Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of Organic-Ligand Concentrations for the 2026 WIPP Compliance Recertification Application Performance Assessment Interim-State Analysis (CRA-2026 IS)

Work Carried Out under Task 3 of the Analysis Plan for WIPP Near-Field Geochemical Process Modeling, AP 153, Rev. 1.
To be included in the AP-153 records package

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1 INTRODUCTION

The Waste Isolation Pilot plant (WIPP) was initially certified as a 10-panel repository for long-term waste disposal for transuranic (TRU) waste, which served as the design layout and basis for the performance assessment (PA) calculations for the 2019 Compliance Recertification Application Deferred Performance Assessment (CRA-2019 DPA). Due to operational constraints, not all this volume is available for waste disposal. In March 2024 the DOE submitted the Replacement Panels Planned Change Request (RPPCR) seeking EPA approval of two replacement waste disposal panels. Although the RPPCR is expected to be approved prior to submittal of 2026 Compliance Recertification Application (CRA-2026), the replacement panels will not accommodate the entire allowable waste volume as specified in the WIPP Land Withdrawal Act (LWA) (U.S. Congress 1992), leading to the consideration of seven additional waste panels. Thus, the CRA-2026 performance assessment (PA) will consider two repository designs: an interim state repository with 12 panels (CRA-2026 IS) and a final-state repository with 19 panels (CRA-2026 FS), which provides sufficient storage for disposal of the entire WIPP LWA waste volume.

This report documents the scaling of the organic ligands used in the baseline actinide solubility calculations the results of which will be included in the CRA-2026 PA for the interim state repository. A separate report (Domski, 2025) documents the scaling of the organic ligands for the final state repository, which provides sufficient storage for disposal of the entire WIPP LWA waste volume.

This analysis report provides the interim-state repository concentrations of the organic ligands acetate, citrate, ethylenediaminetetraacetate (EDTA), and oxalate dissolved in two standard Waste Isolation Pilot Plant (WIPP) brines as a function of the volumes of these brines in the repository. These brines are Generic Weep Brine (GWB) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6). GWB is a synthetic brine representative of intergranular Salado Formation (Fm.) brines at or near the stratigraphic horizon of the repository (Krumhansl et al., 1991; Snider, 2003). ERDA-6 (Popielak et al., 1983) is a synthetic brine representative of fluids in brine reservoirs in the Castile Fm., which underlies the Salado Fm.

The scaled concentrations of the organic ligands will be used to calculate An(III), An(IV), and An(V) baseline concentrations for the CRA-2026 IS.

Note that the calculations documented in this analysis report are a deviation from AP-153 Revision 1 (Brush et al., 2012) because the analysis plan does not provide a description of how the calculations should be performed. The procedure for the calculation of organic ligand concentrations is documented in this report in a transparent and reproducible manner.

Table 1 defines the abbreviations, acronyms, and initialisms used in this report.

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
acetate	CH_3COO^- or $CH_3CO_2^-$
acetic acid	CH_3COOH or CH_3CO_2H

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Abbreviation, Acronym, or Initialism	Definition
AP	analysis plan
C	carbon
CCA	(WIPP) Compliance Certification Application
CCDF	complementary cumulative distribution function
citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
citric acid	$(CH_2COOH)_2C(OH)(COOH)$ or $(CH_2CO_2H)_2C(OH)(CO_2H)$
CRA-2004	the first (WIPP) Compliance Recertification Application
CRA-2009	the second (WIPP) Compliance Recertification Application
CRA-2009	third (WIPP) Compliance Recertification Application
CRA-2014	fourth (WIPP) Compliance Recertification Application
CRA-2019	fifth (WIPP) Compliance Recertification Application
DBR	direct brine release (a release to the surface)
DOE	(U.S.) Department of Energy
EDTA	ethylenediaminetetraacetic acid, $(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$ or $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)_2$.
g	gram(s)
H	hydrogen
kg	kilogram(s)
L	liter(s)
M	molar
m	meter(s) or molal
mol	moles
N	nitrogen
Na	sodium
Na-acetate	CH_3COONa or CH_3CO_2Na
NaH_2citrate	$(CH_2COOH)_2C(OH)(COONa)$ or $(CH_2CO_2H)_2C(OH)(CO_2Na)$
NaH_3EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)(CH_2COONa)$ or $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2Na)$
NaH-oxalate	$(COOH)(COONa)$ or $(CO_2H)(CO_2Na)$
O	oxygen
oxalate	$(COO)^{2-}$ or $C_2O_4^{2-}$
oxalic acid	$(COOH)_2$ or $H_2C_2O_4$
PA	(WIPP) performance assessment
PABC	(WIPP) Performance Assessment Baseline Calculation(s)

