

## Clumped isotope effects during C<sub>2</sub>H<sub>6</sub> recombination/dissociation reactions calculated using ab-initio canonical transition state theory

Distinguishing biotic compounds from abiotic ones is important in resource geology, biogeochemistry, and the search for life in the universe. Stable isotopes have traditionally been used to discriminate the origins of organic materials, with particular focus on hydrocarbons. However, despite extensive efforts, unequivocal distinction of abiotic hydrocarbons remains challenging. Recent development of clumped-isotope analysis provides more robust information because it is independent of the stable isotopic composition of the starting material. Taguchi reported data from a <sup>13</sup>C-<sup>13</sup>C clumped-isotope analysis of ethane and demonstrate that the abiotically-synthesized ethane shows distinctively low <sup>13</sup>C-<sup>13</sup>C abundances compared to thermogenic ethane Taguchi *et al.*, (2022).

The results reported by Taguchi *et al.*, lack solid kinetics-based evidence of the nature of the <sup>13</sup>C-<sup>13</sup>C clump-isotope values. We performed an *ab-initio* study on the recombination reaction of CH<sub>3</sub> methyl radicals combined with canonical transition state theory to determine the clumped-isotopic constants. We discuss the results obtained so far and made comparisons with the results from chamber experiments. The <sup>13</sup>C-<sup>13</sup>C signature can provide an important step forward for discrimination of the origin of organic molecules on Earth and in extra-terrestrial environments.