

## Serpentine and brucite intergrowths: effects on $\delta^{11}\text{B}$

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A quantitative understanding of fluid:rock interaction is important for understanding the transfer of elements and fluid circulation within the crust. Serpentinites can provide a sensitive record of fluid-rock interaction, particularly via analysis of isotopes of fluid mobile elements, such as boron.

Previous studies of boron in serpentinised rocks have provided a wide range of values. <sup>11</sup>B partitions into seawater, so heavy  $\delta^{11}\text{B}$  values indicate a seawater influence, while lighter  $\delta^{11}\text{B}$  reflects mantle influences. Strong fractionation between the two isotopes at temperatures of serpentinisation enables elucidation of the evolving fluid:rock system with progressive serpentinisation.

However, boron isotopic fractionation is influenced by temperature and pH because <sup>11</sup>B is preferentially incorporated into trigonal environments, such as those found in the  $\text{B}(\text{OH})_3$  aqueous species, while <sup>10</sup>B is preferentially hosted by the  $\text{B}(\text{OH})_4^-$  tetragonal species, which dominates in solution at high pH [1]. Additionally serpentine minerals, particularly early grown serpentine, can be intimately intergrown with brucite. Brucite cations are held in a trigonal site, so the presence of brucite is expected to increase  $\delta^{11}\text{B}$ . If this is not recognised,  $\delta^{11}\text{B}$  values heavier than the true serpentine  $\delta^{11}\text{B}$  values will be inferred, and erroneous interpretations may be made.

In this study, brucite, serpentine and brucite-serpentine intergrowths of partially serpentinised peridotites from ODP Leg 209 and New Caledonia were identified using micro-Raman spectroscopy. Secondary Ion Mass Spectrometry (SIMS) was used to assess the extent to which the presence of brucite affects  $\delta^{11}\text{B}$ . The results enable a quantitative assessment of the magnitude of the effect of brucite on  $\delta^{11}\text{B}$  and the implications of this for interpretation of fluid:rock interaction during serpentinisation.

[1] Foustoukos *et al.* (2008) *Geochimica et Cosmochimica Acta* **72**(22) 5457–5474.

## Direct molecular simulation of aqueous electrolyte solubility

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### Introduction

We describe a new and computationally efficient methodology using Osmotic Ensemble Monte Carlo (OEMC) simulation to calculate the solubility of aqueous electrolytes [1]. We apply it to directly determine solubility without the need for calculating chemical potentials. The method avoids calculations for the solid phase, directly incorporating readily available data from thermochemical tables based on well-defined reference states [2].

### Methodology

The method performs simulations of the aqueous solution at a fixed number of water molecules, pressure, temperature and specified overall electrolyte chemical potential. Insertion/deletion of ions to/from the system is implemented using fractional ion states, and transitions between the states incorporates Wang-Landau sampling.

### Results and Discussion

We have applied the approach to calculate the solubilities of a range of alkali halides, using several water and ionic force-field models from the literature. We consider both individual alkali halides and their mixtures, dissolved in both  $\text{H}_2\text{O}$  and  $\text{HCl-H}_2\text{O}$  solutions. The solubility predictions are generally good. The solubility is very sensitive to the force field employed.

[1] F. Moucka, M. Lisal, J. Skvor, J. Jirsak, I. Nezbeda & W.R. Smith (2011) *J. Phys. Chem. B*, submitted. [2] M. Chase, Jr. (1998) NIST-JANAF Thermochemical Tables, *J. Phys. & Chem. Reference Data Monograph No. 9*, Am. Chem. Society, Am. Inst. Physics.