Tautomers of gas-phase erythrose and their interconversion reactions: insights from high-level ab initio study.

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Streszczenie

d-Erythrose is a C_4monosaccharide with a biological and potential astrobiological relevance. We have investigated low-energy structures ofd-erythrose and their interconversion in the gas phase with the highest-level calculations up-to-date. We have identified a number of structurally distinct furanose and open-chain isomers and predicted α ↔ α and β ↔ β furanose interconversion pathways involving the O-H rotamers. We have estimated relative Gibbs free energies of the erythrose species based on the CCSD(T)/aug-cc-pVTZ electronic energies and MP2/aug-cc-pVTZ vibrational frequencies. By using natural bond orbital theory we have also quantified a stabilization of erythrose conformers and interconversion transition states by intramolecular H-bonds.

Adres publiczny

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Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html