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Sandia National Laboratories
Waste Isolation Pilot Plant

Experimental determination of solubilities of crystalline lead oxalate, $PbC_2O_4(cr)$, in the $NaCl–H_2O$ system

Work Carried Out under Tasks 22 and 24 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

Author:	Yongliang Xiong, Org. 6212	August 5, 2013 Date
Technical Reviewer:	Greg Roselle, Org. 6212	8/5/2013 Date
QA Reviewer:	Shelly R. Nielsen, Org. 6210	8-5-13 Date
Management Reviewer:	Christi D. Leigh, Org. 6212	8-5-13 Date

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1 INTRODUCTION

This analysis report (AR) provides the thermodynamic properties related to solubility of crystalline lead oxalate, PbC_2O_4(cr), determined in NaCl solutions, and it accompanies the manuscript that has been submitted for publication (Xiong et al., 2011).

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 Tasks 22 and 24 of AP-154 (Xiong, 2011c). There are two deviations from AP-154. The first deviation is that the fitting of experimental data is based on the manual fitting, instead of using the Python script. The reason for this is that the Python script, developed by Nemer (2010) was not functioning properly when the manuscript was prepared for publication (Xiong et al., 2011). The script developed by Kirchner (2012) was not qualified for use until May 1, 2012. The second deviation is that the literature data from Kolthoff et al. (1942) are also used for derivation of thermodynamic parameters, in addition to experimental data produced at SNL Carlsbad Facility.

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
A	activity
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	$(COO)_2^{2-}$ 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 thermodynamic properties related to solubility of crystalline lead oxalate, PbC_2O_4(cr), in NaCl solutions produced at SNL (Jang, Xiong, Kim, and Nemer, 2012). Table 2 lists experimental data in NaCl solutions from the afore mentioned report.

The dissolution reaction for PbC_2O_4(cr) can be expressed as,

$$PbC_2O_4(cr) = Pb^{2+} + C_2O_4^{2-} \quad (1)$$

The corresponding solubility product constant of PbC_2O_4(cr) at infinite dilution can be cast as follows,

$$K_s^o = \frac{a_{Pb^{2+}} \times a_{C_2O_4^{2-}}}{a_{PbC_2O_4(cr)}} \quad (2)$$

The formation reaction for PbC_2O_4(aq) is written as,

$$Pb^{2+} + C_2O_4^{2-} = PbC_2O_4(aq) \quad (3)$$

The corresponding cumulative formation constant at infinite dilution is,

$$\beta_1^0 = \frac{a_{PbC_2O_4(aq)}}{a_{Pb^{2+}} \times a_{C_2O_4^{2-}}} \quad (4)$$

Similarly, the cumulative formation reaction for $Pb(C_2O_4)_2^{2-}$ can be written as,

$$Pb^{2+} + 2C_2O_4^{2-} = Pb(C_2O_4)_2^{2-} \quad (5)$$

The corresponding cumulative formation constant at infinite dilution should be,

$$\beta_2^0 = \frac{a_{Pb(C_2O_4)_2^{2-}}}{a_{Pb^{2+}} \times (a_{C_2O_4^{2-}})^2} \quad (6)$$

The experiments in this study were performed in a NaCl medium and therefore complexation of Pb^{2+} with Cl^- needs to be considered in the modeling. Three lead-chloride aqueous complexes are considered: $PbCl^+$, $PbCl_2$(aq), and $PbCl_3^-$. The cumulative formation reactions for these three complexes are as follows,

$$Pb^{2+} + Cl^- = PbCl^+ \quad (7)$$

$$Pb^{2+} + 2Cl^- = PbCl_2(aq) \quad (8)$$

$$Pb^{2+} + 3Cl^- = PbCl_3^- \quad (9)$$

The corresponding cumulative formation constants for lead-chloride complexes at infinite dilution are as follows,

$$\beta^0_{1,Cl} = \frac{a_{PbCl^+}}{a_{Pb^{2+}} \times a_{Cl^-}} \quad (10)$$

$$\beta^0_{2,Cl} = \frac{a_{PbCl_2(aq)}}{a_{Pb^{2+}} \times (a_{Cl^-})^2} \quad (11)$$

$$\beta^0_{3,Cl} = \frac{a_{PbCl_3^-}}{a_{Pb^{2+}} \times (a_{Cl^-})^3} \quad (12)$$

