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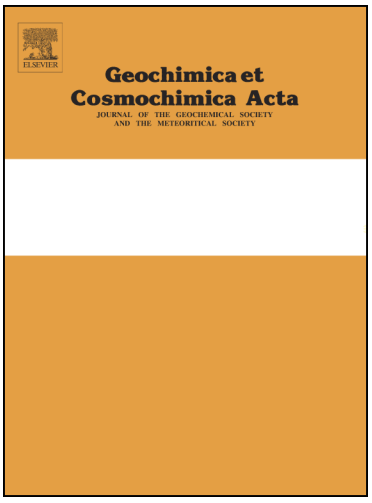

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Molecular and Detailed Isotopic Structures of Petroleum: Kinetic Monte Carlo Analysis of Alkane Cracking

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Abstract

The compositional and bulk isotopic signatures of hydrocarbon compounds are routinely characterized to constrain the origin of oils and natural gases in sedimentary basins. Recent developments in clumped isotope geochemistry have given rise to a suite of measurements that provide new information on the thermal history of low molecular weight hydrocarbon gases. However, to date no study has linked these compositional, bulk and clumped isotope constraints to any mechanistic understanding of how these signatures develop and evolve. In this study, we developed a kinetic Monte Carlo method to predict consistent and simultaneous molecular distributions, bulk isotopic content, and detailed (multiply substituted and site-specific) isotopic structures of hydrocarbons from a cracking model. The detailed isotopic structure of the source (initially modeled as long alkanes), the intermediates, and the product molecules is followed as a function of the level of conversion due to cracking reactions. The bulk ^{13}C content of gaseous alkane products generated via the model is shown to follow the linear natural gas plot at low conversion, but to deviate at high conversions. As examples of the information generated, the populations of center vs. terminal ^{13}C-substituted propane are reported as a function of the starting alkane chain length and conversion and the population of doubly-^{13}C-substituted ethane is described as a function of conversion and for different ^{13}C substitution patterns in the source. The results are compared to experiment where possible and highlight the possibility of constraining hydrocarbon source isotopic structure and the nature of the generation processes leading to the formation of natural hydrocarbon deposits.

1. Introduction

Investigation of the molecular and isotopic structure of petroleum liquids and gases has led to significant understanding of the processes of their formation from source material (Tissot and Welte, 1984; Bernard, 1977; Whiticar 1994; Galimov, 2006) and of their subsequent transformation in the environment. More recent study of multiply-substituted or clumped isotopologues (see Nomenclature) of hydrocarbons adds more information (Eiler, 2007) and offers great promise for further constraining the source and history of hydrocarbon liquids and gases, but understanding of the links between the molecular, bulk and detailed isotopic structures, and the formation processes is still immature.

Models of various kinds have played a role in enhancing our understanding of hydrocarbon formation. Coarse-grained or lumped models of the type kerogen → gas along with kerogen → oil → gas (Burnham, 1989; Pepper and Corvi, 1995a; Pepper and Dodd, 1995b) can be parameterized and compared with observations in order to capture the amounts of these lumps

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