Position-Specific Isotope Compositions of Propane from Natural Gases by Quantitative NMR

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The formation of natural gases and subsequent processes in the subsurface are of great interest for scientific and economic purposes. Conventional, bulk carbon and hydrogen isotopes of natural gases have been widely used to address these processes, but our understanding is still limited. Recently, new dimensions of information on the stable isotopes of natural gases have been explored, including clumped isotopes and position-specific isotope compositions.

We have developed a new method to determine both hydrogen and carbon position-specific isotope compositions of propane from natural gases based on quantitative NMR. The new technique is capable of analyzing intact molecules of propane with precision of <1 per mil and <10 per mil for carbon and hydrogen isotope compositions, respectively. The accuracy of the method has been tested by ^{13}C-labeled compounds as well as an inter-laboratory comparison of a light alkane.

Natural gas samples have been collected from several oil-gas fields in Texas and Oklahoma. The fraction of propane was separated and purified chemically and cryogenically, and their purity and isotopic integrity during the purification have been tested. Our results show that the differences in hydrogen and carbon isotope compositions between the two sites of propane (center vs. terminal C's and H's) range from -187 to +26 per mil and from -4.2 to +3.3 per mil, respectively. Some data of the position-specific isotope compositions are not consistent with theoretical predictions that the central site of propane is enriched in ^{13}C and ^{2}H relative to the terminal site both at isotope equilibrium and by simple cracking of longer hydrocarbons. These position-specific isotope compositions are expected to shed new lights on the origin and history of propane and other natural gases.