Quantum Chemical Study to Verify the Formation of Complex Organic Molecules in Molecular Clouds

*Yu Komatsu[1,2], Kenji Furuya[2]

1. Astrobiology Center, 2. National Astronomical Observatory of Japan

Various complex organic molecules (COMs) have been identified in regions with high temperatures exceeding 100 K, present in both high- and low-mass star-forming regions. Dimethyl ether (DME; CH_3OCH_3) and methyl formate (MF; $HCOOCH_{3)}$ are COMs typically observed in star-forming molecular cloud cores. It was originally thought that these molecules primarily formed through chemical reactions occurring in the hot gas phase after star formation and radical chemical reactions taking place on the warm surface of dust particles. However, recent observations have detected these molecules within molecular cloud cores where stars have not yet developed, and at extremely cold temperatures as low as 10 K. While the formation of DME in interstellar space has been attributed to radiative association in the gas phase [1], this does not fully explain its observed abundance at such low temperatures. Conversely, the formation mechanism of MF in interstellar environments has not been thoroughly investigated.
To understand how DME and MF are formed at extremely low temperatures, we employed an automated chemical pathway search technique based on the transition state theory of quantum chemistry [2, 3] to explore the possible routes through which these molecules can be energetically produced in their electronic ground states [4]. Our calculations revealed energetically favorable gas-phase reactions with no energy barriers for both compounds. For CH_3OCH_3, the reaction network we obtained depicted a detailed pathway starting from CH_3O and CH_3, partially corroborating findings from previous research. In contrast, the formation pathway for MF was found to be more complex. Dust surface reactions and/or photochemical reactions, although not included in our calculations, may play a significant role in MF synthesis. Hence, our study provides theoretical insights into the potential mechanisms for the formation of these COMs, even under extremely cold conditions. The next crucial step is to link these identified reaction pathways with astrophysical models using reaction rate equations to estimate the abundance of COMs in interstellar environments, thus facilitating a comparison between theoretical predictions and observational data.

References
[1] Tennis J., Loison J.-C., and Herbst, E.: 2021, Astrophys. J., 922, 133. [2] Maeda, S. et al.: 2018, J. Comput. Chem., 39, 233–251. [3] Komatsu, Y. and Suzuki, T.: 2022, ACS Earth Space Chem., 6, 10, 2491–2498. [4] Komatsu, Y. and Furuya, K.: 2023, ACS Earth Space Chem., 7, 9, 1753–1760

Keywords: COMs, Quantum Chemistry, Reaction Path Search, Astrochemistry

