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Molecular Isotopic Structure as a Tool for Study of Earth-Surface Materials

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Stable isotopes can trace critical elements from sources to sinks in biogeochemical cycles; establish biogeochemical mechanisms affecting compounds of interest; quantify environmental temperatures; and indirectly constrain humidity, oxidation state, moisture budget or other environmental properties. But this set of methods often struggles with the inability to deconvolve multiple drivers of isotopic variations without prior assumptions.

Advances in technologies and measurement concepts, mostly over the last 25 years, have dramatically improved our ability to address such problems. 'Mass laws' for O and S isotopes have narrowly but powerfully impacted studies of the water cycle, atmospheric photochemistry, and S metabolisms. Potentially broader capabilities are provided by measurements of isotopic structures of molecules — i.e., heterogeneous distributions of isotopes across non-equivalent atomic positions ('site specificity'), and/or the propensities for rare isotopes to combine in the same molecule in amounts different from statistical probabilities ('isotopic clumping'). Molecular isotopic structures of CO_2, N_2O, CH_4, O_2, N_2, and H_2 are now familiar (100+ peer review papers per year) ways of measuring paleotemperature (i.e., carbonate clumped isotope thermometry) and studying cycling of small, biogeochemically active gases.

Perhaps the newest and most complex technical advance is high-dimensionality isotopic fingerprinting of biochemical compounds and pollutants. It is now possible to measure ~5-100 independent statements of isotopic structure simultaneously on a wide range of molecules. These data enable forensic assignment with unprecedented specificity and, when combined with machine-learning classifiers, exceptional sensitivity. Such measurements also enable a new, sophisticated means of studying metabolism and its environmental dependencies. Recent and emerging works prove the value of this approach in studies of sugars, organic acids, amino acids, steroidal compounds, and vanillin and other methoxy-bearing biomolecules. Further expansion of these measurements and, critically, their interpretations through advances in understanding and quantitative modeling of metabolic isotope effects will give rise to a vigorous new sub-discipline of stable isotope geochemistry.