A Computational Evaluation of the Structures of α– and β–D-Glucopyanose and the Contributions to their Stability.

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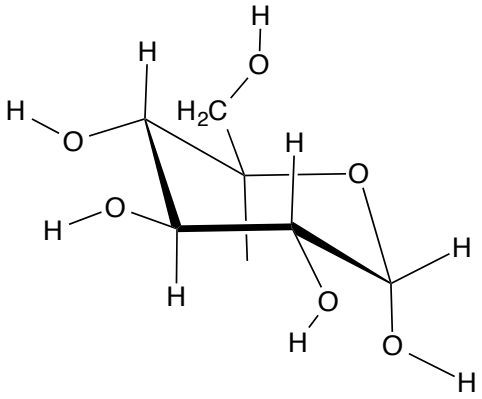
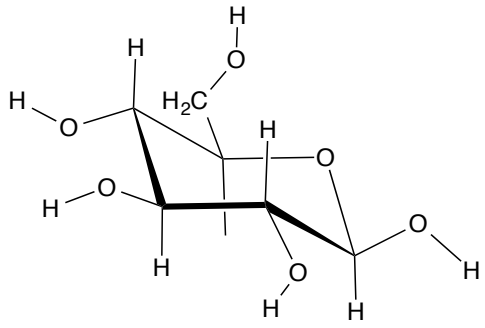
Geometry optimizations at a variety of computational levels were carried out on α– and β–D-glucopyranose and a number of model compounds in order to separate the steric and stereo-electronic contributions to the energies and relative stabilities of the α– versus β– conformers and the *gg*, *gt*, and *tg* rotamers. Changes in the geometry of the conformers give some indicators of the magnitude of the stereoelectronic contributions. Relaxed scans of several dihedrals at the B3LYP/6-311G++(d,p) level show that only the hydroxymethyl substutient on the pyran ring makes any contribution to the set of possible configurations. The relative energies of *gg*, *gt*, and *tg* rotamers from these scans are consistent with other computational studies at this and other levels of calculations. Comparisons of dihedral scans and conformational energies of 2-hydroxymethyl 6-hydroxyl-tetrahydro-*2H*-pyran and 2-hydroxymethyl-tetrahydro-*2H*-pyran with 1,5-anhydro-D-glucitol and D-glucopyranose indicate that the hydroxyl substituents on the pyran ring make little contribution to the stability of the α–, β– conformers and the *gg*, *gt*, and *tg* rotamers of D-glucopyranose.



(1a) α-Glucopyranose



(**1b)** β-Glucopyranose