A Computational Study of Substituted Cyclohexanes and Tetrahydro-*2H*-pyrans to Evaluate the Steric and Stereo-electronic Contributions to the Conformational Energies

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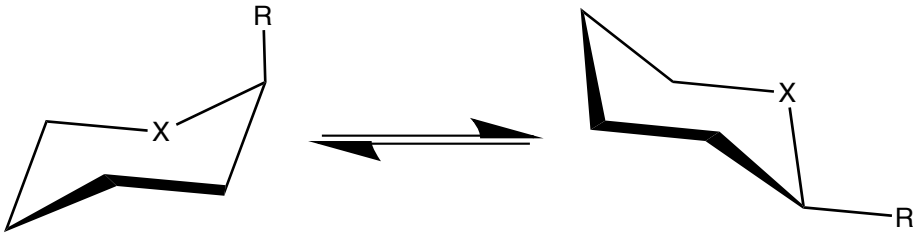
Geometry optimizations at a variety of computational levels were carried out on a series of substituted cyclohexanes and tetrahydro-*2H*-pyrans. Relaxed dihedral scans at the B3LYP/6-311G++(d,p) level helped to identifiy the steric contributions of the position of the rotamers. Analysis of the optimized geometries non-bonded distances contributed to an understanding of the steric contributions. Analysis of bond lengths and bond angles showed changes that reflected possible hyper-conjugation contributions to the stability of some configurations. The series of compounds selected in this study provide a series of model compounds that lead to modeling the contributions to the conformational energies of D-glucopyranose.



1 X = CH_2 , R = CH_3

2 X = O , R = CH_3

3 X = CH_2 , R = OH

4 X = O , R = OH

5 X = CH_2 , R = CH_2OH

6 X = O , R = CH_2OH