

Using VSEPR and VB Theory 1.2

Predicting physical and chemical properties from molecular formulas

Generating Lewis Structures

1. Determine central atom(s) based on largest atom, lowest EN, and ability to make the most bonds.
2. Arrange additional atoms symmetrically around the central atom.
3. Add electrons such that each atom is neutral.
4. Draw single bonds connecting pairs of atoms using one electron from each atom involved.
5. Count the electrons necessary to achieve an octet.
6. If electrons are missing, draw double bonds using one electron from each atom involved.
7. If necessary, transfer an electron from one atom to another to make a bond or satisfy the octet rule.
8. Add an additional electron for each negative charge on anions, preferably on the more EN nuclei.
9. Subtract an electron for each positive charge on cations, preferably on less EN nuclei.
10. 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.
11. Identify alternative locations where electrons can be assigned that still generally fulfill the octet rule and minimize the formal charges.
12. For each structure, double-check that the total number of valence electrons from neutral atoms minus the charge of the particle = number of electrons present in the particle.
13. Evaluate and select the best structure.
14. Use correct arrow notation to convert from one resonance structure to another.
15. Atoms in the first two rows of the periodic table CANNOT exceed their octets.

Determination of Particle Shape and Polarity

1. Determine the number of electron groups.
2. Determine the bond angles and geometric arrangement.
3. If all of the groups cannot be evenly spaced (i.e. trigonal bipyramidal) then put groups with highest electron density in positions with fewest 90° angle interactions.
4. Estimate bond angles. (High electron density electron groups will enlarge 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 to each atom. (2 electron groups = sp, 3 electron groups = sp², etc.)

Practice Exercises

CH ₄	H ₂ O	CHCl ₃	C ₂ H ₆	CSCl ₂	C ₂ H ₄	CO ₂
CHBr	HNO ₃	H ₂ SO ₄	SOCl ₂	CO	NO ₂ ⁻	PCl ₃
PCl ₅	P ₂ O ₅	BBr ₃	C ₂ H ₃ O ₂ ⁻	CNO ⁻	C ₆ H ₆ (benzene)	H ₂ CO ₃