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Abbreviation, Acronym, or Initialism	Definition
PAVT	(WIPP) Performance Assessment Verification Test
RPPA-2022	Replacement Panels performance assessment
WIPP	Waste Isolation Pilot Plant
wt	weight

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2 MASSES OF ORGANIC LIGANDS TO BE EMPLACED IN THE WIPP

Van Soest (2025b, Table 5-9) provided the total masses of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid to be emplaced in the WIPP. Table 2, column labeled "CRA-2026 IS," of this analysis report (see next page) contains the masses of the organic ligands from Van Soest (2025b).

Acetic acid, citric acid, EDTA, and oxalic acid contain one, three, four, and two protons (H^+), respectively, for which Na (or other alkali or alkaline-earth metal cations) can substitute. Acetate, citrate, EDTA, and oxalate are the deprotonated forms of these acids, and have charges of –1, –3, –4, and –2, respectively; these deprotonated species are referred to as "ligands." Table 1 (see Section 1 above) provides the formulas for these acids and ligands. In TRU waste acetate, citrate, EDTA, and oxalate must exist in the zero-net charge by combining with counter ions such as H^+ or Na^+. For this analysis, it was assumed that the acetate, citrate, oxalate, and EDTA as reported by Van Soest (2012), combine with H^+ and are fully protonated. This is conservative, because assuming the presence of any positively charged ions with an atomic mass greater than that of H^+ (e.g., Na^+) would decrease the number of moles of ligands present in the waste and brine.

Table 2 also compares the masses of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid reported by Van Soest (2025b) to those used to calculate the concentrations of organic ligands for the previous WIPP certification- or recertification-related PA calculations. Note that masses of acetic acid, Na acetate, citric acid, Na citrate, Na EDTA, oxalic acid, and Na oxalate were reported for the CRA-2004 PA through the CRA-2009 PABC. Beginning with CRA-2014 PA this changed and the organics were reported as acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid. Reporting the organic masses in this manner is conservative, because reporting the presence of Na-containing forms of these compounds would decrease the number of moles of these ligands present in the waste and brine.

Note also that the inventory reports used for the CRA-2004 PA, the CRA-2004 PABC and CRA 2009 PA, and the CRA-2009 PABC did not specify how many of the acidic hydrogen ions in their reported masses of Na citrate, Na EDTA, or Na oxalate were replaced by Na. Therefore, Brush and Xiong (2003; 2005; 2009) assumed that only one of the acidic hydrogen ions was replaced with Na to calculate the molecular weights of NaH_2citrate, NaH_3EDTA, and NaH-oxalate. This assumption was also conservative (i.e., it resulted in the higher molar quantities of the ligands citrate, EDTA, and oxalate rather than using their salt forms with a higher number of Na^+).

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Table 2. Comparisons of Total Masses (kg) of Organic Compounds Used to Calculate the Concentrations of Organic Ligands for WIPP Certification- or Recertification-Related PA Calculations.

Compound	CRA-2004 PA[B]	CRA-2004 PABC & CRA-2009 PA[C]	CRA-2009 PABC[D]	CRA-2014 PA[E]	CRA-2019 DPA[F]	RPPA[G]
Acetate	None reported	None reported	None reported	9.96×10^3	1.37×10^4	2.32×10^4
Acetic acid	2.01×10^2	1.42×10^2	1.32×10^4	1.41×10^4	1.59×10^4	2.05×10^4
Na-acetate	1.21×10^4	8.51×10^3	9.70×10^3	None reported	None reported	None reported
Citrate	None reported	None reported	None reported	2.55×10^3	2.63×10^3	2.75×10^3
Citric acid	1.69×10^3	1.19×10^3	5.68×10^3	5.23×10^3	5.08×10^3	8.09×10^3
NaH_2citrate	5.66×10^2	4.00×10^2	2.55×10^3	None reported	None reported	None reported
EDTA	None reported	None reported	None reported	3.76×10^2	4.03×10^2	4.29×10^2
NaH_3EDTA	3.63×10^1	2.56×10^1	3.54×10^2	None reported	None reported	None reported
Oxalate	None reported	None reported	None reported	6.50×10^2	7.00×10^2	7.69×10^2
Oxalic acid	1.95×10^4	1.38×10^4	2.66×10^4	1.78×10^4	1.70×10^4	1.80×10^4
NaH-oxalate	4.81×10^4	3.39×10^4	6.46×10^2	None reported	None reported	None reported

