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Why Isotopic Equilibrium Matters for Organic Molecules: DFT Calculations on Methionine

JASON BOETTGER[1] AND JAMES D KUBICKI[2]

[1]The University of Texas at El Paso
[2]University of Texas at El Paso
Presenting Author: jdboettger@utep.edu

Many branches of stable isotope geochemistry have interpreted isotopic compositions in terms of isotopic equilibrium, e.g. for interpreting formation temperatures of Earth materials, paleo-pH, etc. However, most organic compounds are not formed under equilibrium conditions, as chemical disequilibrium is both ubiquitous and necessary in living organisms. The relevance of isotopic equilibrium to interpretation of organic molecules is thus not immediately apparent.

This presentation argues that isotopic equilibrium is relevant and necessary to the interpretation of intramolecular and clumped isotopic signatures in organic molecules. By providing an estimate of what equilibrium signatures would look like, molecular modeling can highlight instances of isotopic disequilibrium in molecules, pointing to e.g. rate-limiting steps in the formation of organic molecules. We apply molecular modeling of the equilibrium isotopic composition of methionine to demonstrate the interpretation of intramolecular isotope compositions through the lens of equilibrium. The isotopic composition of methionine points to the rate-limiting step in its industrial synthesis pathway. Notably, the carbon atom with the lightest isotopic composition is not the same as the site with the greatest isotopic disequilibrium, highlighting the need to understand what isotopic equilibrium would be when making an interpretation. The potential application of molecular modeling of isotopic equilibrium to other systems ranging from central metabolism to preserved biomarkers is addressed.