# A Computational Evaluation the Factors Affecting the Structure of α– and β–D-Glucopyanose in Aqueous Solution

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Previous work has established the stable structures and energetics of α– and β–D-glucopyranose in the gas phase but some examination of the behavior of glucose in aqueous solution is necessary to provide a more realistic picture. By starting with the gas phase optimized geometries of α– and β–D-glucose, thermochemistry calculations were done and gas phase conformational free energies (ΔG°) were calculated. The geometry optimizations were done using 6-31G+(d,p), 6-31G++(d,p), 6-311G+(d,p) and 6-311++(d,p) basis sets with HF, DFT (B3LYP) and MP2 methods. The B3LYP/6-311G++(d,p) gas phase optimized geometries were reoptimized with several solvent models: IEF-PCM (**I**ntegral **E**quation **F**ormalism of the **P**olarized **C**ontinuum **M**odel) , CPCM (the **C**onductor-like **P**olarized **C**ontinuum **M**odel, and SMD (the **S**olvation **M**odel based on electron **D**ensity). CPCM gave results most consistent with experimental values and was used for examining the relationships between energy and geometry.

Two-dimensional scans of energy versus the H-O-C1-O dihedral, the H-O-C6-C5 dihedral and the O-C6-C5-O dihedrals show results consistent with the gas phase results: Only the orientation of hydroxymethyl substituent at C5 ring makes any significant contribution to the energy. The stable rotamers seen in the gas phase *(gg*, *gt*, and *tg* relating the orientation of the hydroxymethyl group at C5) are also seen the solvated molecules but with different relative energies.

Three-dimensional scans of energy versus the two dihedrals in in the hydroxymethyl group (HOCC and OCCO) were done for both α– and β–D-glucopyranose to develop a potential energy surface to confirm the geometries of the low energy structures and establish consistency with the gas phase results. These scans were also relaxed scans in which the geometry was optimized at each 5° step using the B3LYP method with the 6-311G++(d,p) basis set and the CPCM solvation model with water as the solvent.