Footnotes for Table 2 provided on next page.

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Table 2 (continued)

Compound	RPPCR[H]	CRA-2026 FS[I]	CRA-2026 IS[J]
Acetate	1.72×10^4	1.66×10^4	**1.58×10^4**
Acetic acid	1.76×10^4	1.58×10^4	**1.56×10^4**
Na-acetate	None reported	None reported	None reported
Citrate	2.78×10^3	2.77×10^3	**2.62×10^3**
Citric acid	8.82×10^3	8.92×10^3	**8.16×10^3**
NaH_2citrate	None reported	None reported	None reported
EDTA	4.17×10^2	4.45×10^2	**3.92×10^2**
NaH_3EDTA	None reported	None reported	None reported
Oxalate	7.78×10^2	8.06×10^2	**7.15×10^2**
Oxalic acid	1.68×10^4	1.69×10^4	**1.68×10^4**
NaH-oxalate	None reported	None reported	None reported

Footnotes for Table 2:

A. From U.S. DOE (1996b, Table SOTERM-4, column labeled "Inventory Amount") multiplied by a scaling factor of 2.05. U.S. DOE (1996b) obtained this scaling factor from U.S. DOE (1996a, p. 3-1). U.S. DOE (1996b, Table SOTERM-4, column labeled "Inventory Amount") referred to these as "acetate," "citrate," "EDTA," and "oxalate," respectively.
B. From Crawford (2003); used by Brush and Xiong (2003).
C. From Crawford (2003), Crawford and Leigh (2003), and Leigh (2003, 2005a, 2005b); used by Brush and Xiong (2005).

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D. From Crawford et al. (2009); used by Brush and Xiong (2009).
E. From Van Soest (2012)
F. From Van Soest (2018)
G. From Van Soest (2022)
H. From Van Soest (2022a)
I. From Van Soest (2025a)
J. From Van Soest (2025b)

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3 CALCULATIONS OF MOLECULAR WEIGHTS OF ORGANIC LIGANDS

The following atomic weights were used to calculate the molecular weights of acetic acid, citric acid, EDTA, and oxalic acid: H: 1.00794 g/mol; C: 12.0107 g/mol; N: 14.00674 g/mol; O: 15.9994 g/mol; and Na: 22.989770 g/mol (Lide, 2002).

The molecular weights of acetic acid, citric acid, EDTA, and oxalic acid were calculated as follows:

- Acetic acid: (4 × atomic mass H) + (2 × atomic mass C) + (2 × atomic mass O) = (4 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 2 × 15.9994 g/mol) = (4.0318 + 24.0214 + 31.9988) g/mol = 60.0520 g/mol.

- Citric acid: (8 × atomic mass H) + (6 × atomic mass C) + (7 × atomic mass O) = (8 × 1.00794 g/mol) + (6 × 12.0107 g/mol) + (7 × 15.9994 g/mol) = (8.0635 + 72.0642 + 111.9958) g/mol = 192.1235 g/mol.

- EDTA: (16 × atomic mass H) + (10 × atomic mass C) + (2 × atomic mass of N) + (8 × atomic mass O) = (16 × 1.00794 g/mol) + (10 × 12.0107 g/mol) + (2 × 14.00674 g/mol) + (8 × 15.9994 g/mol) = (16.1270 + 120.1070 + 28.0135 + 127.9952) g/mol = 292.2427 g/mol.

- Oxalic acid: (2 × atomic mass H) + (2 × atomic mass C) + (4 × atomic mass O) = (2 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 4 × 15.9994 g/mol) = (2.0159 + 24.0214 + 63.9976) g/mol = 90.0349 g/mol.

