Electrostatic interactions with Spartan'10 and Odyssey

Goal #1: Learn to correlate electrostatic potentials with atomic charges with Spartan'10
Goal #2: Learn to build and manipulate electrostatic potential maps in Spartan'10
Goal #3: Learn about hydrogen bonding and intermolecular interactions with Odyssey

Expected duration: 45-60 minutes

Potential-charge correlations

In classical physics, charged particles generate electromagnetic fields. If the particle is at rest, the field is called an **electrostatic field**.

Fields and forces are closely related. Both are **vectors**, i.e., they combine a number (magnitude) that represents the strength of the field/force and a direction (arrow) that points in the direction of the attractive/repulsive force.

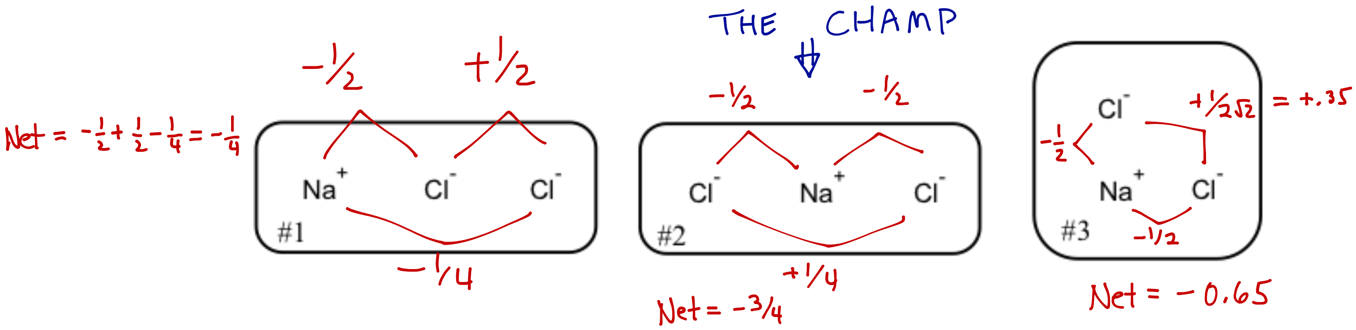
The directional properties of vectors make them hard to display in 3D graphs and charts. Instead, chemists use the **electrostatic potential** to display information about attraction and repulsion.

Potentials are pure numbers. The magnitude of the potential represents how strongly the charged particle interacts with other charges. The sign of the potential tells us whether the charged particle is positively or negatively charged.

The formula that gives a charged particle's electrostatic potential is Q/R, where Q is the particle's charge and R is the distance to the particle. The potential energy of a system containing the original charge and a new charge, Q_{new}, is given by PE = $(QQ_{new})/R = Q_{new}(Q/R)$.

Questions

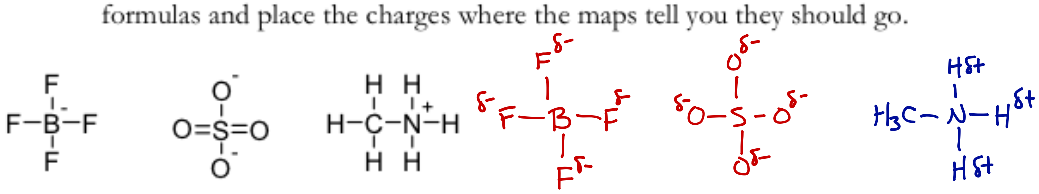
1. For which of these ions is Q>0? Na^{+}, Mg^{+2}, Cl^{-}, SO_4^{-2}
2. Which of these ions create a negative electrostatic potential around themselves? Na^{+}, Mg^{+2}, Cl^{-}, S^{-2}
3. An ion creates a potential of +800 kJ/mol near itself. Is this ion positively charged or negatively charged?
4. Which of these ions creates the most negative potential at a distance of 4 Å from itself? Na^{+}, Mg^{+2}, Cl^{-}, SO_4^{-2}
5. Referring to the ion in Q#4, where would its electrostatic potential be even more negative, at a distance of 2 Å or 6 Å?
6. What should the electrostatic potential be 4 Å from a neutral particle? Does this depend on distance?
   Q=0 → Q/R=0 for all R
7. Calculate the PE of the three systems shown on the next page.
   a. Geometry: assume each ion is 2 Å from its closest neighbor and angles are either 90° or 180°
   b. Energy: calculate in units of electron^2 Å^{-1} and round off to closest 0.1 units



