538203

Sandia National Laboratories
Waste Isolation Pilot Plant

Sensitivities of the Solubilities of +III, +IV, and +V Actinides to The Concentrations of Organic Ligands in WIPP Brines, Rev. 0

Work carried out under the Analysis Plan for CRA Response Activities, AP-112, Rev. 0

Author:	L. H. Brush Laurence H. Brush, 6822	12/15/04 Date
Author:	Yongliang Xiong Yongliang Xiong, 6822	12/15/04 Date
Technical Reviewer:	Nathalie A. Wall, 6822	12/15/04 Date
QA Reviewer:	A. Earl Bradford Earl Bradford, 6820	12/15/04 Date
Management Reviewer:	Mark J. Rigali, 6822	12/15/04 Date

WIPP:1.2.7:PA:QA-L:Pkg 533999

TABLE OF CONTENTS

1 INTRODUCTION

The EPA (Cotsworth, 2004, Enclosure 1, Comment C-23-15) made the following comment regarding the first WIPP Compliance Recertification Application, or CRA-2004 (U.S. DOE, 2004):

> "DOE states that no upper or lower limit need be established for the quantities of organic ligands in the repository because organic ligand concentrations in the solubility calculations had an insignificant impact on actinide solubility. However, review of SOTERM-5.0 does not indicate that a sensitivity analysis was conducted to establish that no upper limit on organic ligands is required. Because new thermodynamic data are available for organic ligands at high ionic strength, the CCA analysis of the potential effects of organic ligands carried out using low-ionic-strength data may no longer be valid.
>
> "The concentrations of actinides calculated for the CCA and CRA are compared in Table 6-13. Comparison of the concentrations in the two sets of calculations indicates that there are significant differences in some of the calculated solubilities for the +III and +V actinides. Based on information in Appendix SOTERM, the principal difference in the solubility calculations appears to be the inclusion of the effects of organic ligands.
>
> "DOE must provide an assessment of the sensitivity of calculated actinide solubilities to organic ligand inventories in the waste."

This analysis responds to the EPA's request that the "DOE must provide an assessment of the sensitivity of calculated actinide solubilities to organic ligand inventories in the waste."

This work was carried out under the Analysis Plan for CRA Response Activities (Kirkes and Wagner, 2004).

2 BACKGROUND

The DOE stated in the WIPP Compliance Certification Application (CCA) that, based on low-ionic-strength calculations with the HYDRAQL code, dissolved nickel (Ni) released during the corrosion of steel waste containers and steels and other Fe-base alloys in the waste will "[render] EDTA [ethylenediaminetetraacetate] unavailable for complexation with the actinides" and – thus – that "complexation of actinides by organic ligands [will be] inconsequential" (U.S. DOE, 1996, Appendix SOTERM, page SOTERM-38). The DOE also stated that, based on low-ionic-strength hand calculations, "complexation of the organic ligands with actinides will be negligible" (U.S. DOE, 1996, Appendix SOTERM, page SOTERM-41).

For the CRA-2004 performance assessment (PA) (U.S. DOE, 2004, Chapter 6), the effects of dissolved acetate, citrate, EDTA, and oxalate on the solubilities of the +III, +IV, and +V actinides (An(III), An(IV), and An(V)) in the WIPP brines Generic Weep Brine (GWB) and Energy Research and Development Administration [Well]-6 (ERDA-6) were incorporated in the speciation and solubility calculations with Fracture-Matrix Transport (FMT). GWB is a synthetic brine representative of intergranular (grain-boundary) fluids from the Salado Formation (Fm.) at or near the stratigraphic horizon of the repository (Snider, 2003). ERDA-6 is a synthetic brine typical of fluids in brine reservoirs in the Castile Fm. (Popielak, et al., 1983). FMT (Babb and Novak, 1997 and addenda; Wang, 1998) is the thermodynamic speciation and solubility code used to calculate An(III), An(IV), and An(V) solubilities for the CCA PA (Novak et al., 1996), the EPA's 1997 Performance Assessment Verification Test (PAVT) (Novak, 1997), and the CRA-2004 PA (Brush and Xiong, 2003a; 2003b; 2003c, Downes, 2003a; 2003b). The FMT calculations for the CCA PA and the 1997 PAVT did not include the effects of acetate, citrate, EDTA, and oxalate. Inclusion of the effects of these organic ligands in the FMT calculations for the CRA-2004 PA superseded the results of the low-ionic-strength hand and HYDRAQL calculations carried out for the CCA.

The DOE has not developed a thermodynamic speciation-and-solubility model for U(VI) in brines (U.S. DOE, 2004, Appendix PA, Attachment SOTERM, SOTERM-3.4.4, pp. 27-28). U is the only actinide expected to speciate in the +VI oxidation state, and the probability that U will speciate as U(VI) is 0.5 (see the second paragraph of Results, below). Therefore, the DOE estimated the solubility of U(VI) in WIPP brines for the CCA PA, the 1997 PAVT, and the CRA-2004 PA (Hobart and Moore, 1996), and Wall and Wall (2004) estimated the effects of organic ligands on its solubility in WIPP brines.

The concentrations of organic ligands used in the FMT calculations for the CRA-2004 PA were: acetate: 5.05×10^{-3} M; citrate: 3.83×10^{-4} M; EDTA: 3.87×10^{-6} M; and oxalate: 2.16×10^{-2} M. Brush and Xiong (2003b) calculated these concentrations based on estimates by Crawford (2003) of the total masses of these organics to be emplaced in the WIPP. Subsequently, however, Crawford and Leigh (2003) corrected their estimates of the masses of these organic ligands. Therefore, Brush and Xiong (2003d) recalculated the following corrected concentrations: acetate: 3.56×10^{-3} M; citrate: 2.71×10^{-4} M; EDTA: 2.73×10^{-6} M; and oxalate: 1.53×10^{-2} M. Because these concentrations are about 70% of their original values, the FMT calculations for the CRA-2004 PA overestimated the effects of these organic ligands on An(III), An(IV), and An(V) solubilities in WIPP brines. Because the extent to which these effects were overestimated was small, and because this increased the conservatism in PA slightly, the solubilities were not recalculated for the CRA-2004 PA after Brush and Xiong (2003d) corrected the organic-ligand concentrations.

