

Part 1.

1. **Define** for each other the following three terms.

An induced dipole is a temporary (or transient) dipole where negative charge is separated from positive charge. Induced dipoles are the most important intermolecular interaction between non-polar molecules.

A hydrogen bond is an intermolecular interaction formed between a hydrogen that has a partial positive charge and a highly electronegative atom in another molecule.

A dipole-dipole is an intermolecular interaction where the partially positively charged end of one molecule is attracted to the partially negatively charged end of another molecular.

2. **Rank** the above interactions in order of **increasing** strength.

Hydrogen bonding >> dipole-dipole interactions >> induced dipole interactions

3. **Think** of a molecule that serves as an example of each interaction and specify why that molecule is a good example.

A molecule that illustrates induced dipole is *n-hexane* because it is non-polar but can have a significant charge separation along its long axis.

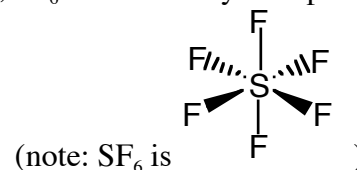
A molecule that illustrates hydrogen bonding is *methanol*, CH_3OH , because it has a hydrogen attached to an oxygen making the H partially positive and this H can be attracted to the electronegative O atom in another methanol molecule.

A molecule that illustrates dipole-dipole is SF_2 because it has a dipole (S is partially positive and the F's are negative) that is aligned between the F-S-F bond.

4. What causes a dipolar bond?

A bond made between two different atoms, and especially if they have very different electronegativities, necessarily is dipolar because one atom will draw electron density towards it more than the other. The 2 e- in the bond are NOT shared equally.

5. The S-F bond is highly polar (why?). However, while SF_2 is a polar molecule, SF_6 is not. Can you explain?

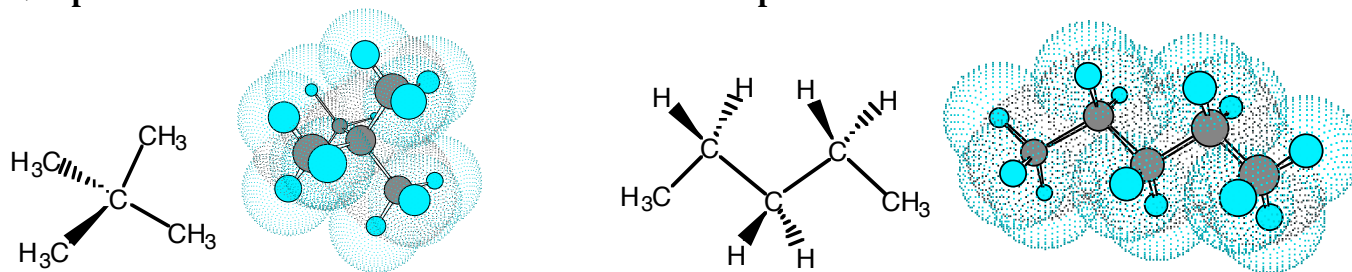


SF_6 is NOT polar and does not have a molecular dipole because the polar S-F bonds are all balanced. The bond dipole for the S-F bond pointing up is offset or cancelled by the S-F bond pointing down.

Another way to describe it is that the bond dipole vectors all cancel.

This does not happen in SF_2 because of the bent shape of the molecule precluding a complete cancellation of bond dipoles.

Pentane, C_5H_{12} , can exist as more than one structure, and these are called isomers. Two isomers are :
Neo-pentane **normal or n-pentane**



Predict which one will have the higher boiling point. (answer given at top of next page; don't look!)

Did you predict the more linear n-pentane? As the answer below shows, it clearly has a higher boiling point. Working backwards, this requires that there be stronger intermolecular interactions in n-pentane. Its long shape means that it can better create an induced dipolar separation of transient + and - charges. The neo-pentane in contrast, is nearly spherical in its shape and so won't stabilize an induced dipole very well.

[neo-pentane b.p. is 9.5 and f.p. -16.5 deg ; n-pentane b.p. is 36.1 and f.p. is -130 deg C]

Part 2. Why a snowflake has 6 points

- Quick!** Build with your molecular model set as many water molecules as you can in 2 minutes, then connect them to build ice. [note: use short pink sticks for full O-H bonds and longer white sticks for O---H bonds). (hint: first join 6 water molecules to make rings, then stack and connect rings, one on top of another)
- Find the 6-fold symmetry in ice! Did you find this?
- Is the temperature the same everywhere in a container of an ice and water mixture? Check out the display on the front desk. Can you explain your observations? How does your explanation relate to your results in (1) above?

