Forcing Chemistry: Comparing Intermolecular Forces Between Ions and Polar Molecules

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1 Abstract

Molecules come in varying shapes, sizes, and compositions. Consequently, different molecules will exercise different properties. One of the most interesting properties of molecules is the intermolecular forces between molecules of the same type and how they govern the behavior of large groups of these molecules.

This project is aimed at comparing the behavior of two molecules that are similar in structure but have different properties when interacting with themselves in large groups. We use a model in VPython to accomplish this. We first outlines some of the background information for intermolecular forces. Then we state some of the goals that we are trying to be accomplished in this project.

2 Background

The largest molecules known of have diameters around 100 nm. Despite its size, it would take over 14.3 million billion of such large molecules to fill a pint glass. What this means is that in order for molecules to aggregate and become recognizable in solid or liquid form, the molecules have to bind together in groups. The forces that are exercised between molecules are called intermolecular forces; those inside of a molecule are intramolecular forces. The intramolecular forces do not affect the intermolecular forces of a molecule. There are a variety of intermolecular forces employed between molecules. We will only be exploring two very different ones: forces between ions (ion-ion) and forces between molecules which have dipole moments (dipole-dipole).

2.1 Attractive Forces

Ion-ion forces are the strongest, as they vary have a direct electrical attraction between the molecules. Ions are molecules that have a different amount of electrons than what their base atom normally has. For example, bromide is a negatively charged atom of bromine because it has one more electron than the average bromine atom. Negatively charged ions are called anions. There can also be positive ions, such as a sodium molecule that has one less electron than the average sodium atom, giving it a plus charge. Positively charged ions are called cations. The force between ions is expressed by this relation:

$$E_p \propto \frac{Q_1 Q_2}{r}$$

where Q_1 and Q_2 are the charges of the two ions and r is the distance between the ions. At a particular distance r, there is the optimum intermolecular distance between the ions for their attraction to be greatest. If the molecules are too far away, they will not be attracted; however, if they are too close together, the repulsive forces between the two molecules will overtake the attractive forces and they will not bond.

The other type of intermolecular force we are looking at is dipole-dipole interactions. Not all molecules have an absolute charge on them like ions do. For example, the molecule methane has no more or less electrons than a typical methane molecule so it does not have an absolute charge. However, because of the difference in the electronegativity of atoms in the molecule, dipole moments can arise. Electronegativity is the tendency for an atom to want to hold onto electrons. Replacing allof the hydrogens in a methane fluorines, which are more electronegative negative atoms, creates diffferent bond polarities in the molecule. However, because the bonds in methane are all equally spread out, these dipole moments in the direction of each of the bonds cancels out and there is not dipole moment on the molecule. However, when only one of the hydrogens in methane is replaced with a fluorine (a fluoromethane molecule), a dipole moment for the whole molecule arises. A dipole moment causes one part of the molecule to have a partial negative charge and the opposite part of the molecule to have a partial positive charge. This is because the dipole moment for the carbon-hydrogen bonds is different than the dipole moment of the carbon-fluorine bond. The charge differential across the molecule causes similar molecules to only align is specific ways; the positive end of a polar molecule will align with the negative end of a polar molecule by Coulumb's Law. This force follows an inverse distance relation like the ion-ion intermolecular interactions:

$$E_p \propto -\frac{\mu_1 \mu_2}{r^3}$$

where μ_1 and μ_2 are the magnitudes of the calculated dipole moments of the molecules interacting. As aforementioned, fluoromethane exercises this type of force between its molecules. There is also a special type of dipole-dipole interaction called hydrogen bonding, but we will not be exploring this as there is no much mathematical basis therein.

2.2 Repulsive Forces

When molecules get too close together, potential energy approaches infinity:

$$\lim_{x \to 0} E_p \propto \frac{1}{r^9} = \infty$$

Molecules tend to occupy states that are at the lowest energy (the Aufbau Principle) so at a positive infinite energy, a molecule would not be happy residing that energy and would much rather recede to a lower energy level. The main cause of this is getting molecules too close together. When the bond distance is less than the sum of the radii of two molecules, then the two molecules aren't just touching but are in fact physically overlapping. This is like trying to push two blocks into each other, it just doesn't work because the laws of physics prohibit it. Aside from distance repulsion there is also electronic repulsion. Like charges repel each other and this force grows larger as the ions get closer together:

$$\lim_{x \to 0} E_p \propto \frac{Q_1 Q_2}{r} = \infty$$

Generally, repulsions between molecules not due to electronics result from the overlapping of molecular orbitals on neighboring molecules. [1]

3 Goals

The minimal goals set for this project aside from becoming proficient in TeX and VPython are the following:

1. Be able to create accurate representations of some molecules including water (H_2O), hydrogen sulfide (H_2S), and ethane (C_2H_6)
2. Be able to create a vector symbolizing dipole moment of polar molecules
3. Show how different molecules tend to orient themselves in a directional electric field
4. Show difference in orientation of a few molecules using different intermolecular interactions (i.e. where H-bonding occurs, etc.)

[1] Atkins, P.; Jones, L. *Chemical Principles: The Quest for Insight, 5^{th} Edition*; W.H. Freeman and Company: New York, NY. 2010. p.172-178

5. Aggregating molecules together in correct orientation with respect to their intermolecular forces