Math 198 proposal

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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. This is hoped to be accomplished using a model in VPython. The first section outlines some of the background information relevant to intermolecular forces and how molecules interact with each other. The next section will state some of the goals that are trying to be accomplished in this project.

2 Background

The largest molecules that can be produced have diameters around 100 nm. Even with that huge molecule, it would take over 62 billion of those molecules to cover 1 square inch. What this means is that in order for molecules to aggregate and become recognizable in solid or liquid form (such as a cup filled with water), 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. Intramolecular forces have no impact on intermolecular forces. There are several different types of intermolecular forces: ion-ion, ion-dipole, dipole-dipole, and van der Waals forces.

2.1 Attractive Forces

Ion-ion forces are the strongest, as they vary have a coulombic (or electrical) attraction between two molecules. In this instance, the two molecules are typically anions and cations. The force between the molecules follows this equation:

$$E_p = \frac{Q_1 Q_2}{4\pi\epsilon_0 r}$$

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.

Ion-dipole forces deal with an ion and a molecule with a dipole moment; that is, a molecule with charge charge differential across the molecule. An example of a molecule with a dipole moment is H_2O, or water. The oxygen atom in water has a partial negative charge with respect to the other atoms in the molecule; the hydrogen atoms have a partial positive charge. The charge differentials across a molecule are typically due to the electronegativity of the atoms that compose the molecule. The equation governing this force is:

$$E_p \propto -\frac{|z|Q\mu}{r^2}$$

where z is the charge number of the ion, Q is the charge of the ion, and μ is the dipole moment of the polar molecule. The inverse square dependency on distance between the molecules mathematically means a weaker force. A practical example of ion-dipole interactions would be dissolving table salt NaCl in water. The positively charged sodium ions would be attracted to the partial negative of the oxygen in the water and the negatively charged chloride ions would be attracted to the partial positive of the hydrogen atoms in the water.

Dipole-dipole forces are demonstrated between molecules that have dipole moments. This force follows an inverse distance relation like the other forces but is even weaker:

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

In the gaseous phase, the relation follows $\frac{1}{r^6}$ because of the weak attraction between molecules because of the smaller likelihood for constantly rotating molecules in the gas phase to align and attract. Chloroform exercises this type of force between its molecules. There is a dipole moment because of the differential charge between the end of the molecule with chlorine atoms and the end with the hydrogen atom.

Water also undergoes dipole-dipole interactions, but its bonds are much stronger due to the phenomenon of hydrogen bonding. For example, hydrogen sulfide has a boiling point of -60 ° C whereas the boiling point of water is 100 ° C [1] Hydrogen bonds only occur between the small, very electronegative

[1] Aylward, G.; Findlay, T. *SI Chemical Data, 5th Edition*; John Wiley & Sons: Hoboken, NJ, 2002.

atoms: hydrogen, nitrogen, oxygen, and fluorine. The strong pull from an electronegative atom can attract the partial positive hydrogen atom and create a very strong bond between two molecules.

The last type of intermolecular force is van der Waals. These forces are all of the forces that have a $\frac{1}{r^6}$ relation to potential energy; what varies is how the numerator relates to energy. In the case of London dispersion forces, the polarizabilty of the molecules is directly related to the energy; in the case of dipole-induced dipole interaction, the polarizabilty of the inducted dipole molecule and the square of the dipole moment of the dipole molecule are directly related to potential energy. These are the weakest types of intermolecular forces. Molecules that have van der Waals intermolecular interactions typically have the lowest melting and boiling points.

2.2 Repulsive Forces

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

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

Molecules tend to occupy states that are at the lowest energy so at a positive infinite energy, a molecule would not be happy residing that energy. Aside from distance repulsion there is also electronic repulsion. In ion-ion interactions, potential energy is positive as it it related to the product of the two charges and takes the sign of the product. Generally, repulsions between molecules not due to electronics result from the overlapping of molecular orbitals on neighboring molecules. [2]

3 Goals

3.1 Minimal Goals

The minimal goals set for this project are the following:

- To become proficient in writing documents in TeX
- To become proficient in using VPython
- Be able to create accurate representations of some molecules including water (H_2O), hydrogen sulfide (H_2S), and ethane (C_2H_6)
- Be able to create a vector symbolizing dipole moment of polar molecules

[2] 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

- Show difference in orientation of a few molecules using different intermolecular interactions (i.e. where H-bonding occurs, etc.)

3.2 Ultimate Goals

Assuming all minimal goals have been completed, the following are the ultimate goals for the project (in order):

1. Aggregating molecules together in correct orientation with respect to their intermolecular forces
2. Demonstrate what happens to molecules and the breaking of intermolecular forces just past the tolerance point of the bond
3. Compare two molecules such as ethane and ethanol (only differing in the hydroxyl group that would participate in H-bonding) and show the difference in their boiling points