Kinetic investigation of a promising synthetic route for several prebiotic molecules: the reaction between vinyl alcohol and radical cyanide

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Vinyl alcohol (Vy) and radical cyanide (CN) are two relatively abundant molecules present in the interstellar medium (ISM). In particular, Vy's microwave transitions have been detected in emission toward the dense molecular cloud SagittariusB2 (N) which is one of the most studied by astronomers because it is rich in prebiotic interstellar complex organic molecules (iCOMs). Vy is the enolic tautomer of acetaldehyde, another very abundant species in the ISM [1]. It can exist in two rotameric forms, *syn* and *anti*, depending on the value assumed by the dihedral angle φ (C=C-O-H), which defines the position of the hydroxyl hydrogen with respect to the double bond [2]. To find out possible iCOMs formation pathways, investigations are ongoing in our group on the gas-phase reactions between Vy's conformers and CN for which, to the best of our knowledge, no kinetic data are available in the literature. The reactions have been preliminarily characterized through a quantum mechanical approach based on the double hybrid functional DSDPBEP86-GD3BJ in conjunction with the jun-cc-pVTZ basis set. Preliminary results suggest that Vy's conformers feature a completely different reactivity with CN. For the *anti* conformer, the hydrogen abstraction leading to radical Vy + HCN is strongly favored with respect to the association of CN to the double bond. For the *syn* conformer, the barrierless association reaction to the double bond shows a strong leading to formation of an intermediate lying at -227.9 kJ mol^{-1} with respect to the reactant asymptote. Work is ongoing in our group in order to refine the potential energy surface through high-level *ab initio* composite schemes and to perform a kinetic analysis through StarRate [3], a program specifically designed for astrochemical reactions, based on a master equation approach coupled to capture theory for the bimolecular association steps and to the Rice-Ramsperger-Kassel-Marcus for the unimolecular evolution of the intermediates.

References

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