In this analysis report, the above cumulative formation constants are taken from the literature (Millero and Byrne, 1984), and associated Pitzer parameters from Millero and Byrne (1984) and Felmy et al. (2000) (Table 3).

Using experimental solubility data of PbC_2O_4(cr) in NaCl solutions from this work, in $K_2C_2O_4$ solutions from Kolthoff et al. (1942), and parameters for lead chloride complexes mentioned above, log K_s^o for Reaction (1), log β_1^o for Reaction (3), log β_2^o for Reaction (5), and associated Pitzer parameters are modeled using EQ3/6 Version 8.0a (Table 3). While utilizing manual fitting, parameters were changed in the database based on experience. The modified database was compiled by running EQPT, and then EQ3/6 calculations were performed using the modified database. After running EQ3/6 calculations, experimental results were compared with the outputted EQ3/6 results in terms of residuals and visual inspection. A series of iterations following the above steps were performed until satisfactory residuals and visual inspection were reached. The parameters obtained are tabulated in Table 3. Finally, the model-predicted solubility curves were compared with the experimental data (see Excel spreadsheet "AR_AP154_Task22_Modeling.xls"). A plot showing such comparisons is shown in Figure 1. The solubility curve for PbC_2O_4(cr) in a NaCl medium was established using EQ3/6 files PbOx001.3i/6i through PbOx5.3i/6i located in the folder "AP154-Task22//NaCl_Pitzer_Model" using the database DATA0.OX1 (Table 4). The solubility curve in a $K_2C_2O_4$ medium was established using EQ3NR files PbOxK-01.3i through PbOxK-10.3i located in the folder "AP154-Task22//K2C2O4_Pitzer_Model" also using the database DATA0.OX1 (Table 4). These files are located in the zip file "AP154_Task22_DataPackage.zip" (Table 4). To demonstrate the performance of the selected set of parameters, the solubility curve for PbC_2O_4(cr) in a NaCl medium predicted by using a different set of parameters is also plotted (dashed line in Figure 1). The dashed solubility curve for PbC_2O_4(cr) in a NaCl medium in Figure 1 was established using EQ3/6 files PbOx001.3i/6i through PbOx5.3i/6i with the database DATA0.OX0. These files for comparison are located in the folder "AP154-Task22//NaCl_Comparison". When considering

these data, it is clear that the selected set of parameters performs well for reproducing solubilities of PbC_2O_4(cr) in NaCl and $K_2C_2O_4$ solutions. Notice that the database DATA0.OX0 contains the parameters from the literature, whereas the database DATA0.OX1 has the parameters evaluated from the experimental data.

It should be mentioned that the lambda parameter for the interaction between PbOx(aq) and Cl^- is zero, and therefore there was no interaction between PbOx(aq) and Cl^- for Task 24.