Table 3 summarizes the molecular weights of these compounds.

Table 3. Formulas and Molecular Weights of Two Forms of Four Ligands that Could be Emplaced in the WIPP.

Compound	Formula Used in This Analysis Report	Mol Wt (g)
Acetic acid	CH_3COOH	60.0520
Citric acid	$(CH_2COOH)_2C(OH)(COOH)$	192.1235
EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$	292.2427
Oxalic acid	$(COOH)_2$	90.0349

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4 BRINE VOLUME USED TO CALCULATE ORGANIC-LIGAND CONCENTRATIONS

Five volumes of GWB or ERDA-6 were used to calculate the concentrations of acetate, citrate, EDTA, and oxalate for CRA-2026 IS PA. The initial minimum volume, 6,314 m^3, of brine, representing the direct brine release (DBR) volume calculated from the updated repository volume parameter (Brunell, 2025) was used to calculate the maximum dissolved concentrations of these organic ligands in a homogeneous, 12-panel PA repository. A DBR is defined as a release of brine that occurs directly from the repository to the surface above the repository (i.e., without lateral transport through an offsite transport pathway such as the Culebra Member of the Rustler Formation). The maximum concentrations of the organic ligands were calculated by assuming that the total masses of these ligands in the waste would dissolve completely in this volume (DBR volume) of brine.

The maximum organic ligand concentrations were then recalculated for brine volumes that are 2, 3, 4, or 5 times this minimum volume by dividing these maximum concentrations by 2, 3, 4, or 5, respectively. This method that has been in place since CRA-2014.

Table 4 (see next page) compares the brine volumes used to calculate the concentrations of organic ligands for WIPP certification- or recertification-related PA calculations. The previous estimates of the minimum volume of brine in the repository required for a DBR were based on the results of previous PA calculations. For example, Stein (2005) used the results of the CRA-2004 PA calculations to estimate a new minimum brine volume of 10,011 m^3, which was used for the actinide-solubility calculations for the CRA-2004 PABC and the CRA-2009 PA. Clayton (2008), however, successfully established a minimum brine volume that is independent of the results of any given PA calculation. Clayton (2008) provided a detailed description of how this minimum volume was established, and it is the same method used by King (2021), Docherty (2024), and Brunell (2025).

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Table 4. Comparisons of Brine Volumes (m^3) Used to Calculate the Concentrations of Organic Ligands for WIPP Certification- or Recertification-Related PA Calculations.

Brine Volume	CCA, PAVT & CRA-2004 PA[A]	CRA-2004 PABC & CRA-2009 PA[B]	CRA-2009 PABC[C]	CRA-2014 PA & CRA-2019 DPA[C,D]	RPPA & RPPCR[E]	CRA-2026 FS[F]	CRA-2026 IS[G]
Minimum	29,841	10,011	17,400	17,400	33,804	9,608	6,314
Additional volume for PA post CRA-2009 PABC	-	-	-	34,800 (2 × min.)	67,608 (2 × min.)	19,216 (2 × min.)	12,628 (2 × min.)
Additional volume for PA post CRA-2009 PABC	-	-	-	52,200 (3 × min)	101,412 (3 × min)	28,824 (3 × min)	18,942 (3 × min)
Additional volume for PA post CRA-2009 PABC	-	-	-	69,600 (4 × min)	135,216 (4 × min)	38,432 (4 × min)	25,256 (4 × min)
Additional volume for PA post CRA-2009 PABC	-	-	-	87,000 (5 × min)	169,020 (5 × min)	48,040 (5 × min)	31,570 (5 × min)

A. [T]he smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996)
B. "[A] reasonable minimum volume of brine in the repository required for a brine release" (Stein, 2005).
C. "[A] reasonable minimum volume of brine in the repository required for a DBR" (Clayton, 2008).
D. Also used 2 ×, 3 ×, 4 ×, and 5 × the minimum brine volume of Clayton (2008).

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E. Also used 2 ×, 3 ×, 4 ×, and 5 × the minimum brine volume of King (2021).
F. Also used 2 ×, 3 ×, 4 ×, and 5 × the minimum brine volume of Docherty (2024).
G. Also used 2 ×, 3 ×, 4 ×, and 5 × the minimum brine volume of Brunell (2025).

