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Sandia National Laboratories
Waste Isolation Pilot Plant

Experimental determination of solubility constant of di-calcium ethylenediaminetetraacetic acid (Ca_2EDTA), $Ca_2C_{10}H_{12}N_2O_8(s)$, in the NaCl–$H_2O$ system

Work Carried Out under Task 29 of AP-154: Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA.
To be included in the AP-154 records package

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WIPP:1.4.2.2:PA:QA-L:558083

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1 INTRODUCTION

This analysis report (AR) provides the solubility constant of di-calcium ethylenediaminetetraacetic acid ($Ca_2EDTA(s)$), $Ca_2C_{10}H_{12}N_2O_8(s)$, determined in NaCl solutions.

The computer code EQ3/6 Version 8.0a (Wolery, 2008; Wolery et al., 2010; Xiong, 2011b) was used for this analysis. Wolery (2008), Wolery et al. (2010) and Xiong (2011b) completed the qualification of Version 8.0a of EQ3/6 according to Sandia National Laboratories' (SNL's) WIPP quality assurance (QA) procedures for WIPP compliance-related actinide solubility calculations, and US EPA approved it on September 27, 2011 (US EPA, 2011).

This analysis was carried out under Task 29 of AP-154 (Xiong, 2011c). There is one deviation from AP-154. The deviation is that the Python script developed by Kirchner (2012) is used instead of the one developed by Nemer (2010).

Table 1 (see next page) defines the generic abbreviations, acronyms, and initialisms used in this report and other analysis reports.

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
acetate	CH_3COO^- or $CH_3CO_2^-$
Am, Am(III)	americium, americium in the +III oxidation state
am	amorphous
anhydrite	$CaSO_4$
AP	analysis plan
aq	aqueous
aragonite	$CaCO_3$,a polymorph of $CaCO_3$ that is metastable with respect to calcite
atm	atmosphere(s)
B, B(III)	boron, boron in the +III oxidation state
Br, Br(−I)	bromine, bromine in the −I oxidation state
brucite	$Mg(OH)_2$
C	carbon
Ca, Ca(II), Ca^{2+}	calcium, calcium in the +II oxidation state, calcium ion
calcite	$CaCO_3$, the thermodynamically stable polymorph of $CaCO_3$
citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
Cl, Cl(−I), Cl^-	chlorine, chlorine in the −I oxidation state, chloride ion
CMS	(Sandia/WIPP software) Configuration Management System
CO_2	carbon dioxide
CO_3^{2-}	carbonate
CRA-2009	the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009
DB	(thermodynamic) database
DOE	(U.S.) Department of Energy
dolomite	$CaMg(CO_3)_2$, a carbonate mineral that is nucleates and grows slowly under low-temperature conditions and is often suppressed (prevented from forming) in geochemical modeling calculations
DRZ	disturbed rock zone
EDTA	ethylenediaminetetraacetate, $(CH_2COO)_2N(CH_2)_2N(CH_2COO)_2)^{4-}$ or $(CH_2CO_2)_2N(CH_2)_2N(CH_2CO_2)^{4-}$
EPA	(U.S.) Environmental Protection Agency
EQ3/6	a geochemical software package for speciation and solubility calculations (EQ3NR) and reaction-path calculations (EQ6)

Table 1 continued on next page

Table 1. Abbreviations, Acronyms, and Initialisms (continued).

Abbreviation, Acronym, or Initialism	Definition
ERDA-6	Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs
f_{CO_2}	fugacity (similar to the partial pressure) of CO_2
Fm.	Formation
FMT	Fracture-Matrix Transport, a geochemical speciation and solubility code
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines at or near the stratigraphic horizon of the repository
gypsum	$CaSO_4 \cdot 2H_2O$
H or H_2, H^+	hydrogen or hydrogen ion
halite	NaCl
H_2O	water (aq, g, or contained in solid phases)
hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
I	ionic strength
K, K(I)	potassium, potassium in the +I oxidation state
kg	kilogram(s)
M	molar
m	meter(s) or molal
magnesite	$MgCO_3$
Mg, Mg(II)	magnesium, magnesium in the +II oxidation state
MgO	magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and various impurities
mM	millimolar
Na, Na(I), Na^+	sodium, sodium in the +I oxidation state, sodium ion
nesquehonite	$MgCO_3 \cdot 3H_2O$
Np, Np(V)	neptunium, neptunium in the +V oxidation state
O or O_2	oxygen
OH, OH^-	hydroxide or hydroxide ion
oxalate	$(COO)^{2-}$ or $C_2O_4^{2-}$
PA	performance assessment
PABC	Performance Assessment Baseline Calculations

Table 1 continued on next page

Table 1. Abbreviations, Acronyms, and Initialisms (continued).