Furthermore, after the FMT calculations for the CRA-2004 PA, Xiong (2004a) modified the thermodynamic database used for these calculations (FMT_021120.CHEMDAT). Xiong (2004a) corrected the molecular weight of oxalate and added the solid calcium (Ca) oxalate to this database. FMT_021120.CHEMDAT contained the solid Na oxalate, but use of this solid as the solubility-controlling phase for oxalate along with recent estimates of the concentrations of oxalate in the WIPP results in dissolved oxalate concentrations of about 2.16×10^{-2} M (Brush and Xiong, 2003b) or 1.53×10^{-2} M (Brush and Xiong, 2003d). These concentrations are certainly much too high to be realistic, because Ca oxalate would precipitate rapidly from any solution with such a high oxalate concentration. They clearly result from the omission of Ca oxalate from FMT_021120.CHEMDAT. To add Ca oxalate, Xiong (2004a) used the mean of three values of the normalized standard chemical potential (μ^0/RT) of whewellite ($CaC_2O_4 \cdot H_2O$). All three of these values were obtained from studies carried out for non-WIPP applications (Nancollas and Gardner, 1974; Tomažič and Nancollas, 1979; and Streit et al., 1998). After making these corrections, Xiong (2004b) released FMT_040628.CHEMDAT.

3 FMT RUNS USED FOR THIS ANALYSIS

We used 12 new and 4 previous FMT calculations to quantify the sensitivities of An(III), An(IV), and An(V) solubilities to the concentrations of organic ligands in the WIPP brines GWB and ERDA-6. We also carried out another 12 new FMT runs that are not described in detail in this analysis report.

The previous FMT calculations used for this analysis (ap098_fmt_run011, ap098_fmt_run017, ap098_fmt_run021, and ap098_fmt_run027) were 4 of the 30 runs for the CRA-2004 PA by Brush and Xiong (2003a; 2003b; 2003c) and Downes (2003a; 2003b). These four runs provided An(III), An(IV), and An(V) solubilities in the absence of organic ligands for (1) GWB and nonmicrobial PA vectors (f_{CO_2} buffered by the brucite-calcite ($Mg(OH)_2$-$CaCO_3$) carbonation reaction); (2) GWB and microbial vectors (f_{CO_2} buffered by the brucite-hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) carbonation reaction); (3) ERDA-6 and nonmicrobial vectors; and (4) ERDA-6 and microbial vectors, respectively. (This order of brines and vectors was used for all four-run sets of calculations in this analysis.) These four runs were conducted using conditions identical to those used to obtain An(III), An(IV), and An(V) solubilities for the CRA-2004 PA (ap098_fmt_run012, ap098_fmt_run018, ap098_fmt_run022, and ap098_fmt_run028), except that ap098_fmt_run011, ap098_fmt_run017, ap098_fmt_run021, and ap098_fmt_run027 did not contain any organic ligands. The results of these previous runs are still valid despite subsequent correction of the molecular weight of oxalate and addition of Ca oxalate to the FMT database by Xiong (2004a) because these runs did not include oxalate (or any other organic ligands). Table 1 lists the conditions specified for all 30 FMT runs for the CRA-2004 PA.

Four new FMT calculations for this analysis (FMT_CRA1V_ORGS_001, FMT_CRA1V_ORGS_002, FMT_CRA1V_ORGS_003, and FMT_CRA1V_ORGS_004) provided An(III), An(IV), and An(V) solubilities with acetate, citrate, EDTA, and oxalate present at concentrations identical to those calculated by Brush and Xiong (2003b) for the CRA-2004 PA (5.05×10^{-3} M, 3.83×10^{-4} M, 3.87×10^{-6} M, and 2.16×10^{-2} M, respectively). These runs yielded An(III), An(IV), and An(V) solubilities identical to those from ap098_fmt_run012, ap098_fmt_run018, ap098_fmt_run022, and ap098_fmt_run028, which provided solubilities for the CRA-2004 PA. Input files for FMT_CRA1V_ORGS_001, FMT_CRA1V_ORGS_002, FMT_CRA1V_ORGS_003, and FMT_CRA1V_ORGS_004 were prepared because it was believed at the time that an additional, significant correction of the FMT database was required Xiong, 2004c; 2004d). When it was determined that this additional correction was unnecessary (Xiong, 2004e; 2004f), these runs were carried out anyway to ensure that – in the absence of Ca oxalate precipitation (prevented by disabling the precipitation of this solid in the input files) – the new and previous runs gave identical results, except for possible insignificant differences due correction of the molecular weight of oxalate (Xiong, 2004a). Because precipitation of Ca oxalate was disabled, the dissolved oxalate concentration specified in the input files (2.16×10^{-2} M) and those obtained in the output file were too high to be realistic. (The concentrations specified in the input files differ slightly from those in the output files because of density changes resulting from equilibration of the brines with minerals such as halite (NaCl), anhydrite ($CaSO_4$), brucite, and calcite or hydromagnesite.) Table 2 provides the conditions specified for all 24 new FMT runs for this analysis.

