Lab 06: Intermolecular Forces

INTRODUCTION

Goals

• Describe how the structure of a molecule determines the intermolecular forces it can exhibit.

- Compare the relative strength of intermolecular forces between different compounds.
- Use experimental data to qualitatively rank the strength of compounds' intermolecular forces and explain relative magnitudes of the individual structural contributions to those intermolecular forces.

Background

In order for a compound to exist in a liquid or solid phase, there must be attractive forces that hold the molecules together, preventing them from moving freely like gaseous molecules. These attractive forces are known as intermolecular forces (IMFs). Although generally weaker than intramolecular forces (e.g., covalent bonding between atoms in a molecule), IMFs are responsible for many of the physical properties of compounds that we observe in our daily lives.

This course studies three types of IMFs: London dispersion forces, dipole-dipole interactions, and hydrogen bonding. Not all molecules exhibit all three of these IMFs; it depends on the structure, shape, and polarity of the molecule.

London dispersion forces:

The electron clouds around atoms and bonds are not static distributions of charge; they may fluctuate over time. As this electron density shifts, it can create an instantaneous asymmetry in the charge distribution, resulting in an **instantaneous dipole moment**. The motion of electrons in one molecule can influence the motion of electrons in a neighboring molecule, causing the instantaneous dipole moments to line up head-to-tail and create an attractive force between the molecules. This attractive force is known as the London dispersion force (LDF).

In general, larger atoms and molecules have larger electron clouds that can fluctuate further from their average position, exhibiting larger LDFs. This explains why molecular bromine, Br_2 , is a liquid at room temperature while molecular chlorine, Cl_2 , is a gas. Bromine has a larger principal quantum number (n), so its electron cloud is larger and can experience larger fluctuations in electron density, leading to greater dispersion forces.

It is worth noting that many students incorrectly perceive LDF as the least significant type of intermolecular force. While the relative strength of LDF may be weak for small molecules, it is ubiquitous to all molecules and plays a significant role in dictating the physical properties of many molecules, especially those with large electron clouds.

Dipole-dipole interaction

Individual covalent bonds between atoms in a molecule will be polar when there is a significant difference in electronegativity between the two atoms involved. The more electronegative atom will have a greater density of electron around it, leading to the buildup of a partial negative charge, denoted as δ^- , around that atom. The less electronegative item will have a lower density of electron cloud, leading to a partial positive charge, denoted as δ^+ . The separation of these two partial charges creates what is known as a dipole moment, usually shortened to dipole. The greater the difference in electronegativity, the larger the disparity between the electron densities will be, leading to larger partial charges and dipole moments. Dipoles can interact with each other; the partial negative charge from one molecule's dipole can attract the partial positive charge from another molecule's dipole. Hydrogen chloride, HCl, is an example of a molecule with a dipole moment – the more electronegative chlorine atom has a partial negative charge while the hydrogen has a partial positive charge. When two HCl molecules are interacting with each other, they will align their molecular dipole in a head-to-tail manner, where the partially positive-charged H in one molecule is aligned with the partially negative-charged Cl in the other molecule.

Note that bond dipole moments have both a magnitude related to the size of the partial charges and the distance between them, and a direction related to the relative orientation of the polar bond. To determine the polarity of a molecule, one must consider both the individual bond dipoles and the molecular geometry. This content has been thoroughly discussed during the first semester of General Chemistry (Chapter 8 in McQuarrie).

Hydrogen bonding:

The attraction between the oxygen of one water molecule and a hydrogen atom of another water molecule is a special case of dipole-dipole interaction known as hydrogen bonding. Hydrogen bonding occurs between different molecules – it is a type of intermolecular forces, not a covalent or ionic bond! Hydrogen bonding is usually established between molecules in which a hydrogen atom is bonded to a highly electronegative atom, such as an oxygen, nitrogen, or fluorine atom. Because a hydrogen atom is very small, the highly concentrated positive charge on it strongly attracts the electronegative atoms in the neighboring molecules, making hydrogen bonding stronger than any typical dipole-dipole interactions. The strength of this interaction is the primary reason why water exists as a liquid at room temperature while hydrogen chloride is a gas, despite HCl also exhibiting a dipole-dipole interaction.

Evaporative colling:

One of the observable physical properties of a compound closely tied to its intermolecular forces is the evaporation and evaporative cooling of liquids. For a molecule on the surface of a liquid to transition to the gas phase, it must possess sufficient kinetic energy to overcome the intermolecular forces with surrounding molecules in the liquid. The temperature of the liquid is linked to the average kinetic energy of its molecules, where some exhibit low kinetic energy, while others have high kinetic energy.

The probability that a given molecule has a specific amount of kinetic energy is determined by the Boltzmann distribution, defined by the temperature of the liquid. Consequently, only a fraction of molecules will possess the required kinetic energy to overcome intermolecular forces and transition to the gas phase. In an open system, where the amount of vapor produced by the evaporation of high-kinetic-energy molecules isn't limited by the vapor pressure of the liquid, the continual evaporation of these higher-energy molecules will lower the liquid's average kinetic energy, shifting the distribution to lower temperatures and inducing cooling.