Abbreviation, Acronym, or Initialism	Definition
periclase	pure, crystalline MgO, the primary constituent of the WIPP engineered barrier
pH	the negative, common logarithm of the activity of H^+
pcH	the negative, common logarithm of the molar concentration of H^+
phase 3	$Mg_2Cl(OH)_3 \cdot 4H_2O$
phase 5	$Mg_3(OH)_5Cl \cdot 4H_2O$
polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$
QA	quality assurance
Rev.	revision
RH	relative humidity
S, S(VI), SO_4^{2-}	sulfur, sulfur in the +VI oxidation state, sulfate ion
s	solid
SCA	S. Cohen and Associates
SNL	Sandia National Laboratories
Th, Th(IV)	thorium, thorium in the +IV oxidation state
TIC	total inorganic C
WIPP	(U.S. DOE) Waste Isolation Pilot Plant
wt %	weight percent
μ^0/RT	dimensionless standard chemical potential

2 METHODS

The objective of this analysis was to obtain the solubility constant for di-calcium ethylenediaminetetraacetic acid, $Ca_2C_{10}H_{12}N_2O_8(s)$, abbreviated as $Ca_2EDTA(s)$, based on solubility data of $Ca_2EDTA(s)$ in NaCl solutions produced at SNL (Jang, Xiong, Kim, and Nemer, 2012). Table 2 lists experimental data in NaCl solutions from that report.

The solubility constant of $Ca_2EDTA(s)$ is important to performance assessment (PA). Regarding EDTA concentrations in the brines, the chemical equilibrium calculations that support PA using the current WIPP thermodynamic database are inventory-limited with respect to species containing EDTA. The addition of the solubility constant for $Ca_2EDTA(s)$ into the WIPP thermodynamic database would make the concentrations of EDTA become solubility-limited, should the EDTA concentrations in inventories increase to level to reach the saturation of $Ca_2EDTA(s)$.

The dissolution reaction for $Ca_2EDTA(s)$ can be expressed as,

$$Ca_2EDTA(s) = 2Ca^{2+} + EDTA^{4-} \quad (1)$$

Based on total calcium and EDTA concentrations from chemical analyses, the solubility constant ($\log K_{sp}$) for Reaction (1) can be obtained by computer modeling.

The experimental solubility data for $Ca_2EDTA(s)$ in NaCl gathered under TP 08-02 and reported in the milestone report (Jang, Xiong, Kim, and Nemer, 2012), are utilized to derive the $\log K_{sp}$ for $Ca_2EDTA(s)$ with the aid of the computer code EQ3/6 Version 8.0a (Wolery et al., 2010; Xiong, 2011b). The essence of the modeling is to minimize the difference between experimental and model predicted values.

Using experimental solubility data of $Ca_2EDTA(s)$ for NaCl solutions (Jang, Xiong, Kim, and Nemer, 2012), $\log K_{sp}$ only for $Ca_2EDTA(s)$ is first evaluated. The value for $\log K_{sp}$ is evaluated by using the Python script (Ca2EDTA_NaCl_PD4.py) which runs the EQ3CodeModule optimization routine (Kirchner, 2012) with EQ3NR input files CaED-1.3i through CaED-112.3i. These files are located in the folder labeled "Ca2EDTA_NaCl" in the zip file "AP154_Task29_DataPackage.zip".

Table 2. Experimental results concerning solubility of $Ca_2EDTA(s)$ in NaCl solutions produced at SNL at 22.5 ± 1.5 °C (from Jang, Xiong, Kim, and Nemer, 2012)*.