Table 2. Experimental results concerning solubility of PbC_2O_4(cr) in NaCl medium 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, day	pH_{Ob} [A]	Solubility Expressed As Total Pb On Molal Scale ($m_{\Sigma Pb}$)
PbOx-0.01-1	0.010	109	6.40	2.52×10^{-5}
		551	6.30	1.37×10^{-5}
		780	6.01	2.02×10^{-5}
		831	6.30	2.23×10^{-5}
		1062	6.46	3.45×10^{-5}
PbOx-0.01-2	0.010	109	6.51	2.38×10^{-5}
		551	6.30	1.56×10^{-5}
		780	6.00	2.14×10^{-5}
		831	6.54	2.66×10^{-5}
		1062	6.37	2.81×10^{-5}
PbOx-0.1-1	0.10	109	6.03	3.84×10^{-5}
		551	6.06	2.67×10^{-5}
		780	5.77	3.04×10^{-5}
		831	6.22	3.19×10^{-5}
		1062	6.24	3.41×10^{-5}
PbOx-0.1-2	0.10	109	5.88	3.84×10^{-5}
		551	5.49	2.82×10^{-5}
		780	5.21	3.17×10^{-5}
		831	5.43	3.36×10^{-5}
		1062	5.31	3.53×10^{-5}
PbOx-1.0-1	1.0	109	6.55	$1.37\pm0.02\times10^{-4}$ [B]
		551	6.80	1.20×10^{-4}
		780	6.88	1.04×10^{-5}
		831	6.88	1.08×10^{-4}
		1062	6.77	1.48×10^{-4}
PbOx-1.0-2	1.0	109	6.53	$1.40\pm0.01\times10^{-4}$ [B]
		551	6.81	1.21×10^{-4}
		780	6.93	1.05×10^{-4}
		831	6.73	1.11×10^{-4}
		1062	6.81	1.39×10^{-4}
PbOx-2.0-1	2.1	109	6.11	$3.05\pm0.01\times10^{-4}$ [B]
		551	5.86	1.99×10^{-4}
		780	5.70	2.76×10^{-4}
		831	5.66	2.71×10^{-4}
		1062	5.63	3.17×10^{-4}
PbOx-2.0-2	2.1	109	6.19	$3.72\pm0.04\times10^{-4}$ [B]
		551	6.10	1.91×10^{-4}
		780	6.38	2.73×10^{-4}
		831	6.00	2.72×10^{-4}

		1062	6.19	3.19×10^{-4}
PbOx-3.0-1	3.2	109	6.14	$7.23\pm0.17\times10^{-4}$ [B]
		551	5.85	$6.306.22\times10^{-4}$
		780	5.98	$6.936.78\times10^{-4}$
		831	5.63	6.73×10^{-4}
		1062	5.71	7.69×10^{-4}
PbOx-3.0-2	3.2	109	6.23	$7.34\pm0.10\times10^{-4}$ [B]
		551	6.07	6.22×10^{-4}
		780	6.30	6.90×10^{-4}
		831	5.85	6.89×10^{-4}
		1062	6.13	7.76×10^{-4}
PbOx-4.0-1	4.4	109	6.56	$1.65\pm0.00\times10^{-3}$ [B]
		551	6.38	1.61×10^{-3}
		780	6.58	1.62×10^{-3}
		831	6.12	1.62×10^{-3}
		1062	6.37	1.77×10^{-3}
PbOx-4.0-2	4.4	109	6.62	$1.67\pm0.01\times10^{-3}$ [B]
		551	6.37	1.62×10^{-3}
		780	6.46	1.68×10^{-3}
		831	6.44	1.64×10^{-3}
		1062	6.38	1.84×10^{-3}
PbOx-5.0-1	5.0	109	7.12	$3.07\pm0.04\times10^{-3}$ [B]
		551	6.88	3.13×10^{-3}
		780	7.05	3.17×10^{-3}
		831	6.72	3.05×10^{-3}
		1062	6.87	3.52×10^{-3}
PbOx-5.0-2	5.0	109	7.15	$3.03\pm0.02\times10^{-3}$ [B]
		551	6.95	3.16×10^{-3}
		780	7.27	3.17×10^{-3}
		831	7.09	3.09×10^{-3}
		1062	6.95	3.29×10^{-3}

[A] pH readings obtained by using a pH electrode, and they can be converted to hydrogen ion concentrations by applying correction factors (see SP 12-14, Roselle, 2012).
[B] Replicate analyses, and uncertainty represents two standard deviations (2σ).
Experimental data contained in this table are from the scientific notebooks WIPP-SOLUBILITY-3, WIPP-SOLUBILITY-10, WIPP- SOLUBILITY-12, WIPP-SOLUBILITY-13 and WIPP-SOLUBILITY-14 and associated binders.