Four new FMT calculations (FMT_CRA1V_ORGS_013, FMT_CRA1V_ORGS_014, FMT_CRA1V_ORGS_015, and FMT_CRA1V_ORGS_016) gave An(III), An(IV), and An(V) solubilities with the same concentrations of organic ligands used for FMT_CRA1V_ORGS_001, FMT_CRA1V_ORGS_002, FMT_CRA1V_ORGS_003, and FMT_CRA1V_ORGS_004 (see preceeding paragraph) *plus* additional organic ligands produced as metabolic byproducts of microbial consumption of papers used to simulate cellulosic materials in the long-term microbial gas-generation experiments at Brookhaven National Laboratory (Gillow and Francis, 2003). Acetic acid and lactic acid were the only microbial metabolites observed by Gillow and Francis (2003) that are of potential concern from the standpoint of their effects on actinide solubilities in aqueous solutions. Therefore, Trone (2004) calculated the mean and median concentrations of acetic and lactic acids observed by Gillow and Francis (2003), and obtained mean and median concentrations of 2.84×10^{-3} M and 1.81×10^{-3} M, respectively, for acetic acid; and mean and median concentrations of 4.8×10^{-4} M and 2.8×10^{-4} M for lactic acid. We then added 2.84×10^{-3} M, the larger value obtained by Trone (2004) for acetic acid, to the concentration of acetate used for the CRA-2004 PA (5.05×10^{-3} M) to obtain 7.89×10^{-3} M; and added 4.8×10^{-4} M, the larger value obtained by Trone (2004) for lactic acid, to the concentration of lactate used for the CRA-2004 PA (0) to obtain 4.8×10^{-4} M. Lactate was not included in the FMT calculations for the CRA-2004 PA because it has never been reported to be present in the WIPP inventory (see, for example, Crawford, 2003; Crawford and Leigh, 2003). Because Gillow and Francis (2003) did not report any citric acid, EDTA, or oxalic acid, the concentrations of these organic ligands used for these runs were identical to those calculated by Brush and Xiong (2003b) for the CRA-2004 PA. Therefore, the organic-ligand concentrations used for these runs were: acetate: 7.89×10^{-3} M; citrate: 3.83×10^{-4} M; EDTA: 3.87×10^{-6} M; lactate: 4.8×10^{-4} M; and oxalate: 2.16×10^{-2} M. Because precipitation of Ca oxalate was disabled in these runs, the dissolved oxalate concentration specified in the input files (2.16×10^{-2} M) and those obtained in the output file were unrealistically high.

Four new FMT calculations (FMT_CRA1V_ORGS_017, FMT_CRA1V_ORGS_018, FMT_CRA1V_ORGS_019, and FMT_CRA1V_ORGS_020) provided An(III), An(IV), and An(V) solubilities with organic-ligand concentrations 10 times higher than those used for FMT_CRA1V_ORGS_013, FMT_CRA1V_ORGS_014, FMT_CRA1V_ORGS_015, and FMT_CRA1V_ORGS_016 (see preceeding paragraph). Therefore, the concentrations used for FMT_CRA1V_ORGS_017, FMT_CRA1V_ORGS_018, FMT_CRA1V_ORGS_019, and FMT_CRA1V_ORGS_020 were: acetate: 7.89×10^{-2} M; citrate: 3.83×10^{-3} M; EDTA: 3.87×10^{-5} M; lactate: 4.8×10^{-3} M; and oxalate: 2.16×10^{-1} M. Once again, precipitation of Ca oxalate was disabled.

Several additional new FMT runs were carried out for this analysis, but are not described in detail in this report. FMT_CRA1V_ORGS_005, FMT_CRA1V_ORGS_006, FMT_CRA1V_ORGS_007, and FMT_CRA1V_ORGS_008 used the corrected organic-ligand concentrations calculated by Brush and Xiong (2003d) (see Background, above) with precipitation of Ca oxalate disabled. For FMT_CRA1V_ORGS_009,

FMT_CRA1V_ORGS_010, FMT_CRA1V_ORGS_011, and FMT_CRA1V_ORGS_012, the organic-ligand concentrations specified in the input files were identical to those of FMT_CRA1V_ORGS_005, FMT_CRA1V_ORGS_006, FMT_CRA1V_ORGS_007, and FMT_CRA1V_ORGS_008, but Ca oxalate was allowed to precipitate in FMT_CRA1V_ORGS_009, FMT_CRA1V_ORGS_010, FMT_CRA1V_ORGS_011, and FMT_CRA1V_ORGS_012. Finally, for FMT_CRA1V_ORGS_021, FMT_CRA1V_ORGS_022, FMT_CRA1V_ORGS_023, and FMT_CRA1V_ORGS_024, the organic-ligand concentrations specified in the input files were identical to those of FMT_CRA1V_ORGS_017, FMT_CRA1V_ORGS_018, FMT_CRA1V_ORGS_019, and FMT_CRA1V_ORGS_020, but Ca oxalate was allowed to precipitate in FMT_CRA1V_ORGS_021, FMT_CRA1V_ORGS_022, FMT_CRA1V_ORGS_023, and FMT_CRA1V_ORGS_024.

All new runs carried out for this analysis used the current FMT database, FMT_041210.CHEMDAT (Xiong, 2004e, 2004f).

