

Beryllium speciation in hydrothermal and magmatic fluids - new insights from first principles molecular dynamics

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Beryllium is a strategic element [1] and, because of a low absorption cross-section for thermal neutrons, it is used in nuclear reactors. Furthermore, the geochemical behavior of Be^{2+} in late magmatic fluids is poorly known [2].

The frequent association of beryllium minerals with fluorite and topaz in hydrothermal beryllium deposits and pegmatite suggests that Be^{2+} is commonly transported in fluoride-rich aqueous solutions in geological environments. It is the aim of this study to make predictions of the speciation of beryllium in geological fluids from ambient conditions up to 700 °C and 600 MPa with focus on monomeric complexes of beryllium with fluoride.

Be is especially difficult to study experimentally as it is highly toxic and virtually invisible to x-rays. For this reason we use first principles molecular dynamics simulations and thermodynamic integration to compute the potential of mean force, from which the equilibrium constants of dissociation reactions of different Be-F species are derived.

We are able to reproduce experimental stability constants [3] of Be-F complexes at room temperature and to interpolate our data in pressure-temperature space. At higher temperatures, there are increasing deviations of our predictions from the extrapolated values of Wood (1992) [4]. We expect that our new results are more accurate at high temperatures as they are derived from a reasonable structure model. In addition, we see a better agreement of our data with high temperature experiments for $\text{BeF}_2(\text{aq})$ [5,6]. Moreover, the simulations reveal that the tetrahedral coordination geometry of Be^{2+} that is dominant at ambient conditions is not stable anymore at high temperature. We conclude that at high fluoride activity $\text{BeF}_2(\text{aq})$ and $\text{BeF}_3(\text{aq})$ are the majority species. With our results we can shed new light on the behavior of beryllium during late magmatic evolution, which needs to be understood to interpret field observations [2].

[1] Lederer et al. (2016) USGS Fact Sheet 2016–3081; [2] Thomas et al. (2010) Contrib. Mineral. Petrol. 161, 483; [3] Mesmer and Baes (1969) Inorg. Chem. 8, 618; [4] Wood (1992) Ore Geol. Rev. 7, 249; [5] Kozmenko et al. (1985) Geochem. Int. 22, 162; [6] Kozmenko et al. (1987) Geochem. Int. 24, 135