Experimental Number	Supporting Medium, NaCl, molal	Experimental time, days	pmH**	Total calcium concentrations, $m_{\Sigma Ca}$	Total EDTA concentrations, $m_{\Sigma EDTA}$
Ca_2EDTA-0.01-1	0.010	390	8.23	7.14E-02	5.92E-02
Ca_2EDTA-0.01-2	0.010	390	8.20	7.16E-02	3.75E-02
Ca_2EDTA-0.1-1	0.10	390	8.37	8.63E-02	6.88E-02
Ca_2EDTA-0.1-2	0.10	390	7.90	8.69E-02	6.79E-02
Ca_2EDTA-1.0-1	1.0	390	8.39	1.35E-01	9.21E-02
Ca_2EDTA-1.0-2	1.0	390	7.92	1.35E-01	9.18E-02
Ca_2EDTA-2.0-1	2.1	390	8.54	1.39E-01	9.16E-02
Ca_2EDTA-2.0-2	2.1	390	8.49	1.42E-01	9.32E-02
Ca_2EDTA-3.0-1	3.2	390	8.71	1.35E-01	8.49E-02
Ca_2EDTA-3.0-2	3.2	390	8.47	1.30E-01	8.26E-02
Ca_2EDTA-4.0-1	4.4	390	8.69	1.17E-01	5.31E-02
Ca_2EDTA-4.0-2	4.4	390	8.63	1.18E-01	7.50E-02
Ca_2EDTA-5.0-1	5.0	390	8.19	1.10E-01	6.80E-02
Ca_2EDTA-5.0-2	5.0	390	8.19	1.10E-01	6.92E-02
Ca_2EDTA-0.01-1	0.010	965	7.79	7.27E-02	5.72E-02
Ca_2EDTA-0.01-2	0.010	965	7.85	7.28E-02	5.70E-02
Ca_2EDTA-0.1-1	0.10	965	7.88	8.36E-02	6.77E-02
Ca_2EDTA-0.1-2	0.10	965	7.81	7.99E-02	6.77E-02
Ca_2EDTA-1.0-1	1.0	965	8.09	1.21E-01	9.10E-02
Ca_2EDTA-1.0-2	1.0	965	7.77	1.22E-01	9.30E-02
Ca_2EDTA-2.0-1	2.1	965	8.18	1.20E-01	9.20E-02
Ca_2EDTA-2.0-2	2.1	965	8.20	1.19E-01	9.45E-02
Ca_2EDTA-3.0-1	3.2	965	8.43	1.08E-01	8.55E-02
Ca_2EDTA-3.0-2	3.2	965	8.30	1.09E-01	8.51E-02
Ca_2EDTA-4.0-1	4.4	965	8.41	9.31E-02	7.54E-02
Ca_2EDTA-4.0-2	4.4	965	8.40	9.16E-02	7.68E-02
Ca_2EDTA-5.0-1	5.0	965	8.11	8.55E-02	7.09E-02
Ca_2EDTA-5.0-2	5.0	965	8.10	8.49E-02	7.04E-02
Ca_2EDTA-0.01-1	0.010	1050	7.84	7.30E-02	5.83E-02
Ca_2EDTA-0.01-2	0.010	1050	7.83	7.27E-02	5.87E-02
Ca_2EDTA-0.1-1	0.10	1050	7.81	8.49E-02	7.21E-02

