

CBIMMS Invited Seminar

Density functional/*ab initio* studies on carbohydrates: Solvation with explicit water molecules and conformational preferences of disaccharides

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Thursday, Nov. 14, 2002

10:00am

Room 141 Hudson Hall

Abstract

Geometry/energy optimization of mono-, penta- and decahydrates of glucose were carried out at the B3LYP/6-311++G** level of theory. Energetically favored hydration sites were found and the stress energy on glucose associated with the interaction of the water molecules was obtained. The enthalpy, entropy, zero point energy, and hydrogen bond energy were found and the free energy compared between hydrogen bonding sites in which one H--O interaction is found and those with double hydrogen bonding sites. The stability of the α - and β -glucose anomers are described and comparisons made to solution results.

β -D-cellobiose and a series of cellobiose analogs were also studied at the B3LYP/6-311++G** level of theory to isolate and understand how the various electronic components of the β -(1->4)-linked disaccharide, contribute to the energetic stability of the molecule in vacuo. Our studies on β -D-cellobiose showed that the most energetically stable conformation was that in which the dihedral angle ϕ_H was Δ flipped Δ by $\sim 180^\circ$ relative to the Δ normal Δ or observed form. From our examination of eight sets of structures in which different combinations of functional hydroxyl and hydroxymethyl groups were removed, it was determined that only β -D-cellobiose and one other analog (β -xylobioside), can form a synergistic or Δ co-operative Δ hydrogen-bonding network that stabilizes the Δ flipped Δ form. Preliminary hydration studies on cellobiose suggest that more than one water molecule is required before the Δ normal Δ conformation is energetically preferred.

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