Intermolecular Forces, Liquids, Solids

Interactions Between Molecules:
What does it take to separate two (or more) molecules from one another?
-or-
What holds molecules close to one another?

Structure/Property Relationships

<table>
<thead>
<tr>
<th>Name</th>
<th>Butane</th>
<th>Acetone</th>
<th>Isopropyl Alcohol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Formula</td>
<td>C₄H₁₀</td>
<td>C₃H₆O</td>
<td>C₃H₈O</td>
</tr>
<tr>
<td>Molar Mass</td>
<td>58 g/mol</td>
<td>58 g/mol</td>
<td>60 g/mol</td>
</tr>
<tr>
<td>Structure</td>
<td><img src="image1" alt="Butane Structure" /></td>
<td><img src="image2" alt="Acetone Structure" /></td>
<td><img src="image3" alt="Isopropyl Alcohol Structure" /></td>
</tr>
<tr>
<td>Boiling Point</td>
<td>-0.6 °C</td>
<td>56 °C</td>
<td>82 °C</td>
</tr>
</tbody>
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Why is there this discrepancy in boiling point?
INTERMOLECULAR FORCES!
Isopropyl alcohol > acetone > butane

IM Forces and Physical Properties

Why this difference in bp? Let's take a closer look at these molecules:

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</tr>
<tr>
<td>Nonpolar Bonds Present</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polar Bonds Present</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molecular Polarity</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Apparently, nonpolar molecules have weaker intermolecular forces. Why?
**Electrostatic interactions of molecules**

Interactions that result from charges!

- Governed by Coulomb's Law:
  \[ \text{Force} = \frac{q_1 \cdot q_2}{4\pi\varepsilon_0 r^2} \]

- Types of electrostatic "species" possible:
  1. Ions-
  2. Dipoles-
  3. Induced Dipoles-

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**Possible Types of IM Interactions aka “van de Waals forces”**

1. **Ion-Dipole Interactions**
   - Remember back to discussion of water as a solvent: Water hydrates an ionic solute.

   ![Image of ion-dipole interaction]

2. **Dipole-Dipole Interactions**
   - Interactions of \( \delta^+ \) end of one dipole with the \( \delta^- \) end of another.

   ![Image of dipole-dipole interaction]
**Possible Types of IM Interactions**

3. **Dipole-Induced Dipole Interactions**

   ![Dipole-Induced Dipole Interactions](image)

4. **Induced Dipole-Induced Dipole Interactions**
   - “Dispersion Forces”
   - Aka London Forces
   - **Present in ALL molecules**!

   ![Dispersion Forces](image)

   In one instant: Nanoseconds later:

   ![Dispersion Forces](image)

   - Attractive
   - Repulsive

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**Hydrogen Bonding**

Specialized case of dipole-dipole interaction

- Occurs b/w
  1. H bound to O, N, F
  2. Lone pair of e⁻ on another N, O, F

- Water forms hydrogen bonded array
  - special!

![Hydrogen Bonding](image)
Properties of Liquids:
Try to relate these to IM

1. Heat of Vaporization ($\Delta H_{\text{vap}}$)
2. Vapor Pressure (atm or mm Hg)
3. Boiling Point
   - “Normal boiling point”: v.p. = 1 atm
4. Surface Tension
   - Cohesive vs adhesive forces
5. Viscosity

Properties of Liquids:
More on Vapor Pressure

- V.P. depends on
  - Interaction b/w molecules
  - Energy available (“heat”)

- Can model V.P. using Clausius-Clapeyron Eqn.

$$\ln \frac{P_2}{P_1} = \frac{\Delta H_{\text{vap}}}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$
Solids: Structure and Properties

Solids are classified based on identity of material and forces that hold solid together. (Table 12.7)

<table>
<thead>
<tr>
<th>Type of Solid</th>
<th>Forces at Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionic</td>
<td></td>
</tr>
<tr>
<td>Metallic</td>
<td></td>
</tr>
<tr>
<td>Molecular</td>
<td></td>
</tr>
<tr>
<td>Network</td>
<td></td>
</tr>
<tr>
<td>Amorphous</td>
<td></td>
</tr>
</tbody>
</table>

Describe arrangement of particles in a crystalline solid by describing smallest repeat unit of the solid: **Unit Cell**

<table>
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<th>TABLE 12.7 Characteristics of Crystalline Solids</th>
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<tr>
<td>Metallic</td>
</tr>
<tr>
<td>Ionic</td>
</tr>
<tr>
<td>Network covalent</td>
</tr>
<tr>
<td>Molecular Nonpolar</td>
</tr>
<tr>
<td>Polar</td>
</tr>
<tr>
<td>Hydrogen-Bonded</td>
</tr>
</tbody>
</table>
Packing of Spheres

- Closest packed vs. non-closest packed
- Unit cells that result

Crystalline Unit Cells

Seven different "simple" unit cells (crystal systems)
- Defined by distance and angles between lattice points.
- We'll focus on cubic unit cells - if you understand how cubic works, you can extend to the other six!
X-Ray Diffraction

- As x-rays impinge on crystal planes, they are scattered...diffracted
- Angle of scatter depends on spacing in the crystal
  Bragg Equation: \( n\lambda = 2dsin\theta \)
- Changing orientation allows 3-D structure to be calculated.

Cubic Cells

- Three symmetries: simple, bcc, fcc
- Counting atoms in the unit cell:
  - Corners
  - Faces
  - Edges
- Determination of atomic/ionic radii and cell dimensions: 2 keys
  1. Know simple, fcc, bcc
  2. Remember right triangle math!

EXAMPLE: Gold is a face-centered cubic unit cell. The density of the solid is 19.32 g/cm³. Calculate the radius of a gold atom.
Ionic Crystals

- Typically anions are closest packed and cations fit into “holes”
  - 3 Types: Trigonal, Tetrahedral*, Octahedral*
- * most common
  - Relative size of hole and cation drives structure.
    - Maximize M-X, minimize X-X

Properties of Solids

- Enthalpy of Fusion ($\Delta H^\circ_{\text{fusion}}$):
- Freezing point/melting point:
  - “normal” m.p.

- Enthalpy of Sublimation ($\Delta H^\circ_{\text{sublimation}}$):
Phase Diagrams

Map out temperature/pressure/phase relationships for materials.
- Shapes differ as physical properties differ.
- What occurs at each boundary?

- Triple Point:

- Critical Point and supercritical fluids

Water: Sorta Weird, Sorta Not!

Triple point: 0.00098°C, 4.58 Torr; Critical point: 374.1°C, 218.2 atm
- Behavior of s-l line
- Polymorphism