

# Gas-Grain Model for Carbon Isotope Fractionation of COMs in Star-Forming Cores

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Understanding the isotopic composition of ice molecules in star-forming cores is a powerful tool for investigating the origin of organic molecules in solar system objects. Recent high-resolution ALMA observations have measured the carbon isotopic ratios ( $^{12}\text{C}/^{13}\text{C}$ ) of Complex Organic Molecules (COMs) in the Class 0 low-mass protostellar object IRAS 16293-2422B. The measured isotopic values are comparable to the average values in the local interstellar medium or show lower values, that is enriched in  $^{13}\text{C}$ . Several model calculations, observations, and laboratory experiments suggest that COMs are formed on the dust grain surface during star-formation. However, there are no model calculations of carbon isotope fractionations of COMs, and the origin of observed fractionations is not well understood.

In this study, we use a physical model of a star-forming core undergoing gravitational contraction, and performing chemical reaction network calculations considering three phases: the gas phase, the grain surface, and the ice mantle. And then we systematically investigate the carbon isotopic fractionations of COMs including formation of icy COMs prior to star formation and subsequent their sublimation into the gas phase following star formation.

Before the protostar formation, the  $^{12}\text{C}/^{13}\text{C}$  ratios of icy small carbon species exhibit bimodal profile: the derivative species from CO are slightly enriched in  $^{13}\text{C}$ , while those succeeded from C and  $\text{C}^+$  are depleted in  $^{13}\text{C}$  owing to isotope exchange reactions. Icy COMs, originating from simpler species, also show this bimodality or deviation from it due to mixing. Sublimated COMs reflect the  $^{12}\text{C}/^{13}\text{C}$  ratios of their icy counterparts. However, parts of COMs originate from radical and ionised species at higher temperature ( $T > 20$  K), which change the  $^{12}\text{C}/^{13}\text{C}$  ratios of the molecules from that of their ice in the prestellar phase. Eventually, in our base model COMs exhibit more fractionated rather than the observed value. The additional Eley-Rideal (ER) reactions, which is a grain surface reaction having occurred at shorter timescales relative to isotope exchange reactions, lead to formation of COMs originated from less fractionated atomic carbon.

Consequently, the ER reactions mitigates isotope fractionation, and roughly reproduces the non-fractionated observed values. Nonetheless, further investigation is necessary to reproduce the observed values more comprehensively.