Valence-Shell Electron-Pair Repulsion

- Regions on central atom repelled as far as possible

linear trigonal planar tetrahedral trigonal bipyramidal octahedral

Molecular Shape

2 Regions e⁻ ρ

CO₂ :O=C=O:

linear

O—C—O

180°

3 Regions e⁻ ρ: 3 Bonds

NO₃⁻:O=O=O:

trigonal planar

3 Regions e⁻ ρ: 2 Bonds, 1 Lp

SO₂ :O=S=O:

bent, 120°

3 Regions e⁻ ρ: 3 Bonds

NH₃ H–N–H

trigonal pyramidal

4 Regions e⁻ ρ: 3 Bonds, 1 Lp

NH₄⁺ H–N–H

tetrahedral

4 Regions e⁻ ρ: 2 Bonds, 2 Lp

H₂O H–O–H

bent, 109.5°

5 Regions e⁻ ρ: 5 Bonds; 4 Bonds, 1 Lp

PCl₅:Cl=Cl=Cl:

axial equatorial lone-pair equatorial

SF₄:Cl=Cl=Cl:

trigonal bipyramidal see-saw
5 Regions e– p: 3 Bonds, 2 Lp; 2 Bonds, 3 Lp

ClF₃  28 ve–
both lone-pairs equatorial

F
Cl
90°
F

I–
22 ve–
all lone-pairs equatorial

I
I
linear

6 Regions e– p: 6 Bonds

SF₆  48 ve–

F

90°

F

octahedral

6 Regions e– p: 5 Bonds, 1 Lp; 4 Bonds, 2 Lp

IF₅  42 e–
square planar
any position: all same

H
Cl

H
H

H
O

trigonal planar

Complex Molecules
> 1 central atom

acetic acid

trigonal planar

bent

tetrahedral

8 notation: “partial” vector notation: length ∝ difference

H
Cl

Linus Pauling
American 1932

Electronegativity: ability of an atom, in a molecule, to attract e–.
Determining Molecular Polarity

overall e⁻ distribution in molecule

1. Lewis structure
2. VSEPR shape
3. bond polarity: bond vector notation
4. vector sum of bond polarities

polar if unique +, – charge distribution
only need to determine: polar or nonpolar

**CO₂**

\[ \begin{align*}
1 \times C (4 \text{ ve}) & \quad 4 \text{ e}^- \\
2 \times O (6 \text{ ve}) & \quad 12 \text{ e}^- \\
\text{EN O > C (3.5 vs 2.5)} & \quad \text{bond vectors cancel: carbon dioxide is nonpolar}
\end{align*} \]

**SO₂**

\[ \begin{align*}
1 \times S (6 \text{ ve}) & \quad 6 \text{ e}^- \\
2 \times O (6 \text{ ve}) & \quad 12 \text{ e}^- \\
\text{EN O > S (3.5 vs 2.5)} & \quad \text{vectors do not cancel: sulfur dioxide is polar}
\end{align*} \]

**BF₃**

\[ \begin{align*}
24 \text{ ve}^- & \\
\text{trigonal planar} & \quad \text{vectors cancel: boron trifluoride is nonpolar}
\end{align*} \]

**POCl₃**

\[ \begin{align*}
32 \text{ ve}^- & \\
tetrahedral & \quad \text{vectors do not cancel: phosphorous oxychloride is polar}
\end{align*} \]

**PCl₅**

\[ \begin{align*}
\text{trigonal bipyramidal} & \quad \text{vectors cancel: phosphorous pentachloride is nonpolar}
\end{align*} \]
CCl₄  CHCl₃
acetone  H₂O

Polarity

nonpolar

slightly polar

polar

very polar

Molecular Orbital Treatment – CH₄

but, E and shape not correct...
not tetrahedral
bond E’s not equal

sp³ Hybrid Orbitals

Weighted average energy:

E

2s

2p

sp³

sp³

sp³

sp³

Molecular Orbital Treatment – CH₄

sp² Hybrid Orbitals

trigonal planar

sp Hybrid Orbitals

linear