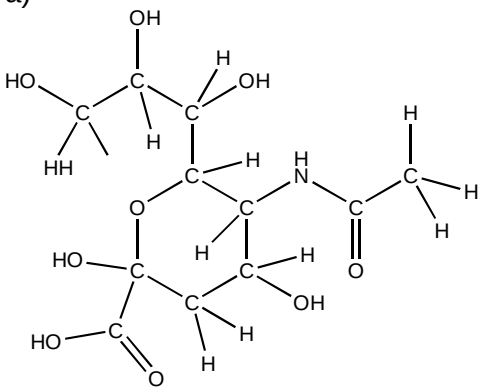
Computational Chemistry: Answers

1. a)



[2]

(b) (i) a ≈ 109.5°; b ≈ 118°; c ≈ 107° [3]

(ii) This is done on the basis of Valence Shell Electron Pair Repulsion (VSEPR) theory.

The carbon atom at *a* is making four single covalent bonds (it has four bonding pairs of electrons around it) and these are arranged tetrahedrally.

The carbon atom at *b* is making two single and one double covalent bonds (it has three groups of electrons around it) and these are arranged in a trigonal planar arrangement. The group of four electrons in the double bond repels the other electrons more than an electron pair and therefore angle *b* is 'squeezed down' to a little less than 120°.

The nitrogen atom at *c* is making three single covalent bonds and also has a lone pair (it has four electrons pairs around it). The electron pairs are arranged tetrahedrally but the lone pair repels the other electrons more than a bonding pair. This 'squeezes down' angle *c* to a little less than 109.5°. [3]

c) All the hydrogen atoms that are part of OH groups and the hydrogen that is part of the NH group. [2]

d) All the oxygen atoms and the nitrogen atom. [2]

e) Fluorine, oxygen and nitrogen [3]

f) A hydrogen bond can form between a hydrogen atom that is covalently bonded to an electronegative atom (F, O or N) and another electronegative atom. [2]

g) (i) The COOH group

(ii) The NH group [2]

h) (i) The H of the COOH group

(ii) The N of the NH group [2]

i) A lone pair of electrons [1]

j) All the atoms bonded directly to an oxygen atom or the nitrogen atom are polarised δ^+. All the oxygen atoms and the nitrogen atom are polarised δ^-. [2]