Recepción de resumenes CCG

Titulo / Autores / Institución

TITULO DE LA PONENCIA

Equilibrium Isotope Fractionation in Carbonate Minerals: Role of Mg-Ca Distribution and Thermal Effects

AUTORES

Paola Patron1, Carolina Martinez1, Alin M. Elena2, Marc Blanchard3 and Carlos Pinilla1,4,*

INSTITUCIÓN

1 Departamento de Física y Geociencias, Universidad del Norte, Km 5 Vía Puerto Colombia, Barranquilla, Colombia. 2STFC Daresbury Laboratory, Sci-Tech Daresbury, Keckwick Lane, Daresbury, Cheshire WA4 4AD, United Kingdom 3 Géosciences Environnement Toulouse (GET), Observatoire Midi-Pyrénées, Université de Toulouse, CNRS, IRD, UPS, 14 avenue E. Belin, 31400 Toulouse, France. 4 School of Chemistry, University of Bristol, Cantock’s Close, BS8 1TS, Bristol, United Kingdom.

CORREO ELECTRÓNICO

ccpinilla@uninorte.edu.co

Estilo preferido

ESTILO DE PRESENTACIÓN

- Presentación Oral

Categoría del resumen

ÁREA TEMÁTICA

Bio - Geo - Química

LÍNEAS TEMÁTICAS BGQ

Petrología, mineralogía y geoquímica

Resumen

PALABRAS CLAVE

Mg and Ca isotopes, carbonate minerals, ab-initio calculations, concentration effects, structural multiplicity

CONTENIDO DEL RESUMEN

Natural carbonates are key to understanding fundamental geochemical processes, particularly through their isotopic composition, which serves as a geothermometer for paleoclimate studies

and helps constrain the global Ca cycle. However, experimental determination of equilibrium isotope fractionation factors for 26Mg/24Mg and 44Ca/40Ca is challenging due to the complexities of mineral precipitation. Computational studies have explored the influence of Mg concentration on equilibrium isotope fractionation factors, typically using expensive density-functional-theory calculations. These studies, however, often substitute only one or two Ca atoms with Mg and rely on minimum-energy configurations at zero temperature, neglecting structural multiplicity and thermal probability effects relevant at ambient conditions.

This study examines Mg and Ca isotope fractionation in the Ca1-xMgxCO3 solid solution (calcite, dolomite, magnesite) and in aragonite, emphasizing the role of Mg substitution, structural multiplicity, and thermal probability. By analysing multiple configurations across various compositions, we observe a significant Mg concentration effect on the reduced partition function ratio using minimum-energy or maximum-probability approaches. However, this effect diminishes when applying a thermally weighted probability average, underscoring the importance of structural multiplicity in estimating equilibrium isotope fractionation factors.

We find that configurations with clustered Mg atoms exhibit reduced lattice distortion and lower Mg β-factor. Additionally, in ordered dolomite, minimized stress and disorder correlate with elevated Mg β-factor. Our results show that averaging fractionation factors over symmetrically non-equivalent structures in Mg-bearing calcite at a given composition can yield variations up to □1 ‰. This highlights the necessity of accounting for compositional complexity when estimating isotope fractionation in solid solutions.

Overall, our findings emphasize the structural implications of Mg incorporation in carbonates and its impact on isotope fractionation. This study enhances our understanding of Mg isotope behaviour in carbonate minerals and contributes to broader geochemical insights into their formation.