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Triple oxygen isotope fractionation between O-bearing organic compounds and water, and their possible uses to study extraterrestrial organics

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Organic compounds (e.g., amino acids, hydrocarbons, carbonyls, carboxylic acids, sulfur and nitrogen bearing compounds, insoluble organic matter (IOM)) are found in carbonaceous chondrite meteorites and their origins remain a subject of active study. Carbonyl and aromatic alcohol compounds contain oxygen (O), the isotopic composition of which might allow us to trace these species to their volatile precursors and the environments where they formed. Specifically, it has been shown that there are large differences in ^{17}O anomaly between early solar system CO, H_2O, rocky bodies, rare pre-solar components, and chemical processing in the nebula and meteorite parent bodies led to large mass-dependent variations in oxygen isotope composition. These signatures must also be recorded by oxygen-bearing meteoritic organic compounds and thus, can be used as a fingerprint to trace where and how these organic compounds formed in the solar system.

We have evaluated the fractionation factors including mass laws for ^{17}O and ^{18}O isotope exchange between several organic compounds and water, calculated using B3LYP/aug-cc-pVTZ level of Density Functional Theory (DFT) at a range of temperatures relevant to formation of these compounds. The fractionation factors have been calculated for both gas phase molecules and molecules solvated in water. The COSMO solvation model is shown to be accurate for carbonyl compounds whereas explicit solvation appears to be preferred for Phenol and Alanine.

All of the organic compounds included in this study (Acetone, Cyclopentanone, Pentanal, Phenol, Alanine) are enriched in ^{17}O and ^{18}O compared to water (e.g., 24.4 – 41.1‰ at 273K for ^{18}O) in the temperature range investigated. This broadly agrees with experimentally measured Acetone-water ^{18}O fractionation factors reported in the literature. Using the calculated fractionation factors and mass laws, we predict triple O isotopic composition of these organic molecules formed in equilibrium from various volatile sources in the solar system.

Finally, we will present initial results of a new Orbitrap-based method for isotope ratio analysis of ^{17}O, ^{18}O and other isotopic properties of O bearing organics — a method capable of addressing the challenges of studies of meteoritic and returned samples.