Ca_2EDTA-0.1-2	0.10	1050	7.81	8.52E-02	6.93E-02
Ca_2EDTA-1.0-1	1.0	1050	8.00	1.21E-01	9.33E-02
Ca_2EDTA-1.0-2	1.0	1050	7.68	1.21E-01	9.09E-02
Ca_2EDTA-2.0-1	2.1	1050	8.13	1.20E-01	9.10E-02
Ca_2EDTA-2.0-2	2.1	1050	8.11	1.23E-01	9.00E-02
Ca_2EDTA-3.0-1	3.2	1050	8.23	1.09E-01	8.36E-02
Ca_2EDTA-3.0-2	3.2	1050	8.20	1.08E-01	8.28E-02
Ca_2EDTA-4.0-1	4.4	1050	8.37	9.15E-02	7.38E-02
Ca_2EDTA-4.0-2	4.4	1050	8.33	9.41E-02	7.49E-02
Ca_2EDTA-5.0-1	5.0	1050	8.14	8.97E-02	6.98E-02
Ca_2EDTA-5.0-2	5.0	1050	8.10	8.57E-02	6.93E-02
Ca_2EDTA-0.01-1	0.010	1099	7.88	7.33E-02	5.32E-02
Ca_2EDTA-0.01-2	0.010	1099	7.86	7.25E-02	5.37E-02
Ca_2EDTA-0.1-1	0.10	1099	7.90	8.42E-02	6.36E-02
Ca_2EDTA-0.1-2	0.10	1099	7.85	8.17E-02	6.37E-02
Ca_2EDTA-1.0-1	1.0	1099	8.03	1.22E-01	8.87E-02
Ca_2EDTA-1.0-2	1.0	1099	7.72	1.24E-01	8.88E-02
Ca_2EDTA-2.0-1	2.1	1099	8.13	1.21E-01	8.83E-02
Ca_2EDTA-2.0-2	2.1	1099	8.11	1.20E-01	8.84E-02
Ca_2EDTA-3.0-1	3.2	1099	8.25	1.07E-01	8.09E-02
Ca_2EDTA-3.0-2	3.2	1099	8.19	1.05E-01	8.13E-02
Ca_2EDTA-4.0-1	4.4	1099	8.33	9.11E-02	6.94E-02
Ca_2EDTA-4.0-2	4.4	1099	8.31	9.35E-03	6.94E-02
Ca_2EDTA-5.0-1	5.0	1099	8.14	8.38E-02	6.42E-02
Ca_2EDTA-5.0-2	5.0	1099	8.14	8.23E-02	6.44E-02
Ca_2EDTA-0.01-1	0.010	1149	7.94	7.24E-02	5.49E-02
Ca_2EDTA-0.01-2	0.010	1149	7.92	6.64E-02	5.44E-02
Ca_2EDTA-0.1-1	0.10	1149	7.96	8.39E-02	6.42E-02
Ca_2EDTA-0.1-2	0.10	1149	7.90	8.40E-02	6.44E-02
Ca_2EDTA-1.0-1	1.0	1149	8.02	1.20E-01	8.97E-02
Ca_2EDTA-1.0-2	1.0	1149	7.73	1.18E-01	9.09E-02
Ca_2EDTA-2.0-1	2.1	1149	8.09	1.20E-01	8.92E-02
Ca_2EDTA-2.0-2	2.1	1149	8.14	1.24E-01	8.91E-02
Ca_2EDTA-3.0-1	3.2	1149	8.35	1.09E-01	8.21E-02
Ca_2EDTA-3.0-2	3.2	1149	8.22	1.11E-01	8.16E-02
Ca_2EDTA-4.0-1	4.4	1149	8.34	9.62E-02	7.11E-02
Ca_2EDTA-4.0-2	4.4	1149	8.35	9.28E-03	7.06E-02
Ca_2EDTA-5.0-1	5.0	1149	8.23	8.11E-02	6.56E-02

