

Calculation on *Cyclopyranose* as C-Nanotube Co-solvent
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The properties of single-wall carbon nanotubes (SWNT) are classified in *zigzag* ($n,0$), *armchair* (n,n) and *chiral* (n,m). A recommended periodic table [1,2] format is discussed [3,4]. The solubility of SWNTs is investigated in a variety of solvents, finding a class of non-hydrogen-bonding Lewis bases that provide good solubility [5]. The investigated solvents are grouped in three classes. Solvchromic parameters, dielectric permittivity, ionization potential, electron affinity, volume and charge transfer have been calculated for different solvents. A molecular modelling study of the linear and cyclic (1→4)-linked oligosaccharides containing respectively 1–6 and 5–6 D-glucopyranose units provides a clear conception of their overall conformations, their contact surfaces and their cavity proportions [6]. This gives a first estimation of their inclusion properties. An expansion of the central channel is suggested for helical D-glucopyranose-SWNT complexes. Free energy of solvation and partition coefficient have been computed for $\alpha(1\rightarrow4)$ -linked D-glucopyranose residues. Dipole moment, ionization potential, electron affinity, volume and charge transfer have been calculated for $\alpha(1\rightarrow4)$ -linked D-glucopyranose residues. Fig. 1 illustrates MOPAC-AM1 standard heat of formation ΔH_f° for D-Glcp_n vs. number of units. Fig. 2 shows MOPAC-AM1 standard heat of formation per unit $\Delta H_f^\circ/n$ for D-Glcp_n vs. number of units. Fig. 3 displays MOPAC-AM1 standard heat of formation per unit for I_n^{z-} vs. number of units. Provisional conclusions follow. (1) Solubility of SWNTs has been investigated in a variety of solvents, finding a class of non-hydrogen-bonding Lewis bases that provide good solubility. Solvents have been grouped in three classes. SWNTs in some organic solvents are positively charged, while in water/Triton X are negative. It is explained on the basis of dielectric permittivity and electron affinity. (2) *CycloD-Glcp_n* are less hydrophilic than linear structures. The decrease of hydrophilicity by cyclation is smaller for D-Glcp₅ than for D-Glcp₆. The lipophilicity characteristics of *cycloD-Glcp_n* point towards the hydrophobic effect as an important factor governing the formation of D-Glcp_n-inclusion complexes with hydrophobic molecules by incorporation into the hydrophobic channel. (3) The positive electron affinity of D-Glcp suggests the formation of colloids of positively charged SWNTs in water. This charge transfer is assumed for all D-Glcp_n. (4) Variation of $\Delta H_f^\circ/n$ for D-Glcp_n shows that shorter chains are more stable than larger ones. *CycloD-Glcp_n* are less stable than linear D-Glcp_n. Variation of $\Delta H_f^\circ/n$ for I_n^{z-} indicates that shorter chains are more stable than larger ones. An expansion of the central channel is suggested for the helical D-Glcp_n-SWNT complexes. Work is in progress on the study of D-Glcp_n- I_m^{z-} , D-Glcp_n-SWNT and crown ether-SWNT complexes. This would give an insight into a possible generality of these conclusions.

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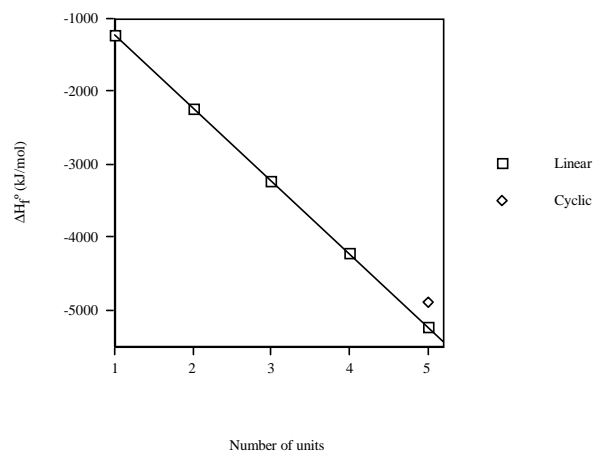


Fig. 1. MOPAC-AM1 standard heat of formation for D-Glcp_n vs. number of units.

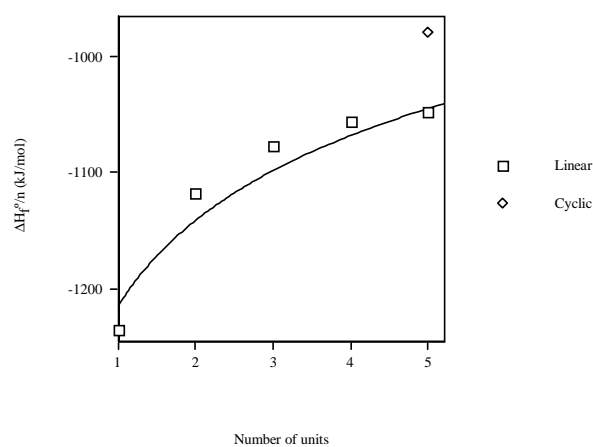


Fig. 2. MOPAC-AM1 standard heat of formation per unit for D-Glcp_n vs. number of units.

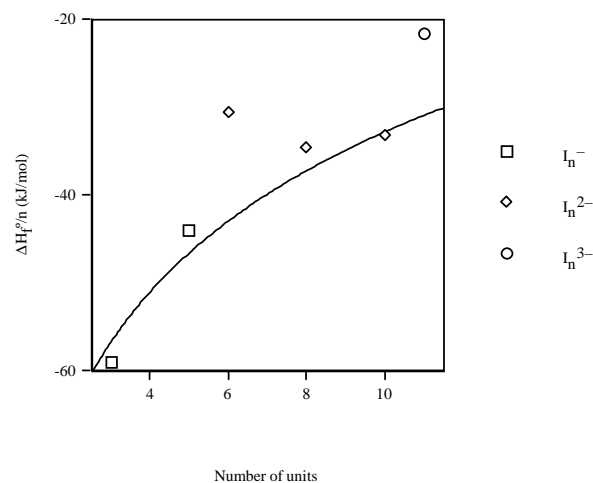


Fig. 3. MOPAC-AM1 standard heat of formation per unit for I_n^{z-} vs. number of units.