MOLECULAR GEOMETRY OR MOLECULAR SHAPE

The determination of molecular shape involves determining BOND ANGLES. We are going to use a very simple theory of molecular shape which only requires Lewis electron dot structures and simple electrostatic ideas; this is called Valence Shell Electron Pair Repulsion Theory (VSEPR).

This approach to molecular shape involves the following steps:

A. Determination of the Central Atom

The central atom is defined as the atom around which all the other atoms are arranged:

• Sometimes clearly identified by the stoichiometry e.g. NH$_3$; PCl$_5$

• F is very rarely a central atom; Cl, Br, and I are never central atoms unless bonded to another halogen or oxygen

• O is not usually central unless bonded to TWO other atoms e.g. H$_2$O; OF$_2$

• H is never a central atom

B. Determination of the Number of Valence Electrons Surrounding the Central Atom

• Draw the Lewis electron dot structure for the molecule

• Determine the number of valence electrons around the central atom
e.g. OF$_2$; Central atom = O

   F - O - F

   Number of valence electrons around O = 8

• Divide the no. of valence electrons around the central atom into PAIRS

• Further re-classify the ELECTRON PAIRS into ELECTRON GROUPS

   If ONE LIGAND atom forms TWO (or THREE) 2-ELECTRON bonds to the central atom we consider ALL FOUR (or SIX) electrons together as a GROUP

C. Distribute GROUPS OF ELECTRONS around the CENTRAL ATOM so that REPULSION of LIKE CHARGES is MINIMIZED

The geometries that MINIMIZE the repulsion between GROUPS of electrons have been mathematically established. From the attached figure, we see that the ELECTRON GROUPS in OF$_2$ will be distributed TETRAHEDRALLY.

This will be THE IDEALIZED ELECTRON GROUP GEOMETRY.

The GEOMETRY OF THE MOLECULE is conventionally considered to be the GEOMETRY of the ATOMS, NOT THE GEOMETRY OF THE ELECTRON GROUPS.

Thus, the IDEAL MOLECULAR GEOMETRY of OF$_2$ is BENT with a $<$ FOF = 109° 27'
<table>
<thead>
<tr>
<th>Number of points</th>
<th>Geometrical description</th>
<th>General Formula</th>
<th>Angles</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Linear</td>
<td>AB₂</td>
<td>180°</td>
<td>BeCl₂(g), CO₂, CS₂</td>
</tr>
<tr>
<td>3</td>
<td>Trigonal planar (Equilateral) triangle</td>
<td>AB₃</td>
<td>120°</td>
<td>BX₃, CO₃²⁻, SO₃</td>
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<tr>
<td>4</td>
<td>Tetrahedron</td>
<td>AB₄</td>
<td>109.5°</td>
<td>CH₄, CX₄, NH₄⁺, SiX₄,</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>BX₄⁺, ClO₄⁻, PO₄³⁻</td>
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<tr>
<td>5</td>
<td>Trigonal bipyramid</td>
<td>AB₅</td>
<td>90°, 120°</td>
<td>PF₅, PCl₅(g), AsF₅</td>
</tr>
<tr>
<td>6</td>
<td>Octahedron</td>
<td>AB₆</td>
<td>90°</td>
<td>SF₆, SeF₆, PF₆⁺, SiF₆²⁻</td>
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