Molecular Polarity

Predicting and Understanding the Behavior of Molecules

Molecular Polarity - How?

Lewis dot structure → geometry → bond polarity (ΔEN) and lone pairs → how is the charge distribution - symmetrical or asymmetrical?

Electrostatic potential map using Chime

Molecular Polarity - Why?

Interactions with other molecules and physical properties such as boiling point, surface tension, and solubility

Intramolecular interactions - within molecule such as proteins

Reaction mechanisms - where attacked

An experimental measurement

The dipole moment, $\mu$, is given by

$$\mu = Qd$$

where $Q$ is the charge and $d$ is the separation distance of the charge.

The unit is the debye, D.

Measurement: Dipole Moment

No voltage applied on metal plates

Voltage applied on metal plates
### Dipole Moments

<table>
<thead>
<tr>
<th>Hydrogen Halide</th>
<th>ΔEN</th>
<th>Bond length (pm)</th>
<th>μ (D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF</td>
<td>1.9</td>
<td>92</td>
<td>1.82</td>
</tr>
<tr>
<td>HCl</td>
<td>0.8</td>
<td>127</td>
<td>1.08</td>
</tr>
<tr>
<td>HBr</td>
<td>0.6</td>
<td>141</td>
<td>0.82</td>
</tr>
<tr>
<td>HI</td>
<td>0.3</td>
<td>161</td>
<td>0.44</td>
</tr>
</tbody>
</table>

Increasing polarity

### Dichloromethane, CH$_2$Cl$_2$

μ$_{calc}$ = 1.50 D

### Ammonia, NH$_3$

μ$_{calc}$ = 1.85 D

### A square planar complex - Pt(NH$_3$)$_2$Cl$_2$

\[ \angle \text{Pt-N} = 80^\circ \]
\[ \angle \text{Pt-Cl} = 101.4^\circ \]

Polar or Non-polar

### Polar or non-polar molecules?

- CCl$_2$F$_2$
- HCN
- SCl$_4$F$_2$
- ICl$_3$
- BCl$_3$
- BrCl