Quantum chemical prediction of possible reactions of interstellar nucleobases

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Nucleobases, which generate the genetic code, i. e. ATCG, were detected from the Murchison meteorite [1]. To take the fact as well into consideration that glycine, the simplest amino acid, was detected both from Murchison meteorite and the comet 67P/C-G, life-related molecules can be constructed easily in an extra-terrestrial environment.

In this study, to estimate possible reactions of nucleobases in the ultracold environment and consider which are key components and where are suitable regions to proceed reactions of such complex molecules, we use the Global Reaction Route Mapping (GRRM) program [2] in order to discover complicated reaction networks, and focus especially on dissociation channels.

At first, we estimated rough profiles of reactions in vacuum with realistic computational costs. As a result, we found two key reaction paths toward pyrimidine from abundant interstellar molecules, HCN, C_2H_2 (Figure 1). Both reactions have high reaction barriers, which indicate the difficulty in ultralow-temperature environment. To avoid the higher barriers, the formation of C_2H_2NCH with lower reaction barrier was evaluated. Key reactions on icy grain surface will be presented. In addition to pyrimidine, the estimated paths toward cytocine, thymine, uracil were also estimated and will be presented.

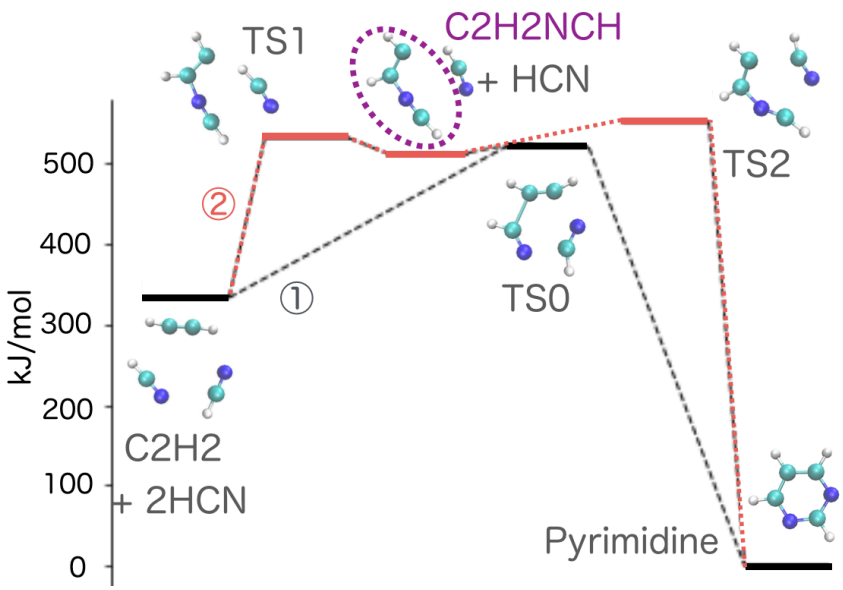

Figure 1: Two reaction paths toward pyrimidine were discovered. The potential energies for stable structures and transition states are shown. Each energy was evaluated at MP2/aug-cc-pVTZ level.

References

[1] Z. Martins et al., 2008, Earth and planetary science Letters 270, 130.
[2] K. Ohno & S. Maeda, 2004, The Journal of Physical Chemistry A 110.28, 8933.