

The methylidyne radical with the benzonitrile reaction potential energies and molecular parameters

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The reaction of the methylidyne (CH) radical with benzonitrile (C₆H₅CN) molecule was studied at a collision energy of 5.0 kJ/mol with ab initio calculations of the potential energy surface (PES). At low temperatures in deep space, a large amount of nitriles are present in the atmosphere of Saturn's moon Titan [1, 2], as well as in interstellar molecular clouds. Reactions of nitriles with the methine radical CH are of interest, as potential initial step in the study of biological molecules. In particular, in the course of the reaction with cyanide molecules, a nitrogenous base, structural blocks in DNA chains, can be formed. In addition, the formation of linear and cyclic radicals is possible with the release of the corresponding products: atoms, molecular particles, ethylene, etc.

Geometries and potential energies of reactants, products, intermediates and transition states for the reaction were found by means of ab initio quantum chemical method ωB97xd/cc-pVTZ [3, 4] and the higher-level corrections were evaluated at the CCSD(T)-F12 level of theory [5, 6, 7] with the cc-pVQZ-f12 basis set [8, 9].

Those results were utilized in Rice–Ramsperger–Kassel–Marcus calculations of the product branching ratios at the zero pressure limit – common approach in modelling of the cold molecular clouds chemistry. Mechanism identified emphasizes importance of the CH+C₆H₅CN reaction as an important supplier of the initial bricks for building heterocyclic hydrocarbons in extreme environments.

References

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