

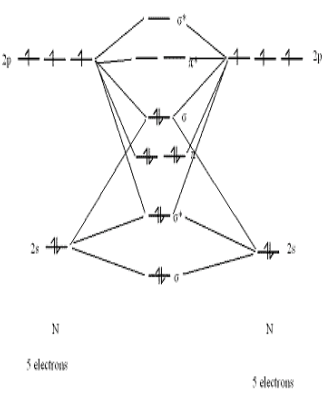
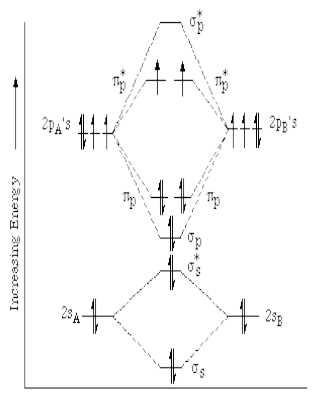


IMF Unit – Lewis Structure, VSEPR Theory, VB Hybridization, MO Theory

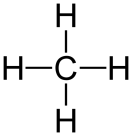
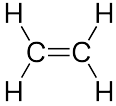

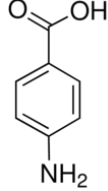
Fill in the chart below.

| Molecule | N ₂ | O ₂ | HF | SeCl ₄ |
|--|--|---|---|---|
| Lewis Structure | $:\text{N} \equiv \text{N}:$ | $:\ddot{\text{O}}=\ddot{\text{O}}:$ | $\text{H}-\ddot{\text{F}}:$ | |
| VSEPR: Electronic geometry of central atom(s)? | Linear | Trigonal Planar | H: Linear F: Tetrahedral | Trigonal Bipyramidal |
| VSEPR: Molecular geometry of central atom(s)? | Linear | Linear | Linear | See-Saw |
| Is the molecule polar? | No | No | Yes | Yes |
| What is the predominate IMF? | Dispersion Forces | Dispersion Forces | H-Bonding | Dipole-Dipole Forces |
| VB: What types of bonds are in the molecule? What atomic and/or hybrid orbitals make up each bond? | 1 σ bond: N(sp) and N(sp) 2 π bonds: N(2p) and N(2p) | 1 σ bond: O(sp ²) and O(sp ²) 1 π bond: O(2p) and O(2p) | 1 σ bond: H(1s) and F(sp ³) | 4 σ bonds: Se(sp ³ d) and Cl(sp ³) |



| | | | | |
|---|---|---|---|---|
| <p>MO: Find the MO diagram for the molecule in a book or on the website and fill it in.</p> |  |  | <p>The MO diagram for this molecule is more complicated and goes beyond the scope of the class. See this website for more info. http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html</p> | <p>The MO diagram for this molecule is more complicated and goes beyond the scope of the class. See this website for more info. http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html</p> |
| <p>What is the bond order? Does it correspond to what you found in the Lewis structure and VB analysis?</p> | <p>$BO = \frac{1}{2}(8-2) = 3$ YES, a BO of 3 predicts the triple bond from VSEPR and VB.</p> | <p>$BO = \frac{1}{2}(8-4) = 2$ YES, a BO of 2 predicts the double bond from VSEPR and VB.</p> | | |
| <p>Diamagnetic or Paramagnetic?</p> | <p>Diamagnetic</p> | <p>Paramagnetic</p> | | |

Fill in the chart below.

| Molecule | methane | ethene | ethyne | 4-aminobenzoic acid |
|--|---|--|---|--|
| Lewis Structure |  |  |  | <p>(Look it up!)</p>  |
| VSEPR: Electronic geometry of central atom(s)? | <p>Tetrahedral</p> | <p>Trigonal Planar</p> | <p>Linear</p> | <p>Trigonal Bipyramidal</p> |
| VSEPR: Molecular geometry of central atom(s)? | <p>Tetrahedral</p> | <p>Trigonal Planar</p> | <p>Linear</p> | <p>See-Saw</p> |



| Is the molecule polar? | No | No | No | Yes |
|---|--|---|---|---|
| What is the predominate IMF? | Dispersion Forces | Dispersion Forces | Dispersion Forces | H-Bonding |
| VB: What types of bonds are in the molecule? What atomic and/or hybrid orbitals make up each bond? | 4 σ bonds: C(sp ³) and H(1s) | 4 σ bonds: C(sp ²) and H(1s) 1 σ bond: C(sp ²) and C(sp ²) 1 π bond: C(2p) and C(2p) | 2 σ bonds: C(sp) and H(1s) 1 σ bond: C(sp) and C(sp) 2 π bonds: C(2p) and C(2p) | 1 σ bond: O(sp ³) & C(sp ²) 1 σ bond: C(sp ²) & C(sp ²) 1 σ bond: O(sp ³) & C(sp ²) 1 σ bond: Cl(sp ²) & C(sp ²) 1 σ bond: N(sp ³) & C(sp ²) 1 σ bond: N(sp ³) & H(1s) 1 π bond: O(sp) & C(2p) |
| MO: Find the MO diagram for the molecule in a book or on the website and fill it in. | | | The MO diagram for this molecule is more complicated and goes beyond the scope of the class. See this website for more info. http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html | The MO diagram for this molecule is more complicated and goes beyond the scope of the class. See this website for more info. http://www.ch.ic.ac.uk/vchemlib/course/mo_theory/main.html |
| What is the bond order? Does it correspond to what you found in the Lewis structure and | $BO = \frac{1}{2}(8 - 0) = 4$ <p>YES, a BO of 4 predicts the 4 bond from VSEPR and VB.</p> | | | |



| | | | | |
|------------------------------|--------------------|--|--|--|
| VB analysis? | | | | |
| Diamagnetic or Paramagnetic? | Diamagnetic | | | |

The HOMO-LUMO gap of a molecule is equal to $\Delta E = 2 \text{ eV}$. What wavelength of electromagnetic radiation do you expect it to absorb?

Work:

$$\Delta E = 2eV \left(\frac{1.60 \times 10^{-19} \text{ Js}}{1eV} \right) = 3.20 \times 10^{-19} \text{ Js}$$

$$E = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{E}$$

$$\lambda = \frac{(6.626 \times 10^{-34} \text{ Js})(3 \times 10^8 \frac{\text{m}}{\text{s}})}{3.2 \times 10^{-19} \text{ J}} = 6.20 \times 10^{-7} \text{ m} = 620 \text{ nm}$$

A molecule absorbs light of $\lambda = 490 \text{ nm}$. What do you predict is the HOMO-LUMO gap of that molecule?

Work:

$$\Delta E_{H-L} = E_{\text{photon}}$$

$$E_{\text{photon}} = \frac{hc}{\lambda}$$

$$E_{\text{photon}} = \frac{(6.626 \times 10^{-34} \text{ Js})(3 \times 10^8 \frac{\text{m}}{\text{s}})}{4.9 \times 10^{-7} \text{ J}} = 4.06 \times 10^{-19} \text{ J}$$

$$\Delta E_{H-L} = E_{\text{photon}} = 4.06 \times 10^{-19} \text{ J} \left(\frac{1eV}{1.60 \times 10^{-19} \text{ J}} \right) = 2.53eV$$