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5 CALCULATIONS OF ORGANIC-LIGAND CONCENTRATIONS

We calculated the concentrations of acetic acid, citric acid, EDTA, and oxalic acid by adding the masses in kg of acetate and acetic acid, citrate and citric acid, and oxalate and oxalic acid from Table 2 of this report (column labeled "CRA-2026 IS"). This is because we assumed that acetate, citrate, and oxalate are present in TRU waste as acetic acid, citric acid, and oxalic acid (see Section 2 above). We then multiplied the total masses of these compounds and EDTA in kg by 1000 g/kg to convert them from kg to grams. Next, we divided these masses by the molecular weights of these compounds from Table 3 of this report, which yielded the total quantities of these compounds to be emplaced in moles. Finally, we divided these molar quantities by 6.314×10^6 L to obtain the concentrations of these compounds in units of mol/L, or M:

- Acetic acid: $((1.58 \times 10^4 \text{ kg} + 1.56 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 6.314 \times 10^6 \text{ L} = 8.29 \times 10^{-2}$ M.

- Citric acid: $((2.62 \times 10^3 \text{ kg} + 8.16 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 6.314 \times 10^6 \text{ L} = 8.88 \times 10^{-3}$ M.

- EDTA: $((3.92 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (292.2427 \text{ g/mol})) \div 6.314 \times 10^6 \text{ L} = 2.13 \times 10^{-4}$ M.

- Oxalic acid: $((7.15 \times 10^2 \text{ kg} + 1.68 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 6.314 \times 10^6 \text{ L} = 3.08 \times 10^{-2}$ M.

Table 5 (see next page) summarizes our calculations of the dissolved concentrations of these organic ligands in the minimum volume of brine required for a DBR from a homogeneous, 12-Panel Repository. The intermediate results have been rounded to three significant figures for entry in Table 5. However, we did not round off until we obtained the final concentrations in our calculations.

Table 6 (see next page) provides the dissolved concentrations of acetate, citrate, EDTA, and oxalate for the minimum brine volume of 6,314 m^3 and for volumes that are 2, 3, 4, or 5 times this minimum volume. In this table, we report as ligands, not acids, because the ligands would potentially form complexes with the actinide elements in the TRU waste that is being emplaced in the WIPP. The intermediate results have been rounded to three significant figures for entry in Table 6. However, we did not round off until we obtained the final concentrations in our calculations.

We first calculated the results shown in Tables 5 and 6 with a hand calculator, then checked them with an Excel spreadsheet (*Org Lig Concs_CRA-2026_12-panel.xlsx*). This spreadsheet will be stored in the SNL/WIPP Records Center along with all other records for AP-153, Task 3 at /data/cvs/CVSLIB/WIPP_ANALYSES/CRA-2026/AP153task3.

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Table 5. Summary of Our Calculations of the Dissolved Concentrations of Organic Ligands in the Minimum Volume of Brine (6,314 m^3) Required for a DBR from a Homogeneous, 12-Panel Repository.

Compound	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	3.14×10^{7}	5.23×10^{5}	8.29×10^{-2}
Citric acid	1.08×10^{7}	5.61×10^{4}	8.88×10^{-3}
EDTA	3.92×10^{5}	1.34×10^{3}	2.13×10^{-4}
Oxalic acid	1.75×10^{7}	1.95×10^{5}	3.08×10^{-2}

Table 6. Dissolved Concentrations of Organic Ligands (M) in the Minimum Volume of Brine Required for a DBR and for Volumes that are 2 ×, 3 ×, 4 ×, and 5 × the Minimum Volume.