Electrostatic potential maps

Because chemical ions contain many charged particles, the electrostatic potential is only meaningful if we look at it from "outside" the ion. A common device for showing electrostatic potentials is the **electrostatic potential map** (or just '**potential map**' for short). The map is drawn on a surface that represents the edge of the molecule's electron cloud.[1] Different colors are used to present different values of the potential and the numerical values that correlate with specific potentials can be reassigned to reveal particular details.

1. Download the file **ions321inter.spartan** to your computer and open it with Spartan. The file contains models of 7 common ions.
2. A color legend ranging from -800 to +800 kJ/mol should be visible. Play with the 'list player' arrows, [list player controls], until you figure out how to look at each ion individually.
3. *CLICK* **Display: Properties**. Play with clicking on the map and on the screen until you can reliably get Molecule Properties and Surface Properties to appear in the window. Things to learn:
   a. What symbol marks the point where you clicked on the map?
   b. Which quantity in the window gives the potential value at the point where you clicked?
   c. Which quantity gives the map's surface area?
4. Which ions are positively charged? Which are negatively charged?
   BLUE RED
5. One ion carries a +1 charge and another carries a +2 charge. How can you distinguish them? (Hint: use the actual value of the potential on the map to guide you.) Why do their maps have the same color? Because ions are same size (same R), potential follows Q. The ion with the larger potential (Val:) is +2.
6. One ion carries a -1 charge and another carries a -2 charge. Distinguish them. Why are their maps nearly the same color? See #5. The ions are not quite the same size, but Q varies by a factor of 2, and R does not. Any potential < −800 is colored RED.
7. Potential maps are provided for BF_4^-, SO_4^{-2}, and $CH_3NH_3^+$. The following structural formulas show the locations of formal charges in these ions as they are commonly drawn. Redraw the structural formulas and place the charges where the maps tell you they should go.

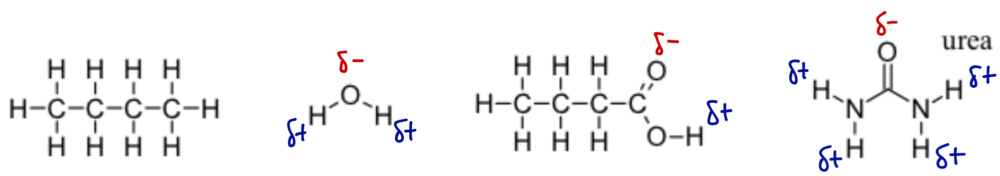


8. Close your model, download the file **neutrals321inter.spartan** to your computer, and open it with Spartan. How many models are there in this file?

[1] Strictly speaking, there is no "edge" to an electron cloud. However, the probability of finding an electron outside these surfaces is practically nil.

9. What color feature of the potential maps in this map suggests that most of these molecules are neutral? Several maps are green. Some have red AND blue w/ lots of green. But the LEGEND is the most important thing. All of the potentials are close to zero.
10. One model is of NaCl. Use the potentials to identify the Na and Cl.
    a. Suppose we added another Cl^- to this model. What color would you place it near to get the lowest PE? BLUE
    b. Suppose we added another Na^+ instead. What color would you place it near to get the lowest PE? RED
    c. Click on different locations in the dark blue and yellow color zones. Do they all have the same potential? Can you account for this? Sure. The same color is used for a range of potentials.
11. Display Surface Properties for one model and adjust the Property Range from -400 to +400 (use the legend to verify that this has happened).