This experiment will examine how the relative rankings of intermolecular forces influence the rate of evaporation and the minimum temperature achieved through evaporative cooling. Subsequently, we will compare these experimental results to the theoretically expected rankings based on the molecular structures of various liquids."

PREPARING FOR LAB 06: INTERMOLECULAR FORCES

• Review the lab procedure, and in your lab notebook, create an outlined version of the procedure (avoid copying verbatim). Ensure that the outline is comprehensive enough for you to execute the experiment seamlessly. Additionally, document each measurement or calculation that needs to be performed, leaving ample space to record numerical values, equations, or data tables with the correct units. Allocate room for qualitative observations at every step; it's recommended to leave more space than you think you'll need to avoid running out or attempting to squeeze in observations and measurements later.

- Don't forget to include the safety data sheet (SDS) information for all the hazardous chemicals you will use during this experiment! Please refer to the instruction on Blackboard on how to prepare your lab notebook and look up SDS information for chemicals.
- This lab uses lots of organic compound, and hence generates organic waste. Organic waste
 must be separated from the aqueous waste and be disposed of in a designated organic waste
 container. Instruction on how to handle multiple waste streams is posted on Blackboard. Make
 sure you read through the instruction, so you are informed of how to dispose the organic waste
 in this lab.

EXPERIMENTAL, LAB 06: INTERMOLECULAR FORCES

Safety

Many of the compounds used in this lab are volatile and will produce flammable and/or toxic fumes. Remember to wear your goggles and gloves, use the minimum amount of each compound necessary to complete the procedure, and close any containers of the compounds when they are not in use. Pay attention to the steps of the procedure that are to be performed in the **fume hood!**

Materials

- Digital thermometer
- Beakers
- 10 mL test tubes
- Test tube rack
- Ring stand and clamp
- Strips of filter paper
- Masking tape

- Methanol, CH₃OH
- 1-propanol, CH₃(CH₂)₂OH
- 1-butanol, CH₃(CH₂)₃OH
- Hexane, CH₃(CH₂)₄CH₃
- Acetone, CH₃(CO)CH₃
- Deionized water, H₂O
- Unknown liquid

Procedure

You should prepare **a data table** in your lab notebook to record the temperature difference and evaporation time for each liquid so you can easily find these data when doing the post-lab.

- 1. For each of the liquids used in the lab, draw the Lewis structure that corresponds to your model in your notebook, indicating the 3D structure with wedged and dashed bonds.
- 2. Using your models and drawn structures, determine which IMFs they'll exhibit, and how they're similar to, or different from, the other molecules.
 - **For group discussion:** predict the ranking of the compounds' rates of evaporation. Write down your ranking in the notebook along with the criteria you used for your ranking.
 - Note down any pairs of compounds for which the ranking is ambiguous. For example, a particularly large molecule without a permanent dipole moment might be hard to qualitatively compare to a much smaller molecular that has hydrogen bonding.
- 3. Using the pipette provided with one of the solvents, add enough of the liquid into a test tube to cover the end of the thermometer probe but not enough to spill out when you dip the thermometer in the liquid, about 3 5 mL. Place the test tube in a test tube holder in the fume hood. Return the pipette to the holder attached to the stock container so they don't get mixed up!

4. Immerse the thermometer in the liquid and wait until the temperature is stable. Record this as the initial temperature, T_i. Remember to hold the thermometer by the plastic head, not the metal probe – you don't want to measure the temperature of your hand!

- 5. To measure the evaporation process, remove the thermometer from the liquid and place it in the clamp on the stand, ensuring the thermometer isn't touching the stand or the tabletop. (*Try not to shake off the droplets as you move the thermometer!*) Have another member of your group start the stopwatch as soon as the thermometer is removed from the liquid.
 - Record any qualitative observations you have during the evaporation process.
 - Once the temperature begins rising again, stop the stopwatch. Record the minimum temperature T_{min} and the time on the stopwatch in seconds, t_{evap} , in your lab notebook. Calculate the change in temperature, ΔT , between T_i and T_{min} .
 - Calculate the rate of evaporation: Rate_{evap} = $\Delta T/t_{evap}$
- 6. If the rates of evaporation are too similar to distinguish between for two liquids: try wrapping a strip of filter paper around the tip of the thermometer and attaching it with masking tape above. This will increase the amount of liquid in contact with the thermometer tip, which should make the evaporation time longer and, therefore, a more pronounced temperature change.
- 7. Repeat steps 3 to 6 for the remaining labeled solvents and the unknown. Try to be as consistent as possible with the amount of each liquid you use! Using the same amount of liquid will give the best results for the experiment.
- 8. Before you start cleaning up, read back through the procedure and make sure you have all the measurements written down in your notebook, not just in the notebooks of other members in your group. Additionally, confirm that you have measurements for all **seven liquids**!
- 9. Discard any excess organic liquid into a designated organic waste beaker. Water can be dumped into the sink, but the non-water solvents are organic and need to be disposed of into an organic waste container!

The solvents are all volatile and any residues will evaporate, so they do not need to be washed. Turn off the thermometers and return them as well as any shared equipment you used. Return any glassware you used back to the drawer.