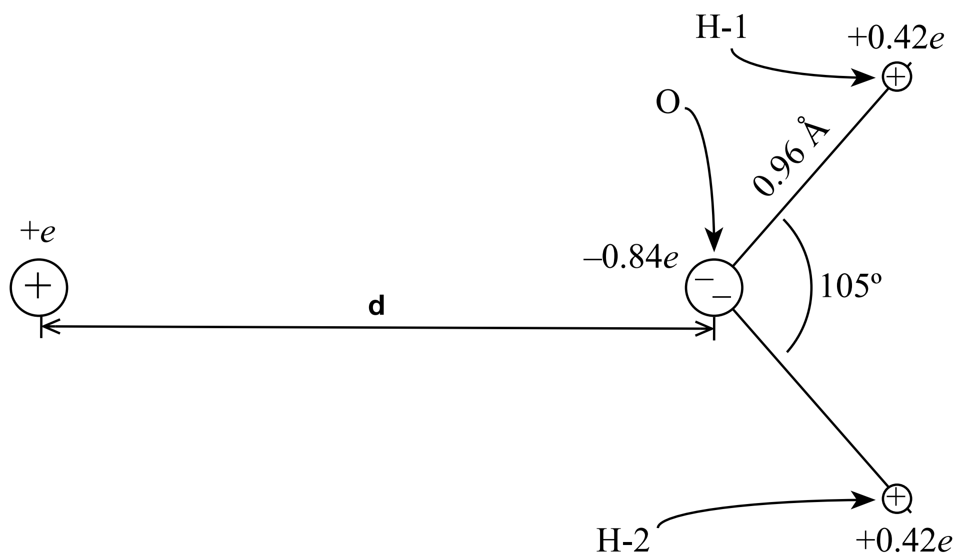
IPLS Recitation 05 – Hydrogen bonding

Name: __________________________ Lab table # ______ at (circle one): 12:00 / 3:00

If it is positioned appropriately, a neutral water molecule will be attracted to a charged particle, a phenomenon called hydrogen bonding. The attraction is pretty weak and short-ranged, but hydrogen bonding is critically important because all biochemistry occurs in aqueous environments. In this recitation, you will calculate the attractive force between a water molecule and a positive ion from first principles.[1]



Values pulled more or less randomly from this page.

A water molecule is positioned as shown, a distance d (in nm) from a singly charged positive ion. Use the effective (net) charge on the hydrogens and oxygen, as well as physical dimensions of the molecule, from the figure above.

(a) Calculate the force that the ion exerts on the water molecule, for $d = 1$ nm. I suppose you could do this by hand, but I highly recommend you use a spreadsheet. You can start from scratch, or grab a copy of "Workbook 05 blank" which has a skeleton to work from.

[1] As you will see, it is tedious doing this by hand, which is why most people use dedicated molecular dynamics packages that have these calculations pre-programmed – but this should give you an appreciation of the physics involved in MD simulations.

(b) Repeat your calculation for $d = 2, 4, 8, 16$ and 32 nm. Plot $F_{net}(d)$.

(c) Compare your results to a normal Coulomb force law, which falls off like $1/d^2$. You should see that hydrogen bonding falls off more rapidly than the Coulomb force. This is what people mean when they say that hydrogen bonding is a short-range force.

(d) The orientation of the water molecule matters as well. Think through (or implement it, if you have time!) how you would change your spreadsheet to calculate the force when the water molecule is rotated through some angle θ.