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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-H₂O 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

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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.

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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.

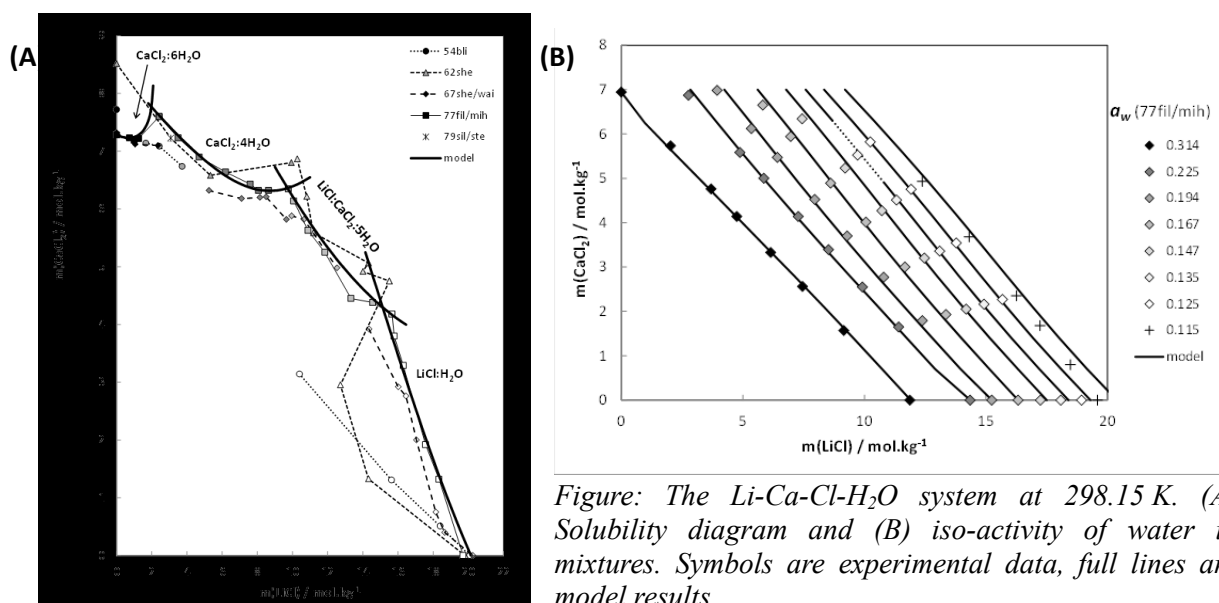


Figure: The Li-Ca-Cl-H₂O system at 298.15 K. (A) Solubility diagram and (B) iso-activity of water in mixtures. Symbols are experimental data, full lines are model results.

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