3.091 Fall Term 2004 Homework #5 addendum October 8

 Beryllium and nitrogen can react to form the molecule, beryllium nitride (BeN). To show that BeN is stable and paramagnetic use LCAO-MO theory (linear combination of atomic orbitals - molecular orbitals) to construct an energy-level diagram that includes the energy levels of the atoms and the bonding and antibonding orbitals of the molecule. Indicate the occupation of the orbitals with arrows. The filling sequence of molecular 2p orbitals in BeN



2. In the liquid state, to which will an argon atom bond more strongly, another argon atom or a krypton atom? Explain.

Kr. Kr is larger than Ar and has more electrons

- + Kr is more polarizable than Ar
- + Kr is capable of stronger van der Waals bonding
- **3.** Both ammonia (NH₃) and phosphine (PH₃) are gases at room temperature. Identify which compound has the higher boiling point and explain your reasoning.

NH₃. Both are polar (trigonal pyramids) but ammonia is capable of hydrogen bonding.

4. Construct an energy-level diagram using LCAO-MO theory (linear combination of atomic orbitals into molecular orbitals) to show that the cyanide ion, CN^- , is stable. The filling sequence of the molecular 2*p* orbitals in CN^- is π_{2p} , σ_{2p} , π^*_{2p} , σ^*_{2p} .



total of 10 valence electrons: 4 from C, 5 from N, and 1 acquired by electron transfer to make the moiety net negative

conclude that cyanide ion is stable owing to the occupancy of only σ_{2p} and π_{2p} bonding orbitals

5. For each pair of compounds, identify the one with the *higher* boiling point. Justify your choice. (i) GeH₄ and SiH₄; (ii) GeH₄ and AsH₃; (iii) HCl and HF.

(i) GeH₄. larger molecule \therefore more polarizable \therefore stronger van der Waals bonds

(ii) AsH₃. it is polar while GeH₄ is nonpolar. both have almost equal mass, but dipole-dipole interaction is stronger than London dispersion force

(iii) HF. both molecules are polar but hydrogen bonding operative in only HF

6. Draw a 3-dimensional representation of the molecular geometry (not simply the Lewis structure) of hydrazine, H₂N–NH₂.



7. Hydrazine and hydrogen chloride have nearly identical molecular weights, yet hydrazine boils at 113.5°C and is a liquid at room temperature, while hydrogen chloride boils at -85°C and is a gas at room temperature. Explain with reference to electronic structure and bonding.

hydrazine is nonpolar while HCl is polar but hydrazine is capable of hydrogen bonding so it has the higher boiling point