Molecular Dynamics Modelling of Zn²⁺ Speciation in Hydrothermal Fluids

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In order to properly understand the role of crustal fluids in geological processes it is necessary to know the chemistry of the dissolved species. Previous experimental work has considered the role of temperature up to 350°C at either the saturated vapour pressure (Ruaya and Seward 1986, Bourcier and Barnes 1987) or at an applied pressure (Cygan et al., 1994), however these methods have generally only considered dilute solutions with $[Zn^{2+}] < 0.1$ m. In addition they have considered only the simplest clusters when fitting their experimental data. It is not possible to predict the existence of more complex species for which no thermodynamic data is available.

We have used molecular dynamics simulations to calculate the speciation of $ZnCl_2$ in aqueous solutions with high ionic strength. We have considered both stoichiometric solutions and concentrated brine solutions. Pressures up to 2 kb and temperatures up to 600°C have been modelled.

We are able to explicitly determine the concentrations of the various clusters that form in solution. We show that in the stoichiometric solutions clusters form which are not considered by experimental data.

Cygan GL, Hemley JJ & D'Angelo WM, *Geochim. Cosmochim. Acta*, **58**, 4841-4855, (1994).

Ruaya JR & Seward TM, *Geochim. Cosmochim. Acta*, **50**, 651-661, (1986).

Bourcier WL & Barnes HL, *Economic Geology*, **82**, 1839-1863, (1987).