4 RESULTS

Table 3 presents the results of runs ap098_fmt_run011, ap098_fmt_run017, ap098_fmt_run021, and ap098_fmt_run027 in the second, third, fourth, and fifth columns, respectively; and FMT_CRA1V_ORGS_001, FMT_CRA1V_ORGS_002, FMT_CRA1V_ORGS_003, and FMT_CRA1V_ORGS_004 in the sixth, seventh, eighth, and ninth columns. In this table (and in Table 4), "Ac" is the abbreviation for "acetate," "Cit" is "citrate," "Lac" is "lactate," "M" is "molar," "microbio" is "microbial PA vectors" (f_{CO_2} buffered by the brucite-hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) carbonation reaction), "nonmicrobio" is "nonmicrobial vectors" (f_{CO_2} buffered by the brucite-calcite carbonation reaction), "orgs" is "organics," "Ox" is oxalate, and "w/o" is "without." Comparison of the second and sixth, third and seventh, fourth and eighth, and fifth and ninth columns demonstrates the effects of acetate, citrate, EDTA, and oxalate at the concentrations used in the FMT calculations for CRA-2004 PA on An(III), An(IV, and An(V) solubilities for each combination of brine (GWB or ERDA-6) and PA vector (nonmicrobial or microbial). (Again, note that the organic-ligand concentrations specified in the input files differ slightly from those in the output file because of density changes resulting from equilibration of the brines with minerals such as halite (NaCl), anhydrite ($CaSO_4$), brucite, and calcite or hydromagnesite.) The results in Table 3 demonstrate that: (1) these organic ligands at these concentrations increased An(III) solubilities by factors of 1.35, 1.36, 1.94, and 1.95 times their solubilities in the absence of organic ligands for GWB and nonmicrobial vectors, GWB and microbial vectors, ERDA-6 and nonmicrobial vectors, and ERDA-6, and microbial vectors, respectively (this order of brines and vectors is repeated for all other four-run sets of results described below); (2) organic ligands at these concentrations had essentially no effect of An(IV) solubilities; and (3) they increased An(V) solubilities by factors of 4.23, 4.32, 19.9, and 9.44.

The conclusion that acetate, citrate, EDTA, and oxalate at these concentrations had a modest effect on An(III) solubilities is important because the +III oxidation state is the most important actinide oxidation state expected in the WIPP. This oxidation state is the most important because: (1) the order of importance of the radioelements in TRU waste based on their potential effects on the long-term performance of the WIPP is Pu ≅ Am >> U > Th > Np; and (2) the oxidation-state distributions of these radioelements implemented in PA consists of a probability of 0.5 that these radioelements will speciate entirely as Pu(III), Am(III), U(IV), Th(IV), and Np(IV); and a probability of 0.5 that they will speciate entirely as Pu(IV), Am(III), U(VI), Th(IV), and Np(V). However, it is noteworthy that comparison of the mean Complimentary, Cumulative Distribution Function (CCDF) for normalized direct brine releases (DBR) from the repository and the mean CCDF for normalized total releases shows that: (1) at a probability of 0.001, the mean DBR were just 12.2% of the mean total releases; and (2) at a probability of 0.1, the mean DBR were only 0.115% of the total releases (Vugrin, 2004).

The conclusion that organic ligands at these concentrations had no effect on An(IV) solubilities is significant because the +IV oxidation state is the second-most important oxidation state expected in the WIPP (see above). Therefore, based on the effects of organics on An(III) and An(IV) solubilities (by far the two most important oxidation states expected in the repository), the overall effects of organics on long-term repository performance were relatively small.

Finally, the significant effect of organic ligands on An(V) solubilities had essentially no impact on the long-term performance of the WIPP because: (1) Np is the only actinide expected to speciate in the +V oxidation state (see above), (2) the probability that Np will speciate as Np(V) is 0.5, and (3) from the standpoint of its potential effects on long-term performance, Np is much less important than Pu, Am, U, or Th.

Therefore, based on the effects of acetate, citrate, EDTA, and oxalate at the concentrations used for the CRA-2004 PA on An(III), An(IV), and An(V) solubilities, the overall effects of organics on the long-term performance of the repository were still negligible.

Table 4 presents the results of runs FMT_CRA1V_ORGS_013, FMT_CRA1V_ORGS_014, FMT_CRA1V_ORGS_015, and FMT_CRA1V_ORGS_016 in the second, third, fourth, and fifth columns, respectively; and FMT_CRA1V_ORGS_017, FMT_CRA1V_ORGS_018, FMT_CRA1V_ORGS_019, and FMT_CRA1V_ORGS_020 in the sixth, seventh, eighth, and ninth columns.

Addition of microbially produced acetate and lactate (Gillow and Francis, 2003) in the manner described above had no effect on An(III) solubilities, essentially no effect on An(IV) solubilities, and a slight effect on An(V) solubilities (compare the results in the second, third, fourth, and fifth columns of Table 4 with those in the sixth, seventh, eighth, and ninth columns in Table 3). These organic ligands at these concentrations increased An(V) solubilities by factors of 4.34, 4.40, 20.0, and 9.52 relative to their solubilities in the absence of organic ligands (compare the results in the second, third, fourth, and fifth columns of Table 4 with those in the second, third, fourth, and fifth columns of Table 3). These factors are slightly higher than those of 4.23, 4.32, 19.9, and 9.44 observed for organic ligands at the concentrations used for the CRA-2004 PA. Therefore, the effect of addition of microbially produced acetate and lactate on long-term repository performance would also be negligible.

Multiplying the concentrations of organic ligands that included microbially produced acetate and lactate by 10 had a greater effect on An(III), An(IV), and An(V) solubilities than addition of these microbial metabolites to the concentrations used for the CRA-2004 PA. Multiplying these concentrations by 10 increased An(III) solubilities by factors of 2.93, 2.93, 5.23, and 5.42 (compare the results in the sixth, seventh, eighth, and ninth columns of Table 4 with those in the sixth, seventh, eighth, and ninth columns in Table 3). The resulting An(III) solubilities exceeded those predicted in the absence of organic ligands by factors of 3.96, 3.97, 10.1, and 10.6 (compare the results in the sixth, seventh, eighth, and ninth columns of Table 4 with those in the second, third, fourth, and fifth columns in Table 3). Multiplying the concentrations of organic ligands that included microbially produced acetate and lactate by 10 had essentially no effect on An(IV) solubilities in two cases (GWB, nonmicrobial vectors; and GWB, microbial vectors); and slightly greater effects, albeit in opposite directions, in the other two cases (ERDA-6, nonmicrobial vectors; and ERDA-6, microbial vectors). Multiplication by 10 increased An(V) solubilities by factors of 7.22, 7.47, 5.59, and 7.13; the resulting An(V) solubilities exceeded those predicted without organic ligands by factors of 30.5, 32.3, 111, and 67.3. Nevertheless, these An(V) solubilities would still have no significant impact on long-term performance for the reasons discussed above.