Ca_2EDTA-5.0-2	5.0	1149	8.18	8.14E-02	6.58E-02
Ca_2EDTA-0.01-1	0.010	1197	7.86	7.10E-02	5.50E-02
Ca_2EDTA-0.01-2	0.010	1197	7.87	7.13E-02	5.54E-02
Ca_2EDTA-0.1-1	0.10	1197	7.90	8.46E-02	6.48E-02
Ca_2EDTA-0.1-2	0.10	1197	7.91	8.49E-02	6.51E-02
Ca_2EDTA-1.0-1	1.0	1197	8.00	1.21E-01	9.07E-02
Ca_2EDTA-1.0-2	1.0	1197	7.72	1.21E-01	9.01E-02
Ca_2EDTA-2.0-1	2.1	1197	8.10	1.18E-01	9.05E-02
Ca_2EDTA-2.0-2	2.1	1197	8.07	1.20E-01	8.98E-02
Ca_2EDTA-3.0-1	3.2	1197	8.23	1.05E-01	8.04E-02
Ca_2EDTA-3.0-2	3.2	1197	8.19	1.07E-01	8.14E-02
Ca_2EDTA-4.0-1	4.4	1197	8.31	9.25E-02	7.15E-02
Ca_2EDTA-4.0-2	4.4	1197	8.30	9.12E-03	7.12E-02
Ca_2EDTA-5.0-1	5.0	1197	8.19	8.49E-02	6.62E-02
Ca_2EDTA-5.0-2	5.0	1197	8.15	8.13E-02	6.60E-02
Ca_2EDTA-0.01-1	0.010	1348	7.85	7.31E-02	5.54E-02
Ca_2EDTA-0.01-2	0.010	1348	7.86	7.26E-02	5.56E-02
Ca_2EDTA-0.1-1	0.10	1348	7.88	8.55E-02	6.67E-02
Ca_2EDTA-0.1-2	0.10	1348	7.88	8.60E-02	6.72E-02
Ca_2EDTA-1.0-1	1.0	1348	7.99	1.23E-01	9.42E-02
Ca_2EDTA-1.0-2	1.0	1348	7.72	1.23E-01	9.23E-02
Ca_2EDTA-2.0-1	2.1	1348	8.11	1.21E-01	9.21E-02
Ca_2EDTA-2.0-2	2.1	1348	8.10	1.22E-01	8.96E-02
Ca_2EDTA-3.0-1	3.2	1348	8.23	1.10E-01	8.33E-02
Ca_2EDTA-3.0-2	3.2	1348	8.19	1.08E-01	8.30E-02
Ca_2EDTA-4.0-1	4.4	1348	8.33	9.41E-02	7.28E-02
Ca_2EDTA-4.0-2	4.4	1348	8.32	9.38E-03	7.21E-02
Ca_2EDTA-5.0-1	5.0	1348	8.20	7.89E-02	6.14E-02
Ca_2EDTA-5.0-2	5.0	1348	8.19	8.58E-02	6.62E-02
Ca_2EDTA-0.01-1	0.010	1456	7.88	7.32E-02	5.75E-02
Ca_2EDTA-0.01-2	0.010	1456	7.88	7.30E-02	5.71E-02
Ca_2EDTA-0.1-1	0.10	1456	7.85	8.54E-02	6.74E-02
Ca_2EDTA-0.1-2	0.10	1456	7.90	8.63E-02	6.80E-02
Ca_2EDTA-1.0-1	1.0	1456	7.98	1.22E-01	9.35E-02
Ca_2EDTA-1.0-2	1.0	1456	7.71	1.23E-01	9.26E-02
Ca_2EDTA-2.0-1	2.1	1456	8.07	1.21E-01	9.23E-02

Ca_2EDTA-2.0-2	2.1	1456	8.05	1.22E-01	9.19E-02
Ca_2EDTA-3.0-1	3.2	1456	8.17	1.10E-01	8.46E-02
Ca_2EDTA-3.0-2	3.2	1456	8.14	1.10E-01	8.48E-02
Ca_2EDTA-4.0-1	4.4	1456	8.24	9.41E-02	7.40E-02
Ca_2EDTA-4.0-2	4.4	1456	8.24	9.37E-03	7.44E-02
Ca_2EDTA-5.0-1	5.0	1456	8.12	7.64E-02	6.14E-02
Ca_2EDTA-5.0-2	5.0	1456	8.12	8.53E-02	6.89E-02

*Experimental data after 1197 days were not reported in Jang, Xiong, Kim, and Nemer (2012). It should be noted that there is a typo in that report; "1150 days" should be "1197 days". Experimental data after 1197 days were generated after that report (see Pages 6–7 for sampling on 1348 days and 34-35 for sampling on 1456 days in WIPP–Solubility–27).
**In Jang, Xiong, Kim, and Nemer (2012), pH reading were reported. Values of pmH reported in this analysis report are calculated by using the correction factors (A_M) for pH readings, and conversion factors (Θ) from molarity to molality, $pmH = pH_{ob} + A_M - \log \Theta$ (Xiong et al., 2010). The correction factors are from Rai et al. (1995). The conversion factors are calculated from densities for NaCl solutions, which are from Sőhnel and Novotný (1985). Please see the spreadsheet "XIONG_Ca2EDTA_NaCl_AR.xls".

Table 3. Locations of the Excel Spreadsheets, EQ3/6 I/O Files Associated with Calculations for This Analysis.