Table 3 Equilibrium constants at infinite dilution, 25°C and 1 bar, Pitzer interaction parameters, and Brønsted-Guggenheim-Scatchard SIT interaction coefficients in Na^+—K^+—Pb^{2+}—Cl^-—$C_2O_4^{2-}$ system

Reactions	log K_s^o, log β_1^o, or log β_2^o	Reference and Remarks
$PbC_2O_4(cr) = Pb^{2+} + C_2O_4^{2-}$	-11.13 ± 0.15 (2σ)	This study, based on solubility of $PbC_2O_4(cr)$ in NaCl medium presented in the present work, Pitzer model
$Pb^{2+} + C_2O_4^{2-} = PbC_2O_4(aq)$	5.85 ± 0.10 (2σ)	This study, based on solubility of $PbC_2O_4(cr)$ in NaCl medium presented in the present work, Pitzer model
$Pb^{2+} + 2C_2O_4^{2-} = Pb(C_2O_4)_2^{2-}$	8.05 ± 0.15 (2σ)	This study, evaluated from solubilities of $PbC_2O_4(cr)$ in $K_2C_2O_4$ medium from Kolthoff et al. (1942), Pitzer model
$Pb^{2+} + Cl^- = PbCl^+$	1.48	Millero and Byrne (1984), evaluated by using Pitzer model; uncertainty not given
$Pb^{2+} + 2Cl^- = PbCl_2(aq)$	2.03	Millero and Byrne (1984), evaluated by using Pitzer model; uncertainty not given
$Pb^{2+} + 3Cl^- = PbCl_3^-$	1.86	Millero and Byrne (1984), evaluated by using Pitzer model; uncertainty not given

Pitzer Binary Interaction Parameters					
Species *i*	Species *j*	$\beta^{(0)}$	$\beta^{(1)}$	C^ϕ	
Pb^{2+}	Cl^-	0.26	1.64	0.088	Millero and Byrne (1984)
$PbCl^+$	Cl^-	0.15	0	0	Millero and Byrne (1984)
Na^+	$PbCl_3^-$	–0.0605	0	0.091	This study
K^+	$Pb(C_2O_4)_2^{2-}$	0	–1.86	0.198	This study
Na^+	$Pb(C_2O_4)_2^{2-}$	0	–1.86	0.198	This study, in analog to K^+—$Pb(C_2O_4)_2^{2-}$
Pitzer Mixing Interaction Parameters and Interaction Parameters Involving Neutral					

Species					
Species *i*	Species *j*	Species *k*	λ_{ij} or θ_{ij}	ζ_{ijk}	
Cl^-	$PbCl_2(aq)$		–0.14		This study
Na^+	$PbCl_2(aq)$		–0.11		Felmy et al. (2000)
Na^+	Pb^{2+}		0.10		Felmy et al. (2000)
Na^+	$PbCl_2(aq)$	Cl^-		0	This study
Na^+	$PbC_2O_4(aq)$	Cl^-	0	0	This study

