A Bayesian approach to identify the provenance of methane gases using rare isotopologues

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Methane plays an outsized role in both the Earths' natural carbon cycle, as a potent greenhouse gas, and the global economy, as a critical energy source. It can be produced by various microbial pathways but also by non-biologic processes, namely: (i) the degradation of organic macromolecules at high temperature, or (ii) carbon dioxide reduction by hydrogen in the presence of mineral catalysts.

Despite recent advances in mass spectrometry that have enabled measurements of the concentrations of methane clumped isotopologues, ($\Delta^{13}CH_3D$ and $\Delta^{12}CH_2D_2$) in addition to traditional isotopes measurements (¹³C and D), there are significant overlaps in empirically-defined genetic fields for methane in both bulk and clumped isotope spaces. Therefore, in many environments, quantifying the relative contribution of microbial methanogenesis versus non-biological methane production remains imprecise. For example, the provenance of methane is often uncertain in serpentinization systems, where the H₂ gas produced is consumed by methanogenesis that could be either microbial or abiotic, or a mixture of the two. This issue is even more complicated on other Solar System bodies, such as Enceladus and Titan, where methane is found, because there is little to no access to the geochemical and isotopic context for the gases.

To better quantify the identification of methane provenance and assess its potential for the search for life beyond Earth, we are applying a Bayesian probabilistic framework to delineate microbial from non-biologic methane within the bulk isotope and clumped isotope space.

We use a compilation of both bulk and clumped isotopes measurement of methane gases for which their origins have been determined independently from isotopic measurements. This approach yields a posterior probability map for the various possible origin pathways for methane. This approach offers a first-order interpretation of methane isotopic composition and provides a quantitative tool to assess methane biogenicity.

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