Description or Title of File(s)	Location of File(s)
Spreadsheet XIONG_Ca2EDTA_NaCl_AR.xls	In zip file AP154_Task29_DataPackage.zip, library LIBAP154_FILES
EQ3/6 DB DATA0.PD4	In zip file AP154_Task29_DataPackage.zip, library LIBAP154_FILES
EQ3/6 I/O files: CaED-1.3i/o through CaED-112.3i/o	In zip file AP154_Task29_DataPackage.zip, library LIBAP154_FILES
Python scripts: Ca2EDTA_NaCl_PD4.py Ca2EDTA_NaCl_beta(0)_PD4.py	In zip file AP154_Task29_DataPackage.zip, library LIBAP154_FILES
Optimization result files: Results_logK_Ca2EDTA_pd4.txt Results_logK_Ca2EDTA_beta0_pd4.txt	In zip file AP154_Task29_DataPackage.zip, library LIBAP154_FILES

The EQ3/6 provisional thermodynamic database (DB) DATA0.PD4, which is modified from DATA0.FM1 (Xiong, 2011a), was used for this analysis. Please see Paul Domski's memo about details of data0.pd4. The DATA0.PD4 database is in AP154_Task29_DataPackage.zip,

LIBAP154_FILES, in the CMS. All supporting EQ3/6 input and output (I/O) files are also located in the above zip file.

3 RESULTS

Using experimental data listed in Table 2, log K_{sp} only for $Ca_2EDTA(s)$ is first evaluated. The optimization results indicate that the residual is minimized to be 142.0 when log K_{sp} is -14.44 (see Results_logK_Ca2EDTA_PD4.txt, which is located in the above mentioned zip file). Notice that the relatively high residual may result from a large number of data points up to 112. Second, K_{sp} for $Ca_2EDTA(s)$ and $\beta^{(0)}$ for Na^+—$CaEDTA^{2-}$ are simultaneously evaluated. The optimization results indicate that the residual is minimized and decreased to 114.4 when log K_{sp} and $\beta^{(0)}$ for Na^+—$CaEDTA^{2-}$ are –13.91 and 0.4644, respectively (see Results_logK_Ca2EDTA_beta0_PD4.txt, which is located in the above mentioned zip file).

Table 4 provides the Pitzer parameter and log K_{sp} derived in this study. In the DATA0.FM1, the Pitzer interaction parameters for Na^+—$CaEDTA^{2-}$ are based on the analogs from Na^+—$MgEDTA^{2-}$. In Model I, experimental data are fitted for log K_{sp} only, using all default Pitzer parameters for Na^+—$CaEDTA^{2-}$ in DATA0.FM1. In Model II, experimental data are fitted for both log K_{sp} and $\beta^{(0)}$. As the residuals from Model II are significantly lower than those from Model I, the parameters in Model II are preferred.

To the author's best knowledge, there are not published solubility data for $Ca_2EDTA(s)$, and an extensive literature search has not located any published solubility constants for $Ca_2EDTA(s)$. Therefore, experimental solubility data produced at Sandia National Laboratories Carlsbad Facility and the thermodynamic parameters obtained based on these data would have a direct impact on PA. Incorporation of the thermodynamic parameters obtained in this analysis would make EDTA concentrations in brines become solubility-limited, should EDTA concentrations calculated from the inventory exceed the solubility limit of $Ca_2EDTA(s)$.

Table 4. The thermodynamic parameters obtained in this analysis

Pitzer Parameters				
Species, *i*	Species, *j*	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
Na^+	$CaEDTA^{-2}$	0.2134 [A]	1.74 [A]	0.00869 [A]
Na^+	$CaEDTA^{-2}$	0.4644 [B]	1.74 [B]	0.00869 [B]
Equilibrium Constants for Dissolution Reaction of $Ca_2EDTA(s)$				
Reaction			log K_{sp} at 25 °C	
$Ca_2EDTA(s) = 2Ca^{2+} + EDTA^{4-}$			−14.44 [A]	
$Ca_2EDTA(s) = 2Ca^{2+} + EDTA^{4-}$			−13.91 [B]	

[A] Model I, using all default Pitzer parameters for Na^+—$CaEDTA^{2-}$ in DATA0.FM1 to fit for logK_{sp} only.

[B] Model II, using default Pitzer parameters, $\beta^{(1)}$ and C^{ϕ} for Na^+—$CaEDTA^{2-}$ in DATA0.FM1 to fit for both logK_{sp} and $\beta^{(0)}$.

4 CONCLUSIONS

In this analysis report, thermodynamic parameters regarding dissolution of $Ca_2EDTA(s)$ are obtained. With these parameters, concentrations of EDTA in brines would become solubility-limited, should the concentrations of EDTA in brines calculated from the inventory exceed the solubility limit of $Ca_2EDTA(s)$.

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