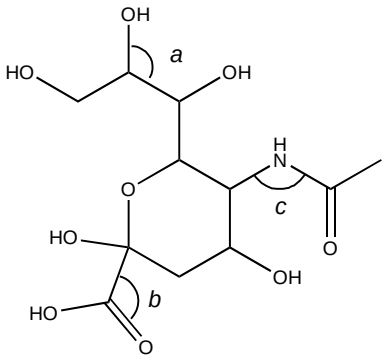
Computational Chemistry: Questions

1. The structural formula of sialic acid is shown below:



a) This formula does not show either carbon atoms or hydrogen atoms that are bonded to carbon atoms. Copy the formula and draw in all the carbon and hydrogen atoms. [2]

b) (i) Estimate the sizes of the bond angles labelled *a*, *b* and *c*.

_____[3]

(ii) Explain carefully the basis on which you made your estimations.

_____

_____

_____

_____[3]

c) Mark on your copy of the formula all the hydrogen atoms that could take part in hydrogen bonding with an electronegative atom on another molecule. [2]

d) Mark on your copy of the formula all the electronegative atoms that could take part in hydrogen bonding with a suitable hydrogen atom on another molecule. [2]

e) Name the three elements that are sufficiently electronegative to take part in hydrogen bonding.

_____[3]

f) Complete the following description of hydrogen bonding. You may need to use several words in each of the gaps.

A hydrogen bond can form between a hydrogen atom that is _____ and _____. [2]

g) Mark on your copy of the formula

(i) an acidic group

(ii) a basic group. [2]

h) Mark on your copy of the formula

(i) a hydrogen atom that is likely to be lost as a H^+ ion

(ii) an atom that is likely to accept a H^+ ion. [2]

i) Consider your answer to (h) (ii). What feature must an atom have to allow it to accept an H^+ ion?

_____

_____

_____[1]

j) Mark on your copy of the formula all the atoms that are polarised δ^+ and all those that are polarised δ^-. [2]