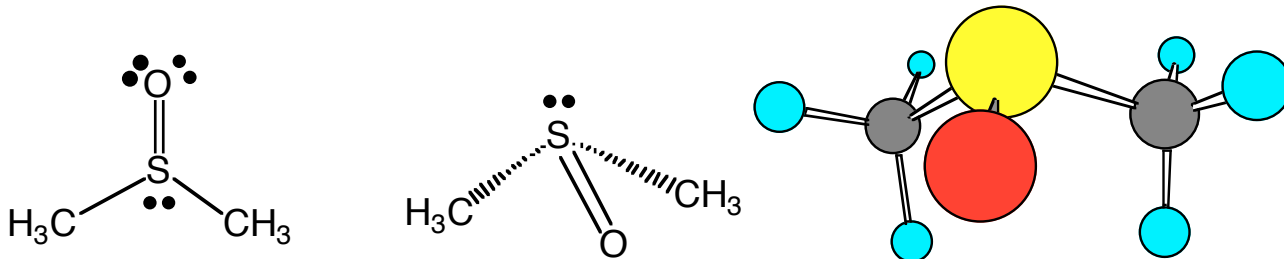
The temperature at the bottom of the cylinder was ~6 deg C while the temperature at the top was 0-2 deg, depending on when you looked at it. The difference in temperature shows that water at 4-6 deg range is more dense than water nearer the freezing point, 0 deg C. Frozen water, ice, has the open structure you should have found in Part 2.(1) and is very unusual in having a less dense solid state than liquid state. Therefore the colder water near the freezing point is already adopting some open, and less dense, ice-like structures that make it more dense.

4. Also on the front desk are 2 beakers, each containing a colorless substance in both liquid and frozen form. One beaker holds water and the other holds dimethylsulfoxide (DMSO), whose structure is below in 3 views (as 3 different models!).

- Which molecule is in which beaker? What can you deduce about frozen DMSO?

DMSO was in beaker A, with the frozen solid sitting on the bottom of the beaker. DMSO is a "normal" substance whose solid phase is more dense than its liquid phase. Water was in beaker 2, where the "ice cube" was floating since ice is less dense than water.

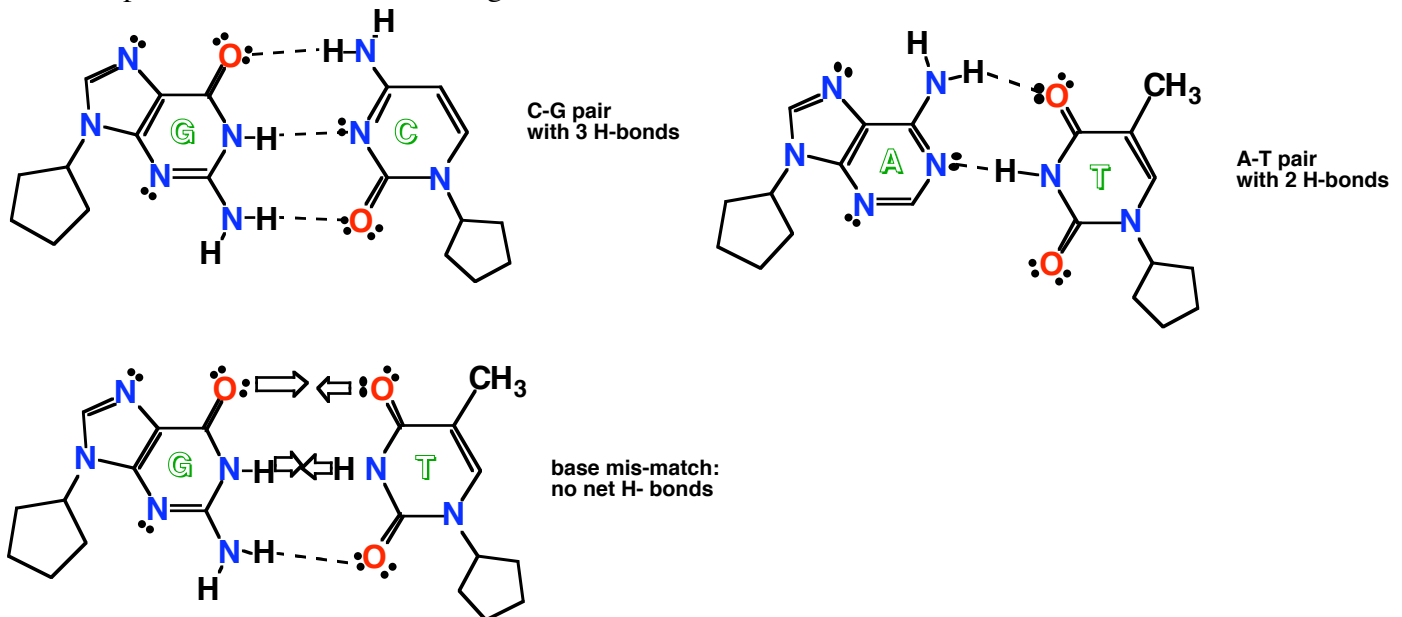
b) Compare the structure of DMSO to that of water and consider the intermolecular interactions possible for each: how are they alike? How do they differ? Note that the freezing point (f.p.) of water is, of course, 0 deg C and the f.p. of DMSO is 18 deg C.



