Extending the carbonate clumped isotopes paleothermometer to new mineral systems: a computer modelling approach

Clumped isotope paleothermometry is now routinely used on carbonates and carbonate-bearing minerals, oxygen in the atmosphere, methane, ethane, and carbonate dioxide. The principle of clumped isotopes is that heavy isotopes confer a lower vibrational energy to a molecular system, and thus there is a relationship between amount of clumped isotopes and the temperature at which a compound was formed. The most practical application of clumped isotope paleothermometry is with the carbonate system, as it is relatively easy to measure and yields important information about the past conditions of our planet. However, in principle clumped isotopes should exist in any mineral or solid phase.

The goal of this PhD will be to establish for the first time the relationship between the clumping values within new mineral systems, and temperature. This will include mineral systems such as various silicates, some sulfates, and ionic substances. The approach taken will be:

1) To model the relationship between vibrational energy and stability from first principles, using computational approaches. This work will lead to the first papers on the clumped isotope of these mineral systems, and thus will likely be highly cited
2) Once promising mineral systems are identified, the student will do a survey of existing measuring techniques that could, at least in theory, help measure the clumping value of these systems.

This work will form an important theoretical basis for applying clumped isotope geochemistry to greater range of mineral systems. This, in theory, will open the possibility of measuring clumped isotopes in settings that lack carbonates, including other planets. The PhD Student will gain training in advance geochemical methods, fundamentals of mineral physics, and advanced numerical modelling.

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