Quantum Theory - A Reminder

Classical Theory  ⇒  Quantum Theory
E = any value  ⇒  E = hν
Energy is wave-like  ⇒  Wave-Particle Duality
Matter is particle-like  ⇒  Energy and Matter are the same
Determinism  ⇒  Heisenberg Uncertainty Principle

Models for the Atom

Electrons occupy atomic orbitals
What do they do in the orbitals?        What do they look like?        What shape and colour are they?
Meaningless

Lewis Structures - A Reminder

Period

1) Determine the Lewis structure(s) for the molecule
2) For molecules with resonance, use any of the possible structures to predict the molecular structure
3) Sum the electron pairs around the central atom
4) Count each multiple bond as a single effective pair
5) The arrangement of the pairs is determined by minimising electron-pair repulsions
6) If necessary, arrange electron groups in space according to "size". Multiple bond > Single bond
Non-bonding (‘lone’) electron pair > Single bond

Predicting Shape Using VSEPR

Valence Shell Electron Pair Repulsion (VSEPR) Theory

Groups of valence electrons around a central atom stay as far apart as possible to minimise electron-electron repulsions.

- an electron group may take part in a single, double, or triple bond, or a lone pair
- by shape we mean the relative positions in space of the bonded nuclei
- the notation AXmE n (used by Silberberg) works as follows:
  - A is the central atom under consideration
  - X are atoms bonded to A (there are m of these)
  - E are lone pairs on A (there are n of these)
- bond angles are the angles made by the nuclei of X with A (i.e. X – A – X)

Lewis Structures - A Reminder

Chemical Formula: NF₃

Place atom with lowest EN in center, add A-group numbers, draw single bonds, subtract 2e⁻ for each bond, give each atom 8e⁻ (2e⁻ for H)

Lewis Dot Diagrams - given what we now know about electrons in orbitals, are they really valid/relevant/useful ...?

Consider the reaction of Be with H₂

Be : + 2 x (H)  ⇒  H : Be : H

[He] 2s² + 2 x {1s²}  ⇒  H : Be : H

- Be has two paired valence electrons, so how can it form electron pairs as shown in the Lewis Diagram?
- What do the dots mean anyway, etc. ...?
The Steps in Determining a Molecular Shape

- Molecular formula
- Lewis structure
- Electron-group arrangement
- Bond angles
- Molecular shape (A, X, E)

See Figure 10.1

Count all groups around central atom (A)

Note lone pairs and double bonds

Count bonding and nonbonding groups separately

The Single Molecular Shape of the Linear Electron-Group Arrangement

<table>
<thead>
<tr>
<th>Class</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>AX₂</td>
<td>Linear</td>
</tr>
</tbody>
</table>

Examples: CS₂, HCN, BeF₂

A = 

X = 

E = 

Key

The Two Molecular Shapes of the Trigonal Planar Electron-Group Arrangement

<table>
<thead>
<tr>
<th>Class</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>AX₃</td>
<td>Trigonal planar</td>
</tr>
</tbody>
</table>

Examples: SO₃, BF₃, NO₂⁻, CO₂⁻

AX₁E

Bent (V shaped)

Examples: SO₂, O₃, PdCl₂, SnBr₂

Trigonal Planar Arrangement of BF₃

F—B—F angle is 120°:

Trigonal Planar Arrangement of NO₃⁻

Trigonal Planar Arrangement of CH₂O

Bent (V shaped) Arrangement of SnCl₂

The Three Molecular Shapes of the Tetrahedral Electron-Group Arrangement

<table>
<thead>
<tr>
<th>Class</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>AX₄</td>
<td>Tetrahedral</td>
</tr>
</tbody>
</table>

Examples: CH₄, SiCl₄, SO₄²⁻, ClO₄⁻

AX₃E

Trigonal pyramidal

Examples: NH₃, PF₃, ClO₃⁻, H₃O⁺

AX₂E₂

Bent (V shaped)

Examples: H₂O, OF₂, SCl₂

Tetrahedral Arrangement of Methane

109.5°

109.5°

109.5°
Polarity of Bonds

- Recall ideas on electronegativity

A bond will always have a degree of ionicity/polarity if the two bonded atoms are not equivalent.

- by ‘not equivalent’, we mean either different elements, or the same element with different environments

\[
\text{Dipole moment (}\mu\text{)} = \text{charge} \times \text{distance} = \delta \times r
\]

Polarity of Molecules and Ions

1) Determine the shape of the molecule using VSEPR theory
2) Determine which bonds have a degree of ionicity (all those where the bonded atoms are not equivalent)
3) Determine whether the bond dipoles cancel each other out due to the symmetry of the molecule - if not, the molecule is polar.

\[
\begin{align*}
\text{H}_2\text{F} & \quad \text{Cl} \quad \text{F} \quad \text{F} \quad \text{O} \quad \text{O} \quad \text{O} \\
\text{Di}p\text{ole moment (}\mu\text{)} & = \text{charge} \times \text{distance} = \delta \times r
\end{align*}
\]

Summary

- Electron groups dictate the shapes of molecules

Lewis Structures
- how many groups of electrons around an atom
- VSEPR (including repulsion of different electron groups)
- Molecular Geometry

- Polarity

COMING NEXT:
How Lewis Structures are in accord with our Quantum view of the atom