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A new set of Pitzer interaction parameters to describe solution properties and solid-liquid equilibria in the Li-Ca-Cl-H₂O system at 298.15 K.

A. Lassin^{1*}, A.-L. Thadée¹, A. Lach¹, L. André¹, S. Guignot¹, J.-P. Serin², P. Cézac²

¹ BRGM – 3 avenue Claude Guillemin, 45100 Orléans, France;

² LaTEP – rue Jules Ferry, 64000 Pau, France

* tel. +33 238 643 025, e-mail: a.Lassin@brgm.fr;

The Li-Ca-Cl-H₂O 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-H₂O [5,6]. The objective of the present work is thus to develop a new set of Pitzer interaction parameters for the Li-Ca-Cl-H₂O system consistent with these latter models, at 298.15 K. This task was done in two steps. First, the description of the Ca-Cl-H₂O 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-CaCl₂ 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-H₂O chemical system at 298.15 K.

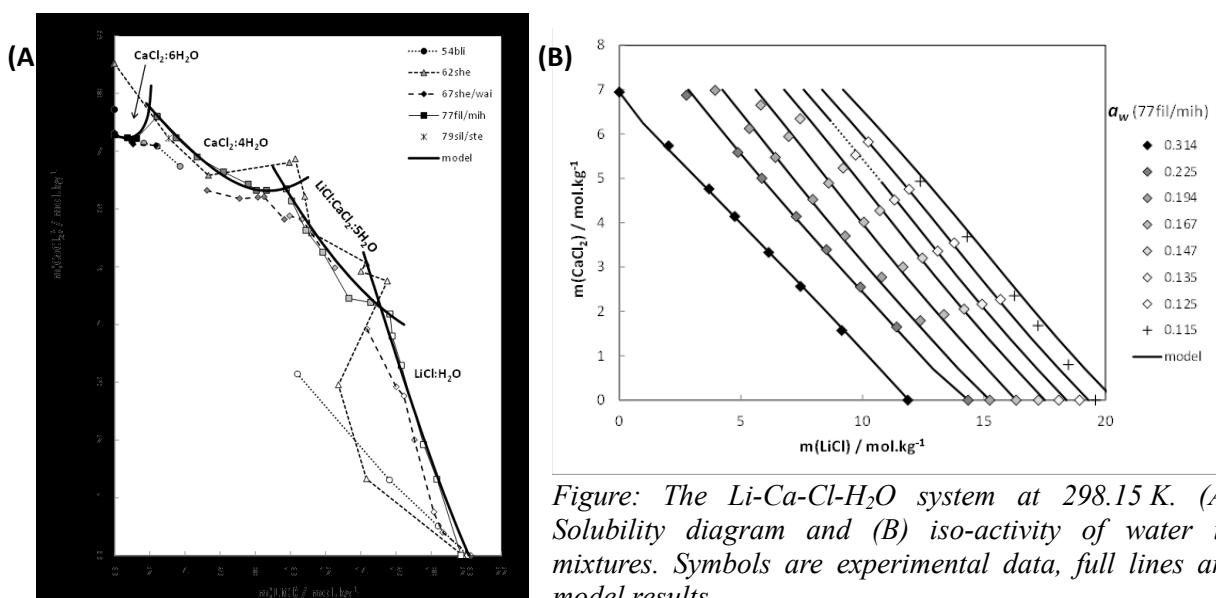


Figure: The Li-Ca-Cl-H₂O system at 298.15 K. (A) Solubility diagram and (B) iso-activity of water in mixtures. Symbols are experimental data, full lines are model results.

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