

# A story of cyclohexane

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Cyclohexane and its derivatives are the simplest models with a six-membered ring in organic and biological molecules and has been the subject of extensive experimental and theoretical investigations to understand the puckered structures and interconversion of the six-membered ring in cyclohexane and its derivatives.<sup>[1,2]</sup> In particular, the conformational transitions of the pyranose ring was responsible for the elasticity of polysaccharides<sup>[3]</sup> and was an essential factor in the synthesis and hydrolysis of glycosidic bonds in saccharides.<sup>[4]</sup>

We explored the interconversion pathways along the puckering transitions in cyclohexane on the two-dimensional projection of the Cremer-Pople sphere<sup>[5]</sup> using density functional theory (DFT) methods and assessed the CCSD(T), MP2, and dispersion-corrected DFT methods with various basis sets for the relative energies of local minima and transition states for the feasible puckering transitions.<sup>[6]</sup> In addition, we calculated the activation free energies and relative free energies for puckering transitions of cyclohexane in the gas phase and in chloroform, and compared with the corresponding experimental values. The feasible pathways along the puckering transitions in cyclohexane obtained here will be used as initial information for exploring the pathways of the helix inversion of a  $\beta$ -peptide pentamer<sup>[7]</sup> via cooperative ring flipping of the cyclohexane ring moiety of each residue along the peptide chain.

## References

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