

First-principle calculations of Equilibrium Mg isotopic fractionations among Mg-phosphates and the implications for tracing the existence of struvite in planetary waters

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Life's origination requires accumulation of nutrients, including ammonium and phosphate, in the planetary waters. There are, however, very limited evidence of the availability of these nutrients. One direct way is to look for indicative minerals. For example, co-existence of ammonium and phosphate could form struvite in favorable environments relevant with the early Earth and some icy moons (such as Enceladus). However, struvite is ephemeral and would tend to decompose to form other Mg-phosphate minerals under relatively mild temperatures [1]. There is still some residual fingerprint, such as the Mg isotopic compositions. One prerequisite to trace the existence of struvite using Mg isotopes is the understanding of Mg isotope fractionation during struvite precipitation. In this study, the equilibrium Mg isotopes fractionation factors of struvite and other Mg-phosphates are investigated by first-principle calculations. Our result shows a heavier-Mg isotopes enrichment in the order of farringtonite > raadeite ~ brucite > bobierite > cattite ~ kovdorskite > struvite > dittmarite > chopinite > newberyite > magnesite. The isotopic fractionation factors between brucite and magnesite are estimated for comparison and our result agrees well with previous studies [2].

This work suggests the equilibrium Mg isotopes fractionation between aqueous solutions and struvite are negligible, which suggests the struvite will have similar Mg isotopes as the aqueous phase. In contrast, the equilibrium fractionation factors between newberyite and aqueous solutions are $\delta^{26/24}\text{Mg}_{\text{aqueous-newberyite}}=1.74\%$ at 300K, which suggests newberyite would enrich lighter Mg isotopes. The struvite tends to form in ammonium-rich liquid, while newberyite tends to form in ammonium-poor liquid [3]. Although those phosphate will decompose, their Mg isotopic compositions would persist in the solid products, which potentially revealing the abundance of ammonium in early earth or other planetary waters.

References:

[1] Feng T., Gull M., Omran A., Abbott-Lyon H. and Pasek M. A. (2021), *Acs Earth Space Chem* 5, 1647–1656.

[2] Wang W., Zhou C., Liu Y., Wu Z. and Huang F. (2019), *Geochim Cosmochim Acta* 250, 117–129.