DMSO like water is a polar molecular; the dipole would be pointing towards the O atom, the most electronegative atom in the molecule. DMSO can make dipole-dipole interactions, just as water does. It cannot however form H-bonds as water does and so does not have this additional intermolecular interaction to stabilize its molecules in the solid state. Part 3. Note: if you have already done 1 in lab, you may move on to 2, 3 and 4

- The four units that hold DNA together are “bases” and have the names adenine (A), thymine (T), cytosine (C) and guanine (G). Using the template diagrams provided, align the bases pair-wise and determine how many H-bonds can be made for each pair (e.g., A-T, A-C, A-G, A-A, etc)

Draw the pairs with the best H-bonding and indicate the H-bonds with dashed ---- lines.



2. The ratio of G-C pairs to A-T pairs determines the stability of DNA towards added heat. When heat is added, i.e. the temperature is increased, the two DNA strands separate, “unwind”: this is called “DNA melting”

a) From your observation in (1) above, which do you predict will be more stable at higher temperature, DNA with more G-C pairs vs. A-T pairs, or DNA with more A-T pairs vs. G-C pairs?

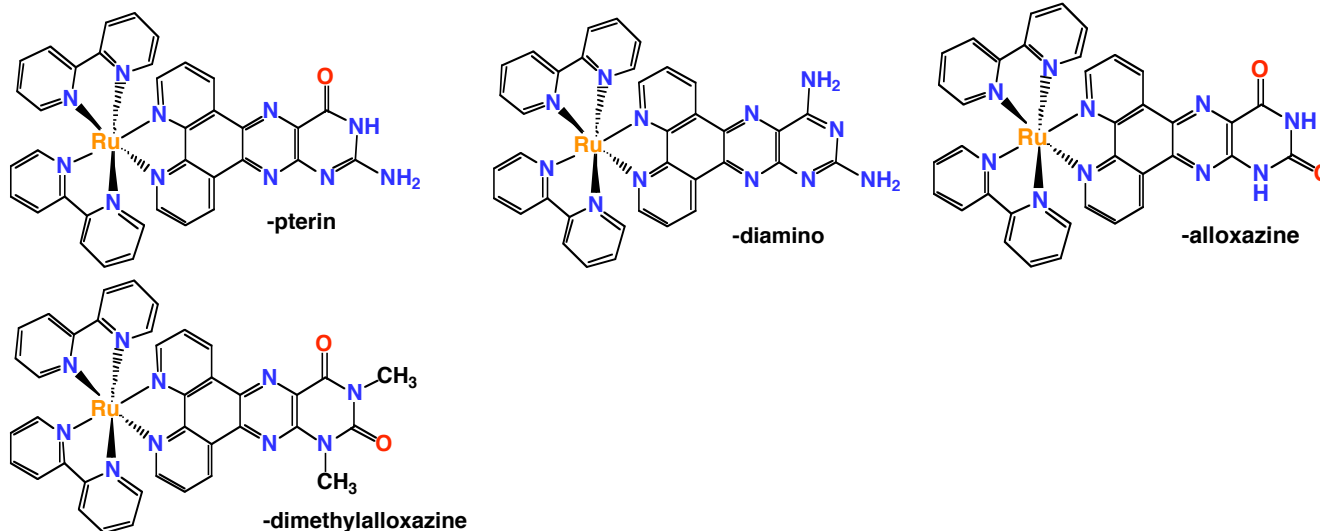
Since H-bonds contribute to more stability between molecular—and DNA bases—and since the C-G pair has 3 bonds, instead of only 2 as in A-T, one might expect DNA having a greater number of C-G pairs to be more stable at higher temperature.

b) How might H₂O help DNA to unwind? Would DMSO be able to help in the same way? So would you predict that DNA melting would occur at a higher or a lower temperature in DMSO?

When the bases separate, they break H-bonds and “expose” H’s or O’s or N’s. If there is water around the DNA, it can come in to replace the base-base interactions. So the H-O-H can H-bond with O or N by donating its H atom. Or, the O in water can make an H-bond with an –NH₂ group as in adenine.

DMSO, although polar, would be more limited in taking the place of a missing base. The O in DMSO could H-bond to an –NH₂ group as in adenine, but it has not H atom available to donate to the O’s or N’s with lone pairs. (The H’s in the CH₃ groups are not partially positive because H and C have similar electronegativities).

One of the research projects in the Burgmayer research group is studying the interactions between DNA and complexes of ruthenium (Ru), whose structures are shown below with abbreviated names.



3. (a) Rank the ruthenium compounds below in order of increasing ability to make H-bonds to DNA.

pterin > alloxazine ~ diamino >> dimethylalloxazine
 3 H-bonds 2 H-bonds no (or maybe 1) H-bond

