

Chapter 9

Molecular Geometry and Bonding Theories

Chapter 9 suggested problems

10th Ed. and 11th Ed.: 21, 27, 35, 47, 49, 51, 76, 96

Class Notes

I. Hybrid orbitals

A. Orbital shapes

1. s
2. p
3. d

B. Orbital overlap is essential for chemical bonding to occur; the greater the overlap the stronger the bond

1. Show overlap between hydrogen and oxygen in water
2. Overlap is an important factor in bond strength but certainly not the only factor

C. If carbon has four valence electrons ($2s^2 2p^2$), how can it form four bonds?

1. In the 1930s Linus Pauling suggested that one of the 2s electrons is promoted to the empty 2p orbital, resulting in the formation of four hybrid orbitals that are intermediate in energy and shape
2. Diagram of orbitals vs. energy
3. This hybridization theory can be easily and accurately used to describe bonding in many molecules

atom	molecule	valence configuration	hybridization	remaining orbitals	geometry	bond angle
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Be	BeH ₂	2s ²	sp	2 p orbitals	linear	180°
B	BF ₃	2s ² 2p ¹	sp ²	1 p orbitals	trigonal planar	120°
C	CH ₄	2s ² 2p ²	sp ³	none	tetrahedral	109.5°
P	PCl ₅	3s ² 3p ³	dsp ³	4 d orbitals	trigonal bipyramidal	120° 90°
S	SF ₆	3s ² 3p ⁴	d ² sp ³	3 d orbitals	octahedral	90°

D. Multiple bonds

1. Double bonds - consist of one sigma bond and one pi bond

a. Sigma bonds

- i. Cylindrical probability distribution around the bond axis
- ii. Sigma bonds are created by the overlap of hybridized orbitals

b. Pi bonds

- i. Probability out of the plane (above and below) the bond axis
- ii. Pi bonds are created by the overlap of the unhybridized p orbitals

2. Triple bonds consist of one sigma bond and two pi bonds

II. VSPER - Valence Shell Paired-Electron Repulsion

- A. There is an excellent correlation between the type of hybridization that occurs in a molecule, the number of bonds formed, the number of nonbonding pairs of electrons on the central atom, and the geometry of the molecule
- B. The mutual repulsion of pairs of electrons cause them to arrange themselves as far apart spatially as possible
- C. Lone pairs take up slightly more space than bonding pairs and are more repulsive as a consequence
- D. Multiple bonds count as one bonding pair - see Tables 9.2, 9.3

total pairs	bonding pairs	nonbonding pairs	geometry	bond angles	hybridization	example
2	2	0	linear	180	sp	BeH ₂

3	3	0	trigonal planar	120	sp^2	BF_3
	2	1	bent		sp^2	NO_2
4	4	0	tetrahedral	109.5	sp^3	CH_4
	3	1	pyramidal		sp^3	NH_3
	2	2	bent		sp^3	H_2O
5	5	0	trigonal bipyramidal	120, 90	dsp^3	PCl_5
	4	1	seesaw		dsp^3	SF_4
	3	2	t-shaped		dsp^3	ClF_3
	2	3	linear		dsp^3	XeF_2
6	6	0	octahedral	90	d^2sp^3	SF_6
	5	1	square pyramidal		d^2sp^3	BrF_5
	4	2	square planar		d^2sp^3	XeF_4

III. Polar bonds and polar molecules

A. Polar covalent bonds - bonding electrons are not shared equally due to differences in electronegativity between the bonding atoms

1. If the bonding atoms are the same (e.g. H_2 , N_2 , O_2 , F_2 , etc.) the bonding atoms are shared equally (50%/50%)
2. If the bonding atoms are not the same the bonding electrons spend more time around the more electronegative atom
3. This causes partial charges to arise on the bonding nuclei

B. As a general rule, molecules with one or more polar bonds are themselves polar which affects interactions with other molecules

C. The polarity of molecules is measured in Debye units (D)

D. Polar molecules are said to have a dipole moment, the magnitude of which indicates the magnitude of the partial charges in the molecule

E. The exceptions: those molecules with polar bonds in which symmetry results in

negation of molecular polarity

F. Lone pairs ruin this, negating symmetry unless all axial or equatorial positions are filled with lone pairs

G. Examples

1. BF_3 vs. BF_2H
2. CCl_4 vs. CCl_3H
3. NH_3 , ClF_3 , XeF_2 , BrF_5 and XeF_4

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