5 REFERENCES

Babb, S.C., and C.F. Novak. 1997 and addenda. "User's Manual for FMT Version 2.3: A Computer Code Employing the Pitzer Activity Coefficient Formalism for Calculating Thermodynamic Equilibrium in Geochemical Systems to High Electrolyte Concentrations." Albuquerque, NM: Sandia National Laboratories. ERMS 243037.

Brush, L.H., and Y.-L. Xiong. 2003a. "Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application, Analysis Plan AP-098, Rev. 1." April 14, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 527714.

Brush, L.H., and Y.-L. Xiong. 2003b. "Calculation of Organic Ligand Concentrations for the WIPP Compliance Recertification Application." Analysis report, April 14, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 527567.

Brush, L.H., and Y.-L. Xiong. 2003c. "Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application." Analysis report, May 8, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 529131.

Brush, L.H., and Y.-L. Xiong. 2003d. "Calculation of Organic Ligand Concentrations for the WIPP Compliance Recertification Application and for Evaluating Assumptions of Homogeneity in WIPP PA." Analysis report, September 11, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 531488.

Cotsworth, E. 2004. Untitled letter with enclosure to R.P. Detwiler with third set of CRA comments and requests for additional information, September 2, 2004. Washington, DC: U.S. Environmental Protection Agency Office of Air and Radiation. ERMS 536771.

Crawford, B. 2003. "Updated Estimate of Complexing Agents in Transuranic Solidified Waste Forms Scheduled for Disposal and Emplaced at WIPP." Letter to C.D. Leigh, April 8, 2003. Carlsbad, NM: Los Alamos National Laboratory. ERMS 527409.

Crawford, B.A., and C.D. Leigh. 2003. "Estimate of Complexing Agents in TRU Waste for the Compliance Recertification Application." Analysis report, August 28, 2003. Carlsbad, NM: Los Alamos National Laboratory. ERMS 531107.

Downes, P.S. 2003a. "Spreadsheet Calculations of Actinide Solubilities for the WIPP Compliance Recertification Application." Memorandum to L.H. Brush, April 21, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 528395.

Downes, P.S. 2003b. "Spreadsheet Calculations of Actinide Solubilities for the WIPP Compliance Recertification Application in Support of AP-098, 'Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application, Analysis Plan AP-098, Rev. 1.'" Analysis report, July 22, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 530441.

Gillow, J.B., and A.J. Francis. 2003. "Microbial Gas Generation under Expected Waste Isolation Pilot Plant Repository Conditions: Draft Final Report, Rev. 0, October 6, 2003." Upton, NY: Brookhaven National Laboratory. ERMS 532877.

Hobart, D.E., and R.C. Moore. 1996b. "Analysis of Uranium(VI) Solubility Data for WIPP Performance Assessment: Implementation of Analysis Plan AP-028." Analysis report, August 12, 1996. Albuquerque, NM: Sandia National Laboratories. ERMS 236488.

Kirkes, G.R., and S.W. Wagner. 2004. "Analysis Plan for CRA Response Activities." AP 112, Rev. 0, April 26, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 534690.

Nancollas, G.H., and G.L. Gardner. 1974. "Kinetics of Crystal Growth of Calcium Oxalate," *Journal of Crystal Growth.* Vol. 21, 267–276.

Novak, C.F. 1997. "Calculation of Actinide Solubilities in WIPP SPC and ERDA-6 Brines under MgO Backfill Scenarios Containing either Nesquehonite or Hydromagnesite as the Mg-CO_3 Solubility-Limiting Phase." Memorandum to R.V. Bynum, April 21, 1997. Albuquerque, NM: Sandia National Laboratories. ERMS 246124.

Novak, C.F., R.C. Moore, and R.V. Bynum. 1996. "Prediction of Dissolved Actinide Concentrations in Concentrated Electrolyte Solutions: A Conceptual Model and Model Results for the Waste Isolation Pilot Plant (WIPP)." Unpublished presentation at the 1996 International Conference on Deep Geological Disposal of Radioactive Waste, September 16-19, 1996, Winnipeg, Manitoba, Canada. ERMS 418098, SAND96-2695C.

Popielak, R.S., R.L. Beauheim, S.R. Black, W.E. Coons, C.T. Ellingson and R.L. Olsen. 1983. *Brine Reservoirs in the Castile Formation, Waste Isolation Pilot Plant Project, Southeastern New Mexico.* TME 3153. Carlsbad, NM: U.S. Department of Energy WIPP Project Office.

Snider, A.C. 2003. "Verification of the Definition of Generic Weep Brine and the Development of a Recipe for This Brine." Analysis report, April 8, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 527505.

Streit, J., L.-C. Tran-Ho, and E. Konigsberger. 1998. "Solubility of the Three Calcium Oxalate Hydrates in Sodium Chloride Solutions and Urine-Like Liquors," Monatsheft für Chemie. Vol. 129, 1225–1236.

Tomazic, B., and G.H. Nancollas. 1979. "The Kinetics of Dissolution of Calcium Oxalate Hydrates," *Journal of Crystal Growth*. Vol. 46, 355–361.

