MgSO4 phases: hydration, spectroscopy and S isotope partitioning

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We study the relative stability of several magnesium sulfate minerals using first-principles calculations based on the density functional theory in the ABINIT implementation. These phases might be present on the surface of Mars or on a variety of smaller icy bodies form the outer solar system. Our calculations show that, if involved in the water cycle of Mars, the magnesium sulfates must be already present as hydrated phases: the anhydrous phases are easily absorbing water and, in turn, the complete dehydration of these phases requires large temperature, unattainable on Mars. We equally compute the Raman and infrared spectra of several phases to offer reference spectra for *in situ* spectroscopic identification. Apart from the appearance of the water bands, the hydration also changes the position of several lower-frequency bands. Using the spectroscopic calculations we determine the influence of hydration on the S isotope partitioning. We show that it is highly dependent on the temperature. For temperatures specific to the surface of Mars, hydration of the anhydrous phase leads to an enrichment in the S34. The effect on the already hydrated phase is opposite: further hydration enriches lighter isotopes.

Partitioning of trace elements between Na-bearing majoritic garnet and melt at 8.5 GPa and 1500–1900°C

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The new experimental data on trace element partitioning between Na-bearing majoritic garnet and melt at 8.5 GPa and 1500–1900°C applicable to partial melting of Na-rich eclogite is presented. The Na-bearing garnet is a liquidus phase of the system at 1850–1650°C being accompanied by enstatite-rich pyroxene at lower temperatures. With the temperature decrease, Na concentration in garnet increases up to >1 wt % Na_2O due to progressive incorporation of Na majorite ($Na_2MgSi_5O_{12}$). Most of the studied trace elements are incompatible, except for Er, Tm, Yb (in some runs), Lu, and Sc (in all runs), which partition into garnet. The main feature of the trace-element partitioning in our experiments is the different behaviour of the LREE (La, Ce, Pr) in comparison with MREE and HREE (Nd, Sm, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, and Lu). Significant increase of D values for LREE with increase of Na_2O concentration in garnet is observed. As predicted from lattice strain, partitioning coefficients for REEs entering the X site of garnet exhibit a near-parabolic dependence on ionic radius. Other elements including the LILE (Rb, Sr, Ba), Sc, as well as Zn, Ta, and Pb have a clear affinity for aluminosilicate melt. The results of the study are applied to the formation of inclusions of Na-bearing majoritic garnets in diamonds and equilibrium melts, which are significantly enriched in LREEs being very similar to kimberlitic and OIB melts.

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