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The control of organic matter input and thermal maturity of source rocks on the molecular and intramolecular isotope of natural gas

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Position-specific isotope analysis of propane in natural gas of Turpan-Hami Basin was carried out, and the carbon isotope composition of natural gas and propane molecule during the thermal evolution of type I and type III kerogen was simulated. The results show that different kerogen types and thermal evolution degrees are the main controlling factors that determine the carbon isotope distribution at the thermogenic propane position.

The organic matter is mainly derived from aquatic organisms. There are more organic matter with straight-chain structure in kerogen. Propane is mainly formed by the n-propyl pathway. Kinetic isotopes effect acts on the terminal carbon position of propane, $\delta^{13}C_{central}$ $\delta^{13}C_{terminal}$, $\Delta_{C\text{-}T}$ ($\delta^{13}C_{central}$-$\delta^{13}C_{terminal}$) is positive. For organic matter with more branched-chain structure, such as type III kerogen, the kinetic isotope effect mainly acts on the central carbon during the formation of propane by the i-propyl pathway, resulting $\Delta_{C\text{-}T}$ is negative. In addition, propane was mainly formed by the i-propyl pathway in the early mature stage. With the increase of maturity, the i-propyl was gradually consumed and n-propyl was gradually involved in the reaction, $\Delta_{C\text{-}T}$ changed from negative to positive. In general, the input of organic matter and sedimentary environment control the type and thermal evolution of kerogen, and the different structures of organic matter determine the different formation pathways of propane, which ultimately leads to the difference in its intramolecular isotope composition. The formation and cracking of propane in the maturation process is a dynamic process related to the type of organic matter. Consequently, the isotopic composition of propane position can indicate the reaction pathway and precursor molecular structure of natural gas, provide a basis for the formation mechanism of natural gas and the chemical structure of kerogen in geological period.