Trone, J.T. 2004. "Routine Calculation of the Mean and Median Values of Acetic and Lactic Organic Acids Detected in Cellulose Samples." Memorandum to L.H. Brush, November 5, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 537806.

U.S. DOE. 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant, Vol. 1-21.* DOE/CAO-1994-2184. Carlsbad, NM: U.S. Department of Energy Carlsbad Area Office.

U.S. DOE. 2004. *Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant, Vol. 1-8.* DOE/WIPP 2004-3231. Carlsbad, NM: U.S. Department of Energy Carlsbad Field Office.

Vugrin, E. 2004. "Routine Calculation of CRA Mean Total Releases and Mean DBR Releases at Probabilities of 0.1 and 0.001." Memorandum to L.H. Brush, December 14, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 538179.

Wall, N.A. and D.E. Wall. 2004. "Discussion on the Influence of Organic Ligands on the Solubility of U(VI)." Memorandum to Records, November 30, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 537938.

Wang, Y. 1998. "WIPP PA Validation Document for FMT (Version 2.4), Document Version 2.4." Carlsbad, NM: Sandia National Laboratories. ERMS 251587.

Xiong, Y.-L. 2004a. "A Correction of the Molecular Weight of Oxalate in FMT_021120.CHEMDAT, and Incorporation of Calcium Oxalate Monohydrate (Whewellite) into CHEMDAT with Its Recommended Dimensionless Standard Chemical Potential (μ^0/RT) Value." Memorandum to L.H. Brush, June 8, 2004? Carlsbad, NM: Sandia National Laboratories. ERMS 535813.

Xiong, Y.-L. 2004b. "Release of FMT_040628.CHEMDAT." E-mail to J.J. Long, June 28, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 536022.

Xiong, Y.-L. 2004c. "An Update on the Dimensionless Standard Chemical Potential of $NpO_2Ac(aq)$ in FMT CHEMDAT." Memorandum to L.H. Brush, November 11, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 537838.

Xiong, Y.-L. 2004d. "Release of FMT_041116.CHEMDAT." E-mail to J.J. Long, November 16, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 537942.

Xiong, Y.-L. 2004e. "A Correction of the Dimensionless Standard Chemical Potential of $NpO_2Ac(aq)$ in FMT_041116.CHEMDAT." Memorandum to L.H. Brush, December 10, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 538162.

Xiong, Y.-L. 2004f. "Release of FMT_041210.CHEMDAT." E-mail to J.F. Kanney and B.L. Buell. December 10, 2004. Carlsbad, NM: Sandia National Laboratories. ERMS 538178.

6 TABLES

Table 1. FMT Runs Carried Out for the CRA-2004 PA Calculations (Brush and Xiong, 2003c). All runs archived in the CMS in lib_ap098_fmt. Runs that provided solubilities for the CRA-2004 PA calculations shown in bold font.

Run ID	Brine	f_{CO_2} Buffer	Organics
ap098_fmt_run001	Brine A	Brucite-calcite	No
ap098_fmt_run002	Brine A	Brucite-calcite	Yes
ap098_fmt_run003	Brine A	Brucite-magnesite	No
ap098_fmt_run004	Brine A	Brucite-magnesite	Yes
ap098_fmt_run005	Brine A	Brucite-hydromagnesite$_{4323}{}^{A}$	No
ap098_fmt_run006	Brine A	Brucite-hydromagnesite$_{4323}{}^{A}$	Yes
ap098_fmt_run007	Brine A	Brucite-hydromagnesite$_{5424}{}^{A}$	No
ap098_fmt_run008	Brine A	Brucite-hydromagnesite$_{5424}{}^{A}$	Yes
ap098_fmt_run009	Brine A	Brucite-nesquehonite	No
ap098_fmt_run010	Brine A	Brucite-nesquehonite	Yes
ap098_fmt_run011	GWB	Brucite-calcite	No
ap098_fmt_run012	**GWB**	**Brucite-calcite**	**Yes**
ap098_fmt_run013	GWB	Brucite-magnesite	No
ap098_fmt_run014	GWB	Brucite-magnesite	Yes
ap098_fmt_run015	GWB	Brucite-hydromagnesite$_{4323}{}^{A}$	No
ap098_fmt_run016	GWB	Brucite-hydromagnesite$_{4323}{}^{A}$	Yes
ap098_fmt_run017	GWB	Brucite-hydromagnesite$_{5424}{}^{B}$	No
ap098_fmt_run018	**GWB**	**Brucite-hydromagnesite**$_{5424}{}^{2B}$	**Yes**
ap098_fmt_run019	GWB	Brucite-nesquehonite	No
ap098_fmt_run020	GWB	Brucite-nesquehonite	Yes
ap098_fmt_run021	ERDA-6	Brucite-calcite	No
ap098_fmt_run022	**ERDA-6**	**Brucite-calcite**	**Yes**
ap098_fmt_run023	ERDA-6	Brucite-magnesite	No
ap098_fmt_run024	ERDA-6	Brucite-magnesite	Yes
ap098_fmt_run025	ERDA-6	Brucite-hydromagnesite$_{4323}{}^{A}$	No
ap098_fmt_run026	ERDA-6	Brucite-hydromagnesite$_{4323}{}^{A}$	Yes
ap098_fmt_run027	ERDA-6	Brucite-hydromagnesite$_{5424}{}^{B}$	No
ap098_fmt_run028	**ERDA-6**	**Brucite-hydromagnesite**$_{5424}{}^{B}$	**Yes**
ap098_fmt_run029	ERDA-6	Brucite-nesquehonite	No
ap098_fmt_run030	ERDA-6	Brucite-nesquehonite	Yes

A. Hydromagnesite$_{4323}$ = $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$.
B. Hydromagnesite$_{5424}$ = $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$.