Organic Ligand	Minimum Required for a DBR	2 × Minimum	3 × Minimum	4 × Minimum	5 × Minimum
Acetate	8.29×10^{-2}	4.15×10^{-2}	2.76×10^{-2}	2.07×10^{-2}	1.66×10^{-2}
Citrate	8.88×10^{-3}	4.44×10^{-3}	2.96×10^{-3}	2.22×10^{-3}	1.78×10^{-3}
EDTA	2.13×10^{-4}	1.06×10^{-4}	7.09×10^{-5}	5.31×10^{-5}	4.25×10^{-5}
Oxalate	3.08×10^{-2}	1.54×10^{-2}	1.03×10^{-2}	7.71×10^{-3}	6.17×10^{-3}

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6 COMPARISONS WITH PREVIOUS RESULTS

Table 6 (see Section 5 above) provides the concentrations of acetate, citrate, EDTA, and oxalate that will be used for the baseline actinide-solubility calculations for the CRA-2026 IS. Table 6 provides these concentrations for the minimum volume of GWB or ERDA-6 (6,314 m^3) required for a DBR from the repository, and for volumes that are 2, 3, 4, or 5 times this minimum volume. Table 7 (see below) compares the CRA-2026 IS acetate, citrate, EDTA, and oxalate concentrations calculated for the minimum brine volume to those used for previous certification- or recertification-related PA calculations. Inspection of Table 7 shows an increase in the all of the organic ligands concentration compared to previous PA's, this is due to the smaller DBR volume and could result in changes to the actinide solubilities for the CRA-2026 IS compared to previous recertifications.

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Table 7. Comparison of the Dissolved Concentrations of Organic Ligands in the Minimum Volume of Brine Required for a DBR from a Homogeneous, interim-state 12-Panel Repository.

Organic Ligand	CRA-2004 PA[B] (M)	CRA-2004 PABC[C] and CRA-2009 PA (M)	CRA-2009 PABC[D] (M)	CRA-2014 PA[E] (M)	CRA-2019 DPA[F] (M)	RPPA[G] (M)
Acetate	5.05×10^{-3}	1.06×10^{-2}	1.94×10^{-2}	2.30×10^{-2}	2.83×10^{-2}	2.15×10^{-2}
Citrate	3.83×10^{-4}	8.06×10^{-4}	2.38×10^{-3}	2.33×10^{-3}	2.30×10^{-3}	1.67×10^{-3}
EDTA	3.87×10^{-6}	8.14×10^{-6}	6.47×10^{-5}	7.40×10^{-5}	7.92×10^{-5}	4.35×10^{-5}
Oxalate	2.16×10^{-2}	4.55×10^{-2}	1.73×10^{-2}	1.18×10^{-2}	1.13×10^{-2}	6.18×10^{-3}

Organic Ligand	RPPCR[H] (M)	CRA-2026 FS[I] (M)	CRA-2026 IS[J] (M)
Acetate	1.72×10^{-2}	5.62×10^{-2}	8.29×10^{-2}
Citrate	1.79×10^{-3}	6.33×10^{-3}	8.88×10^{-3}
EDTA	4.22×10^{-5}	1.58×10^{-4}	2.13×10^{-4}
Oxalate	5.76×10^{-3}	2.05×10^{-2}	3.08×10^{-2}

A. U.S. DOE (1996b, Appendix SOTERM, Table SOTERM-4)
B. Brush and Xiong (2003)
C. Brush and Xiong (2005)

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D. Brush and Xiong (2009)
E. Brush and Domski (2013)
F. Sisk-Scott (2019)
G. Domski (2022)
H. Domski (2023)
I. Domski (2025)
J. This Report

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7 CONCLUSIONS

This analysis report provides updated concentrations of the organic ligands acetate, citrate, EDTA, and oxalate dissolved in GWB and ERDA-6 as a function of the volume of these brines in the repository. These concentrations will be used to calculate the baseline actinide solubilities as a function of brine volume for the CRA-2026 IS. This PA will use solubilities that depend on the volume of brine released from the repository.

Table 6 (see Section 5 above) provides the concentrations of acetate, citrate, EDTA, and oxalate that will be used for the baseline actinide-solubility calculations for the CRA-2026 IS. Table 6 provides these concentrations for the minimum volume of GWB or ERDA-6 (6,314 m^3) required for a DBR from the repository, and for volumes that are 2, 3, 4, or 5 times this minimum volume. Table 7 (Section 6) compares our new acetate, citrate, EDTA, and oxalate concentrations calculated for the minimum brine volume to those used for previous certification- or recertification-related PA calculations. Inspection of Tables 6 and 7 shows that the concentrations of acetate, citrate, EDTA, and oxalate increased due to the smaller minimum brine volume compared to previous PA's, this could influence actinide solubility.

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