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Problem-Solving Using VSEPR and VB Theory

going from molecular and ionic formulas to properties of substances

General Recipe for Connectivity Determination

1. Determine center atom(s) based on largest atom then lowest EN.
2. Arrange additional atoms around the center.
3. Add electrons for each neutral atom.
4. Draw single bonds connecting pairs of atoms using one electron from each atom involved.
5. Draw double bonds, if single electrons remain on adjacent atoms.
6. Add an additional electron for each negative charge on anions, preferably on more EN nuclei.
7. Subtract an electron for each positive charge on cations, preferably on less EN nuclei.
8. Attempt to fulfill octet rule, minimize formal charges, and to place negative formal charges on high EN nuclei/positive formal charges on low EN nuclei.
9. Switch an electron pair from one nucleus to another if necessary.
10. Identify alternative locations where electrons can be assigned that still generally fulfill the octet rule and minimize the formal charges.
11. For each structure, double-check that the total valence electrons from neutral atoms - the charge of the particle = number of electrons used.
12. Select the best structure.
13. Use correct arrow notation to convert from one resonance structure to another.

General Recipe for Shape Determination

1. Determine the number of electron groups.
2. Determine basic shape. (AX_mE_n)
3. If all of the groups cannot be evenly spaced (i.e. trigonal bipyramidal) then put groups with highest electron density in positions with least 90º angle interactions.
4. Estimate bond angles. (High electron density electron groups will increase the adjacent bond angles.)
5. Determine the size and direction of bond dipoles (include resonance factors)
6. Determine the molecular dipole size and direction (include resonance factors)
7. Assign the hybridization of each atom.

Practice Exercises

CH_4	H_2O	$CHCl_3$	C_2H_6	C_3H_8	C_2H_4	CO_2
$CO(CH_3)_2$	HNO_3	H_2SO_4	$SOCl_2$	CO	NO_3^-	PCl_3
PCl_5	P_2O_5	BBr_3	$H_3C_2O_2^-$	CNO^-	C_6H_6 (benzene)	