

TABLE SI-1

A Summary of Equilibrium Constants at 25° C and Zero Ionic Strength Investigated in Lead Solubility Modeling Computations

Reaction	*LEADSOL log K	**SASIAS log K	***MINEQL+ v 4.5 log K	****Powell et. al. (2009) log K
$\text{Pb}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{PbOH}^+$	-7.23	-7.25	-7.697	-7.46
$\text{Pb}^{2+} + 2\text{H}_2\text{O} \rightleftharpoons \text{Pb}(\text{OH})_2^0 + 2\text{H}^+$	-16.93	-16.91	-17.094	-16.94
$\text{Pb}^{2+} + 3\text{H}_2\text{O} \rightleftharpoons \text{Pb}(\text{OH})_3^- + 3\text{H}^+$	-28.1	-28.1	-28.091	-28.03
$\text{Pb}^{2+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Pb}(\text{OH})_4^{2-} + 4\text{H}^+$	-39.7	+	-39.699	-
$2\text{Pb}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{Pb}_2\text{OH}^{3+} + \text{H}^+$	-6.36	-6.4	-6.397	-7.28
$3\text{Pb}^{2+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Pb}_3(\text{OH})_4^{2+} + 4\text{H}^+$	-23.88	-23.9	-23.888	-23.01
$4\text{Pb}^{2+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Pb}_4(\text{OH})_4^{4+} + 4\text{H}^+$	-20.88	+	-19.988	-20.57
$6\text{Pb}^{2+} + 8\text{H}_2\text{O} \rightleftharpoons \text{Pb}_6(\text{OH})_8^{4+} + 8\text{H}^+$	-43.61	-43.6	-	-42.89
$\text{Pb}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{PbCO}_3$	7.1	7.09	6.478	6.45
$\text{Pb}^{2+} + 2\text{CO}_3^{2-} \rightleftharpoons \text{Pb}(\text{CO}_3)_2^{2-}$	10.4	10.29	9.938	10.13
$\text{Pb}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{PbHCO}_3^+$	13.2	+	13.2	12.196
$\text{Pb}^{2+} + \text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{PbHPO}_4$	15.45	15.45	-	-
$\text{Pb}^{2+} + 2\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{PbH}_2\text{PO}_4^+$	21.1	21.049	-	-
$\text{Pb}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{PbSO}_4^0$	2.75	2.75	2.69	2.72
$\text{Pb}^{2+} + 2\text{SO}_4^{2-} \rightleftharpoons \text{Pb}(\text{SO}_4)_2^{2-}$	3.47	+	3.47	-
$\text{Pb}^{2+} + \text{Cl}^- \rightleftharpoons \text{PbCl}^+$	1.6	1.59	1.55	1.50
$\text{Pb}^{2+} + 2\text{Cl}^- \rightleftharpoons \text{PbCl}_2^0$	1.8	1.8	2.2	2.10
$\text{Pb}^{2+} + 3\text{Cl}^- \rightleftharpoons \text{PbCl}_3^-$	1.7	1.7	1.8	2.00
$\text{Pb}^{2+} + 4\text{Cl}^- \rightleftharpoons \text{PbCl}_4^{2-}$	1.4	1.4	1.46	-
$\text{Pb}^{2+} + \text{NO}_3^- \rightleftharpoons \text{PbNO}_3^+$	‡	1.17 §	1.17	-
$\text{Pb}^{2+} + 2\text{NO}_3^- \rightleftharpoons \text{Pb}(\text{NO}_3)_2^0$	‡	1.4 §	1.4	-

$\text{PbCO}_3(\text{s}) \rightleftharpoons \text{Pb}^{2+} + \text{CO}_3^{2-}$	-13.13	-13.88	-13.13	-13.18
$\text{Pb}_3(\text{CO}_3)_2\text{OH}(\text{s}) + 2\text{H}^+ \rightleftharpoons 3\text{Pb}^{2+} + 2\text{CO}_3^{2-} + 2\text{H}_2\text{O}$	-18.8	-19.14	-18.77	-
$\text{Pb}(\text{OH})_2(\text{s}) + 2\text{H}^+ \rightleftharpoons \text{Pb}^{2+} + 2\text{H}_2\text{O}$	13.06	12.69	8.15	-
$\text{Pb}_5(\text{PO}_4)_3\text{OH}(\text{s}) + \text{H}^+ \rightleftharpoons 5\text{Pb}^{2+} + 3\text{PO}_4^{3-} + \text{H}_2\text{O}$	-62.79	-62.8	-62.79	-

*Derived from Table 4-13, AWWARF-TZW Internal Corrosion of Water Distribution Systems, 2nd Edition (1996) Gibbs Free Energy values (LEADSOL)

**Reported in Hunt, D.T.E. & Creasey, J.D WRc Technical Report TR-151 (SASIAS)

***Schecher, W. (2001) Thermochemical Data Used in MINEQL+ version 4.5, Environmental Research Software

****Powell, K.J., Brown, P.L., Byrne, R.H., Gajda, T., Hefter, G., Leuz, A.-K., Sjöberg, S., and Wanner, H., 2009. Chemical speciation of environmentally significant metals with inorganic ligands. Part 3: The $\text{Pb}^{2+} + \text{OH}^-$, Cl^- , CO_3^{2-} , SO_4^{2-} , and PO_4^{3-} systems (IUPAC Technical Report). *Pure and Applied Chemistry*, 81:12. <https://doi.org/10.1351/pac-rep-09-03-05>.

+ Not included in the SASIAS program

‡ Not included in the LEADSOL program

§ Not included in the SASIAS computations in WRc TR-151

- Not included in the database