Table 2. List of New FMT Runs Carried Out in Response to EPA Issue C-23-15 (Organic Ligand Sensitivity). Ac = acetate; Cit = citrate; hydromag = hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$); Lac = lactate; Ox = oxalate.

Run ID	Brief Description of FMT Run	Concentrations of Organic Ligands Specified in FMT Input File
FMT_CRA1V_ ORGS_001	GWB with CRA PA organics,[A] brucite-calcite, no Ca Ox(solid)	Ac = 5.05×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 0 M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_002	GWB with CRA PA organics,[A] brucite-hydromag, no Ca Ox(solid)	Ac = 5.05×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 0 M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_003	ERDA-6 with CRA PA organics,[A] brucite-calcite, no Ca Ox(solid)	Ac = 5.05×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 0 M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_004	ERDA-6 with CRA PA organics,[A] brucite-hydromag, no Ca Ox(solid)	Ac = 5.05×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 0 M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_005	GWB with corrected organics,[B] brucite-calcite, no Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_006	GWB with corrected organics,[B] brucite-hydromag, no Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M

Table 2. List of FMT Runs Carried Out in Response to EPA Issue C-23-15 (Organic Ligand Sensitivity) (cont.).

Run ID	Brief Description of FMT Run	Concentrations of Organic Ligands Specified in FMT Input File (M)
FMT_CRA1V_ ORGS_0007	ERDA-6 with corrected organics,[B] brucite-calcite, no Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_008	ERDA-6 with corrected organics,[B] brucite-hydromag, no Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_009	GWB with corrected organics,[B] brucite-calcite + Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_010	GWB with corrected organics,[B] brucite-hydromag + Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_011	ERDA-6 with corrected organics,[B] brucite-calcite + Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M
FMT_CRA1V_ ORGS_012	ERDA-6 with corrected organics,[B] brucite-hydromag + Ca Ox(solid)	Ac = 3.56×10^{-3} M; Cit = 2.71×10^{-4} M; EDTA = 2.73×10^{-6} M; Lac = 0 M; Ox = 1.53×10^{-2} M

Table 2. List of FMT Runs Carried Out in Response to EPA Issue C-23-15 (Organic Ligand Sensitivity) (cont.).

Run ID	Brief Description of FMT Run	Concentrations of Organic Ligands Specified in FMT Input File (M)
FMT_CRA1V_ ORGS_013	GWB with CRA PA organics^A + microbial Ac & Lac,^{C} brucite-calcite, no Ca Ox(solid)	Ac = 7.89×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 4.80×10^{-4} M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_014	GWB with CRA PA organics^A + microbial Ac & Lac,^{C} brucite-hydromag, no Ca Ox(solid)	Ac = 7.89×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 4.80×10^{-4} M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_015	ERDA-6 with CRA PA organics^A + microbial Ac & Lac,^{C} brucite-calcite, no Ca Ox(solid)	Ac = 7.89×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 4.80×10^{-4} M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_016	ERDA-6 with CRA PA organics^A + microbial Ac & Lac,^{C} brucite-hydromag, no Ca Ox(solid)	Ac = 7.89×10^{-3} M; Cit = 3.83×10^{-4} M; EDTA = 3.87×10^{-6} M; Lac = 4.80×10^{-4} M; Ox = 2.16×10^{-2} M
FMT_CRA1V_ ORGS_017	GWB with 10 × (CRA PA organics^A + microbial Ac & Lac^C), brucite-calcite, no Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_018	GWB with 10 × (CRA PA organics^A + microbial Ac & Lac^C), brucite-hydromag, no Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M

Table 2. List of FMT Runs Carried Out in Response to EPA Issue C-23-15 (Organic Ligand Sensitivity) (cont.).

Run ID	Brief Description of FMT Run	Concentrations of Organic Ligands Specified in FMT Input File (M)
FMT_CRA1V_ ORGS_019	ERDA-6 with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-calcite, no Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_020	ERDA-6 with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-hydromag, no Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_021	GWB with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-calcite + Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_022	GWB with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-calcite + Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_023	GWB with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-calcite + Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M
FMT_CRA1V_ ORGS_024	GWB with 10 × (CRA PA organics[A] + microbial Ac & Lac[C]), brucite-calcite + Ca Ox(solid)	Ac = 7.89×10^{-2} M; Cit = 3.83×10^{-3} M; EDTA = 3.87×10^{-5} M; Lac = 4.80×10^{-3} M; Ox = 2.16×10^{-1} M

Notes for Table 2:

A. Concentrations of Ac, Cit, EDTA, and Ox from Brush and Xiong (2003a).
B. Concentrations of Ac, Cit, EDTA, and Ox from Brush and Xiong (2003c).
C. Obtained by adding the mean concentrations of Ac and Lac observed by Gillow and Francis (2003) (see Trone, 2004) to the waste-derived values.

Table 3. Sensitivity of Actinide +III, +IV, and +V Solubilities to the Concentrations of Acetate, Citrate, EDTA, Lactate, and Oxalate: No Organics and CRA-2004 PA Organics. See text for explanation of abbreviations. See next page for Notes A through H.

