On the test of a new volume variable cluster model method for stable isotope fractionation of solids: Equilibrium Mg isotope fractionations between minerals and solutions

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There is a tremendous interest in developing a cluster-model-based method of isotope fractionation calculation for solids because most of new techniques developed in modern quantum chemistry are for molecules which usually are represented by cluster models. The reason we developed this method is to remedy problems raised from a similar method used by Rustad and co-workers (e.g.,[1]), especially to enhance its implementation on isotope fractionation calculations between solids and aqueous species.

For the test of this so-called volume variable cluster model method (VVCM), we estimated Mg isotope fractionations between various silicate and carbonate minerals. We also study the Mg isotope fractionations between minerals and solutions. These cases usually are thought as the confusing part for isotope fractionation calculations because large disagreements exist among different theoretical groups (e.g., [1] and [2]).

Our results are very close to existing Mg and O isotope experimental data. Especially, for those mineral vs. solution cases, our results are better than previous theoretical estimations, suggesting very useful applications of this method in future.

[1] Rustad *et al*.. (2010) GCA, 74, 6301-6323. [2]Schauble (2011) GCA,75, 844-869.

Grow and Die:The Microbial mud mound and Its Sedimentary Environments of the Middle Permian , Sichuan Basin

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A Microbial mud mound in the Middle Permian Qixia Fm. in Sichuan basin,is first found.This mud mound is belong to Waulsortion ,and supported by mud,the primary builder is fungi.The species diversity is low,high species richness.The main lithology including bioclastic micritic limestone and Thrombolite.The Mud mound can be divided into mound-core,mound-flank,mound-base. Through a multidisciplinary approach, including carbonate petrology and geochemistry of the mud mound and unmound, we reconstruct the development history of the Microbial mud mound and characterize the formation and the evolution of the eastern portions of Sichuan basin. The results of geochemical analysis of the Qixia Fm. shows: all of the paleosalinity Z value greater than 122, $\delta^{13}C$ compositions range from 1.84‰ to 4.58‰(VPDB); δ18O compositions range from -6.33‰ to -4.42‰(VPDB);the Ancient water temperature values compositions range from 33.60℃ to 24.26℃;V/（V+Ni）values compositions range from 0.51228 to 0.77795. It shows that the environment of Qixia period were relatively deep water, hydrodynamic weaker, higher temperature, high salinity and anoxic. According to geochemical analysis,the Microbial mud mound growth environment is low dissolved oxygen content, the higher water temperature and the salinity is higher. After it dead,the water temperature are reduced and salinity began to increase which became a stable super salty hypoxia environment.

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