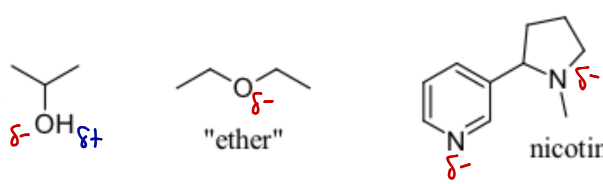
12. Structural formulas of the other models are shown below. Draw δ- and δ+ next to any atom that has a significant potential (>100 or <-100 kJ/mol). Notice that the potentials are much closer to zero than the potentials seen around ions. The δ or 'delta' symbol indicates a partial or fractional charge.



Experiment with building your own maps

Build any of the molecules shown below. Create a potential map and marked partially charged atoms on the structural formula. Repeat for one other molecule.

'rubbing alcohol'



"ether" nicotine

Steps for creating potential maps:

1. Calculate geometry, energy, & electron distribution

   SELECT **Setup: Calculations….** If necessary, adjust menus in Calculate zone to read Equilibrium Geometry at Ground state with Hartree-Fock 3-21G in Vacuum. *CLICK* Submit

2. Generate map

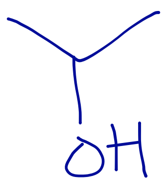
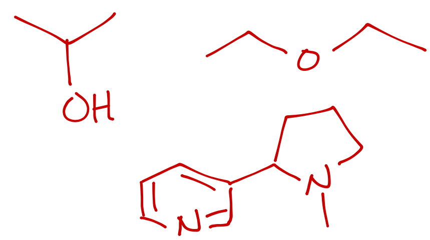
   SELECT **Display: Surfaces**. *CLICK* **Add: Electrostatic Potential Map**. *CLICK* checkbox when map is Completed

3. Adjust map colors

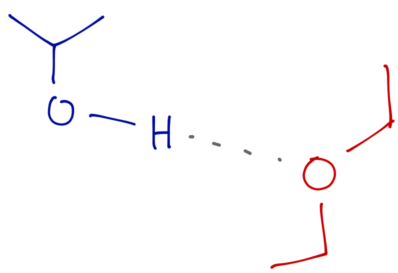
   The default color assignment is red = most negative and dark blue = most positive. *SELECT* **Display: Properties**, display Surface Properties, and adjust Property Range to -400 to +400 (you can display the Legend to verify that this has happened)

Hydrogen bonds

"Hydrogen bonds" are due to electrostatic attraction between a hydrogen with a δ+ charge and another atom with a negative or δ- charge. Identify some molecules on the previous pages that contained suitable hydrogens. Draw two or three of them in the box labeled hydrogen bond donors. Next, identify some molecules that contained atoms with δ- charges. Draw two or three of them in the box labeled hydrogen bond acceptors.

hydrogen bond donors	hydrogen bond acceptors
	

Next, make a drawing that pairs up a hydrogen bond donor with a hydrogen bond acceptor in a way that creates the lowest PE (strongest attraction/hydrogen bond).



PLEASE NOTE

Hydrogen bonds (and other intermolecular interactions) in Odyssey

1. Start Odyssey
2. *SELECT* **Molecular Labs** and perform
    a. #98. Structure & Motion in Ice
    b. #99. Hydrogen Bonding in Mixtures
    c. Then close the **LABS** tab
3. *SELECT* **Applied Chemistry** and #2 Top 10 Organic Chemicals
    a. *SELECT* **Urea → Solid**
    b. *SELECT* **Style: Hydrogen bonds** and rotate model to locate all hydrogen bonds between molecules. Are these consistent with the partial charges in Q#12.

Tips for further study

On your own, try other Molecular Labs relating to intermolecular interactions & solubility. Read Sorrell 2.8. Try Sorrell 2.28-2.32. Learning objectives: be able to 1) identify hydrogen bond donors/acceptors, 2) draw plausible geometries for donor-acceptor pairs, 3) rationalize/predict solubility/volatility phenomena.