Organic Ligand or Actinide	GWB, w/o orgs, nonmicrobio[A] (M)	GWB, w/o orgs, microbio[B] (M)	ERDA-6, w/o orgs, nonmicrobio[C] (M)	ERDA-6, w/o orgs, microbio[D] (M)	GWB, CRA orgs, nonmicrobio, no Ca Ox[E] (M)	GWB, CRA orgs, microbio, no Ca Ox[F] (M)	ERDA-6, CRA orgs, nonmicrobio, no Ca Ox[G] (M)	ERDA-6, CRA orgs, microbio, no Ca Ox[H] (M)
Tot. Ac	0	0	0	0	5.37×10^{-3}	5.37×10^{-3}	5.00×10^{-3}	5.00×10^{-3}
Tot. Cit	0	0	0	0	4.07×10^{-4}	4.07×10^{-4}	3.79×10^{-4}	3.79×10^{-4}
Tot. EDTA	0	0	0	0	4.12×10^{-6}	4.12×10^{-6}	3.83×10^{-6}	3.83×10^{-6}
Tot. Lac	0	0	0	0	0	0	0	0
Tot. Ox	0	0	0	0	2.30×10^{-2}	2.30×10^{-2}	2.14×10^{-2}	2.14×10^{-2}
An(III)	2.27×10^{-7}	2.26×10^{-7}	9.14×10^{-8}	8.67×10^{-8}	3.07×10^{-7}	3.07×10^{-7}	1.77×10^{-7}	1.69×10^{-7}
An(IV)	1.24×10^{-8}	1.19×10^{-8}	5.80×10^{-9}	2.50×10^{-8}	1.24×10^{-8}	1.19×10^{-8}	5.84×10^{-9}	2.47×10^{-8}
An(V)	2.30×10^{-7}	2.36×10^{-7}	1.07×10^{-6}	5.38×10^{-7}	9.72×10^{-7}	1.02×10^{-6}	2.13×10^{-5}	5.08×10^{-6}

A. From ap098_fmt_run011 (Brush and Xiong, 2003a; 2003b; 2003c; Downes, 2003a; 2003b).
B. From ap098_fmt_run017 (Brush and Xiong, 2003a; 2003b; 2003c; Downes, 2003a; 2003b).
C. From ap098_fmt_run021 (Brush and Xiong, 2003a; 2003b; 2003c; Downes, 2003a; 2003b).
D. From ap098_fmt_run027 (Brush and Xiong, 2003a; 2003b; 2003c; Downes, 2003a; 2003b).

Notes for Table 3 (cont.).

E. From FMT_CRA1V_ORGS_001; results identical to those of ap098_fmt_run012 (Brush and Xiong, 2003c; Downes, 2003).
F. From FMT_CRA1V_ORGS_002; results identical to those of ap098_fmt_run018 (Brush and Xiong, 2003c; Downes, 2003).
G. From FMT_CRA1V_ORGS_003; results identical to those of ap098_fmt_run022 (Brush and Xiong, 2003c; Downes, 2003).
H. From FMT_CRA1V_ORGS_004; results identical to those of ap098_fmt_run028 (Brush and Xiong, 2003c; Downes, 2003).

Table 4. Sensitivity of Actinide +III, +IV, and +V Solubilities to the Concentrations of Acetate, Citrate, EDTA, Lactate, and Oxalate: EPA Organics and 10 × EPA Organics. See text for explanation of abbreviations.

Organic Ligand or Actinide	GWB, EPA orgs, nonmicrobio, no Ca Ox[A] (M)	GWB, EPA orgs, microbio, no Ca Ox[B] (M)	ERDA-6, EPA orgs, nonmicrobio, no Ca Ox[C] (M)	ERDA-6, EPA orgs, microbio, no Ca Ox[D] (M)	GWB, 10 × EPA, nonmicrobio, no Ca Ox[E] (M)	GWB, 10 × EPA, microbio, no Ca Ox[F] (M)	ERDA-6, 10 × EPA, nonmicrobio, no Ca Ox[G] (M)	ERDA-6, 10 × EPA, microbio, no Ca Ox[H] (M)
Tot. Ac	8.39×10^{-3}	8.39×10^{-3}	7.81×10^{-3}	7.81×10^{-3}	8.23×10^{-2}	8.23×10^{-2}	7.71×10^{-2}	7.72×10^{-2}
Tot. Cit	4.07×10^{-4}	4.07×10^{-4}	3.79×10^{-4}	3.79×10^{-4}	4.00×10^{-3}	4.00×10^{-3}	3.74×10^{-3}	3.75×10^{-3}
Tot. EDTA	4.12×10^{-6}	4.12×10^{-6}	3.83×10^{-6}	3.83×10^{-6}	4.04×10^{-5}	4.04×10^{-5}	3.78×10^{-5}	3.79×10^{-5}
Tot. Lac	5.10×10^{-4}	5.10×10^{-4}	4.75×10^{-4}	4.75×10^{-4}	5.01×10^{-3}	5.01×10^{-3}	4.69×10^{-3}	4.70×10^{-3}
Tot. Ox	2.30×10^{-2}	2.30×10^{-2}	2.14×10^{-2}	2.14×10^{-2}	2.25×10^{-1}	2.25×10^{-1}	1.81×10^{-1}	1.73×10^{-1}
An(III)	3.07×10^{-7}	3.07×10^{-7}	1.77×10^{-7}	1.69×10^{-7}	8.98×10^{-7}	8.98×10^{-7}	9.23×10^{-7}	9.16×10^{-7}
An(IV)	1.24×10^{-8}	1.18×10^{-8}	5.85×10^{-9}	2.46×10^{-8}	1.25×10^{-8}	1.15×10^{-8}	6.76×10^{-9}	2.02×10^{-8}
An(V)	9.98×10^{-7}	1.04×10^{-6}	2.14×10^{-5}	5.12×10^{-6}	7.02×10^{-6}	7.62×10^{-6}	1.19×10^{-4}	3.62×10^{-5}

A. From FMT_CRA1V_ORGS_013.
B. From FMT_CRA1V_ORGS_014.
C. From FMT_CRA1V_ORGS_015.
D. From FMT_CRA1V_ORGS_016.

Notes for Table 4 (cont.).

E. From FMT_CRA1V_ORGS_017.
F. From FMT_CRA1V_ORGS_018.
G. From FMT_CRA1V_ORGS_019.
H. From FMT_CRA1V_ORGS_020.