuAn#3-
 125  59 112 113 122          UnuAn#4-   U(OH)2(CO3)2= MgCit-         MgEDTA=       NpO2HEDTA=

  14  15  16  17  68  32      CO2         CaCO3     MgCO3       B(OH)3  NpO2OH H3PO4    neutral map ELMAP(3,)
  54  81  42  70 106  84      Th(SO4)2    H2Ox      Am(OH)3(aq) HAc     NpO2Ac HLac
  72  87 110  53  61  62      H3Cit       AmCit     NpO2Lac     Th(OH)4 U(OH)4 U(SO4)2
  49  92 119  76  98 103      Pu(OH)3(aq) PuCit(aq) CaOx(aq)    H4EDTA  ThEDTA UEDTA
 114 126                      MgOx(aq)    UnuNeu#1

'nEQUALACT' 0

 2 (Oxygen)
 'nREDOX' 0
 'nIONEX' 0 0 'nMF'

123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890123456789012
         1         2         3         4         5         6         7         8         9         0         1         2         3
                                                                                                   1         1         1         1
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This database release is described in Giambalvo memo to Brush, 20November02, "Release of FMT database 021120.chemdat."
       (in records package 522977)
Data values without explicit references are from HMW84 or FW86

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