Synthesis of the simplest alcohols and nitrogen-substituted PAHs in the interstellar medium

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Complex organic molecules (COM) are molecules containing six or more atoms of hydrogen, carbon, nitrogen or oxygen - they make up about a third of all molecules found in the interstellar medium [1]. Establishing the ways of their formation is critically important for explaining the fundamental processes governing the poorly understood chemistry of the interstellar medium and for determining organic molecules capable of forming in space conditions. Modern astrochemical models believe that COMs are formed in cold molecular clouds on dust particles - silicate or carbon nanoparticles covered with a thin layer of ice consisting of water, methanol, carbon monoxide, carbon dioxide, ammonia, formaldehyde and methane [2] - as a result of exposure to cosmic radiation at temperatures reaching up to 10 K. During the gravitational collapse of a molecular cloud, molecules from the dust particles can sublimate into the gas phase, since the temperature of the dust particles increases due to the non-isothermal phase of the collapse, and then due to heating from the hot core [1]. These molecules then enter the protoplanetary disk, planets and other bodies in star systems. A recent analysis of the organics in comet 67P has found many organic substances, much more diverse and complex than expected based on currently accepted chemical models [3], therefore, there is still no fundamental understanding of the level of molecular complexity of COM that can be achieved in deep space.

The purpose of the work is to study the radical substitution reaction involving components of space ice, leading to the formation of the simplest alcohols, and about revealing the mechanisms of the chemical conversion of acetonitrile radicals into diazines (pyrimidine and pyridazine) in the gas-phase and ice-phase reactions. Geometry optimization of all possible stationary and transient states was carried out at the long-range corrected hybrid density functional ωB97X-D level of theory with Dunning's correlation-consistent cc-pVTZ basis set in Gaussian 09. The ice- phase conditions were created by applying the SCRF (PCM, solvent water) approach in Gaussian that allows calculations to be performed in the presence of a solvent by placing the solute in a cavity within the solvent reaction field. The energy refinement was carried out according to the extrapolation scheme to the complete basic set E(CBS), the phenomenological velocity constants depending on temperature were calculated in the Abstraction subroutine of the MESS package.

References

1. E. Herbst, The synthesis of large interstellar molecules // International Reviews in Physical Chemistry. — 2017. — Vol. 36. — P. 29.
2. A. C. A. Boogert, P. A. Gerakines, D. C. B. Whittet, Observations of the Icy Universe // Annual Review of Astronomy and Astrophysics. — 2015. — Vol. 53. — P. 541.
3. Altwegg K., Balsiger H., Berthelier J. J. et al. Organics in comet 67P – a first comparative analysis of mass spectra from ROSINA–DFMS, COSAC and Ptolemy // Monthly Notices of the Royal Astronomical Society. — 2017. — Vol. 469. — P. 130.