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A thermodynamic model for {Pb^{2+}–H^+–Na^+–K^+–Mg^{2+}–Cl^-–OH^-}aq at 298 K, 0.1 MPa, and 0 ≤ ionic strength ≤ solid saturation

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A Pitzer ion-interaction model is presented for the Pb^{2+}–H^+–Na^+–K^+–Mg^{2+}–Cl^-–OH^- system at 298 K and 0.1 MPa. Model parameters for interactions not involving Pb species were taken from Harvie et al. [1]. Dimensionless standard state chemical potentials for all Pb species, including solids and excepting Pb^{2+}, were fitted; the NEA value was used for Pb^{2+}. Our model reproduces the most accurate emf and solubility data from infinite dilution to solid saturation for all Pb-chloride salts. The model also reproduces $PbCl_2$(cr) solubility in HCl(aq) ≤ 9 molal.

In contrast to the 21 interaction parameters involving Pb-solute species in Felmy et al. [2], our model uses only 8 – none of which are “ternary” or neutral species terms. The Felmy model is based upon faulty data and uses the Millero & Byrne [3] model parameters for $PbCl_2 + H_2O$. The latter model is valid to I ≤ 1 molal, however, it uses a $C_{Zn,Cl}$ parameter as an analog for $C_{Pb,Cl}$. Adoption of this term, with a sign error, undoubtedly contributed to the peculiar and excessive parameterization in the Felmy model.

[1] Harvie et al. (1984) *Geochim. Cosmochim. Acta* **48**, 723.

[2] Felmy et al. (2000) *Geochim. Cosmochim. Acta* **64**, 3615.

[3] Millero & Byrne (1984) *Geochim. Cosmochim. Acta* **48**, 1145.