A new set of Pitzer interaction parameters to describe solution properties and solid-liquid equilibria in the Li-Ca-Cl-H 2 O system at 298.15 K

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The Li-Ca-Cl-H_2O system has been described in previous works using different modelling approaches [1-3], including the Pitzer equations [4]. These models are self-consistent but cannot be combined with recent developments aiming at describing larger chemical systems such as H-Li-Na-K-Cl-OH-H_2O [5,6]. The objective of the present work is thus to develop a new set of Pitzer interaction parameters for the Li-Ca-Cl-H_2O system consistent with these latter models, at 298.15 K. This task was done in two steps. First, the description of the Ca-Cl-H_2O subsystem has been extended to the metastable super-saturation region by refining the recent model of Lach [7] using the osmotic coefficient data selected by [8]. Then, using osmotic coefficient or water activity data for LiCl-$CaCl_2$ mixtures [9,10] and solubility measurement data [10-12], the new set of specific interaction parameters and solubility products has been determined. Both types of data can be reproduced satisfactorily (see figure below) using the geochemical code PhreeSCALE [13], and it is now possible to envision the extended description of the H-Li-Na-K-Ca-Cl-OH-H_2O chemical system at 298.15 K.

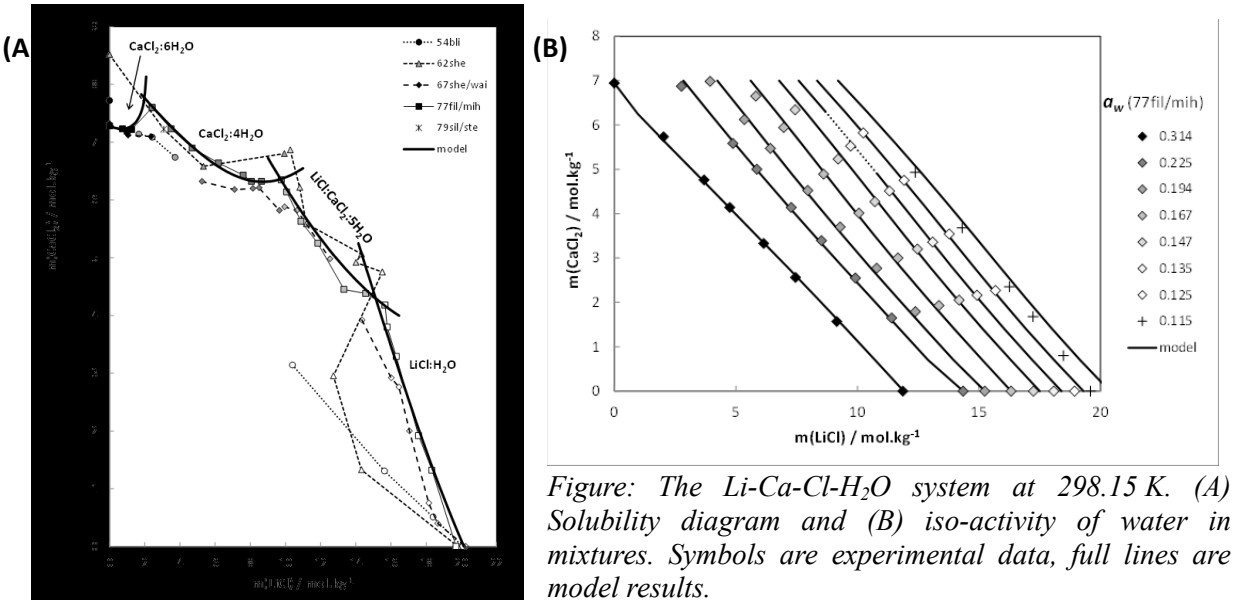

Figure: The Li-Ca-Cl-H_2O system at 298.15 K. (A) Solubility diagram and (B) iso-activity of water in mixtures. Symbols are experimental data, full lines are model results.

References

[1] Christov C., Velikova S. and Ivanova K. (2000) *J. Chem. Thermod.* 32, 1505-1512.
[2] Zeng D., Xu W., Voigt W. and Yin X. (2008) *J. Chem. Thermod.* 40, 1157-1165.
[3] Meng L., Li D., Deng T. and Guo Y. (2014) *Acta Geol. Sinica* 88, 356-358.
[4] K.S. Pitzer, *Activity coefficients in electrolyte solutions*, 2nd ed., CRC Press, Boca Raton, 1991
[5] Lassin A., Christov C., André L. and Azaroual M. (2015) *Amer. J. Sci.* 315, 204-256.
[6] Lach A., André L., Lassin A., Azaroual M., Serin J.-P. and Cézac P. (2015) *J. Sol. Chem.* 44, 1424-1451.
[7] Lach A. (2015) Ph.D. Thesis, Université de Pau et des Pays de l'Adour.
[8] Rard J.A. and Clegg S.L. (1997) *J. Chem. & Engin. Data* 42, 819-849.
[9] Filippov V.K. and Mihelbson K.N. (1977) *Zh. Neorg. Khim.* 22, 1689-1694.
[10] Long G.-M., Yao Y., Wang F.-Q. and Wang R.-L. (1999) *Wuli Huaxue Xuebao* 15, 956-960.
[11] Shevchuk V.G. and Vaisfeld M. (1967) *Zh. Neorg. Khim.* 12, 1064-1069.
[12] Shepelev A.I. (1962) *Ser. Khim. Nauk* 57
[13] Lach A., Boulahya F., André L., Lassin A., Azaroual M., Serin J.-P. and Cézac P. (2016) *Comput. Geosci.* 92 (2016) 58–69