Transformation of acetone into 1-propen-2-ol in the ice phase

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There are some theories of the origin of life on the Earth. One says that the very first important precursors of biomolecules were formed near hot springs, whereas another states that these molecules were created after lightning strikes due to a lot of releasing energy at this moment. However, aromatic compounds have been found in meteorites delivered to the Earth. Therefore, we can not rule out that building blocks for biomolecules are ubiquitous in outer space. This was confirmed by observations via radio telescopes. The thing is that due to the high rarefaction of the interstellar medium, atoms and molecules in the gas phase rarely collide. Organic precursor compounds are formed just during molecular collisions. On the other hand, we know that there are molecular dust clouds in space, from which, in fact, solar systems are formed. The density of the substance in dust grains is high, and the reaction rates are much higher than in a gas. This may explain the evolution of complex compounds in the low-temperature conditions of space [1, 2].

The purpose of the work is about revealing the mechanisms of the chemical conversion of acetone into prop-1-en-2-ol in the ice-phase reaction. The relevance is that the quantum chemical study of the mechanisms of miscellaneous ice-phase chemical reactions is of great importance in astrochemistry and astrobiology since it is one of the ways to find out how complex organic molecular species vital for the origin of life on the Earth were formed in the Universe.

Geometry optimization of different species related to searching for the ice-phase transition state between acetone and prop-1-en-2-ol was carried out at the long-range corrected hybrid density functional ωB97X-D level of theory with the 6-311G(d,p) basis set in Gaussian 09. At the first stage, the integrated water environment surrounding the molecules related to the transition state and imitating ice-phase conditions was not used. Moreover, there is the second stage where these 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. Nevertheless, there are several obtained transition states at the first stage where water molecules helping an atomic hydrogen atom to migrate from carbon to oxygen without using SCRF=(PCM, solvent=water) approach was gradually added. The transition states of the first stage of optimization further were refined by performing a single-point calculation ωB97X-D/6-311G(d,p)+SCRF=(PCM, solvent=water) in Gaussian to check how the energies could change compared to the both approaches of geometry optimization. The final stage will be to refine energies of the second stage of optimization using the explicitly correlated couple clusters technique with single and double excitations, as well as perturbative treatment of triple excitations CCSD(T)-F12 along with Dunning's correlation-consistent cc-pVTZ-f12 basis set in Molpro 2010.

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References

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