

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

Arnault Lassin, Anne-Laure Thadée, Adeline Lach, Laurent André, Sylvain  
Guignot, Jean-Paul Serin, Pierre Cézac

► **To cite this version:**

Arnault Lassin, Anne-Laure Thadée, Adeline Lach, Laurent André, Sylvain Guignot, et al.. A new set of Pitzer interaction parameters to describe solution properties and solid-liquid equilibria in the Li-Ca-Cl-H<sub>2</sub>O system at 298.15 K. 25ème Réunion des sciences de la Terre (RST 2016), Oct 2016, Caen, France. 2016, <<http://rst2016-caen.sciencesconf.org/>>. <hal-01332185>

**HAL Id: hal-01332185**

**<https://hal-brgm.archives-ouvertes.fr/hal-01332185>**

Submitted on 15 Jun 2016

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

A. Lassin<sup>1\*</sup>, A.-L. Thadée<sup>1</sup>, A. Lach<sup>1</sup>, L. André<sup>1</sup>, S. Guignot<sup>1</sup>, J.-P. Serin<sup>2</sup>, P. Cézac<sup>2</sup>

<sup>1</sup> BRGM – 3 avenue Claude Guillemin, 45100 Orléans, France;

<sup>2</sup> LaTEP – rue Jules Ferry, 64000 Pau, France

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

The Li-Ca-Cl-H<sub>2</sub>O 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<sub>2</sub>O [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<sub>2</sub>O 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<sub>2</sub>O 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<sub>2</sub> 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<sub>2</sub>O chemical system at 298.15 K.

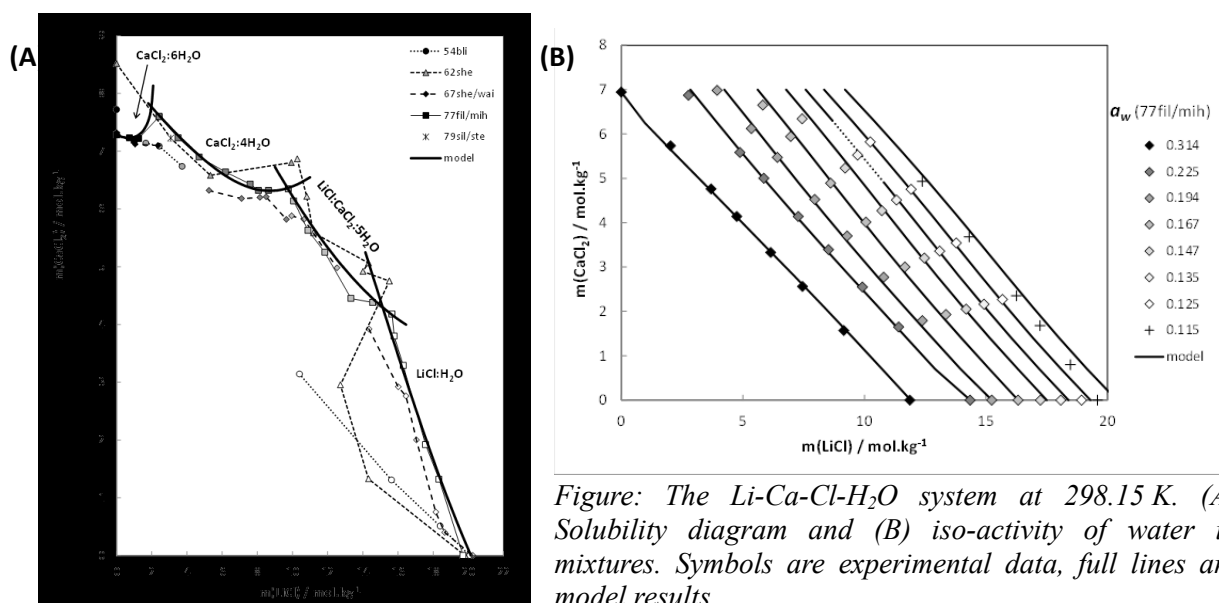


Figure: The Li-Ca-Cl-H<sub>2</sub>O system at 298.15 K. (A) Solubility diagram and (B) iso-activity of water in mixtures. Symbols are experimental data, full lines are model results.

## 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*, 2<sup>nd</sup> 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