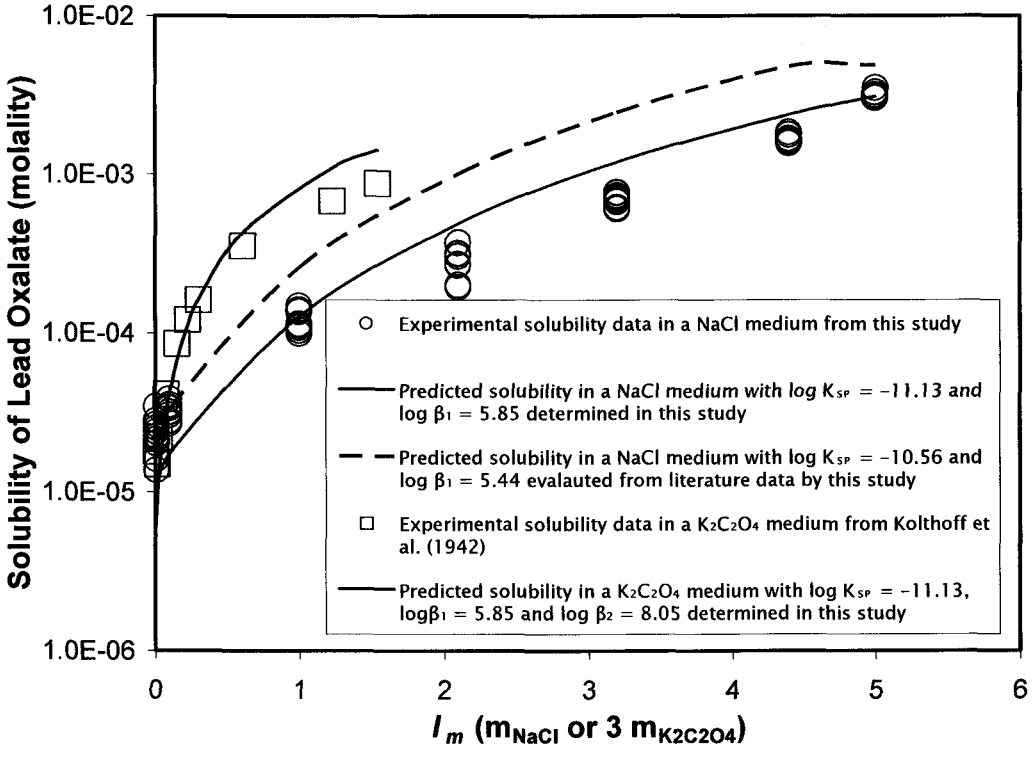

Figure 1. A plot showing solubilities of $PbC_2O_4(cr)$ as a function of ionic strength on molal scale in NaCl and $K_2C_2O_4$ media. Solubility data in NaCl medium are from this study, and solubility data in $K_2C_2O_4$ medium are from Kolthoff et al. (1942).

Table 4. 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 AR_AP154_Task22_Modeling.xls	In zip file AP154_Task22_DataPackage.zip, library LIBAP154_FILES
EQ3/6 DB DATA0.OX0	In zip file AP154_Task22_DataPackage.zip, library LIBAP154_FILES
EQ3/6 DB DATA0.OX1	In zip file AP154_Task22_DataPackage.zip, library LIBAP154_FILES
EQ3/6 I/O files: PbOx001.3i/o and 6i/o through PbOx5.3i/o and 6i/o PbOxK-01.3i/o through PbOxK-10.3i/o	In zip file AP154_Task22_DataPackage.zip, library LIBAP154_FILES

3 RESULTS

Table 3 provides the log K_s^o, log β_1^o, β_2^o, and associated Pitzer parameter in the Na^+—K^+—Pb^{2+}—Cl^-—$C_2O_4^{2-}$ system derived in this study. The parameters obtained in this work perform well in reproducing experimental solubility data in both NaCl and $K_2C_2O_4$ solutions.

To the author's best knowledge, there are not published solubility data for PbC_2O_4(cr) in NaCl solutions. 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 lead oxalate complexes strong competitors with actinides for soluble oxalate, reducing solubility of actinides, as oxalate complexes are strong.

4 CONCLUSIONS

In this analysis report, the log K_s^o, log β_1^o, β_2^o, and associated Pitzer parameters in the Na^+—K^+—Pb^{2+}—Cl^-—$C_2O_4^{2-}$ system are obtained. With these parameters, the interactions of lead as radiation shielding material with oxalate in waste streams can be accurately modeled.

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