Chemistry 4610/5560
Exam I
September 23, 1999

(8) 1. a. Draw all resonance structures for an NO$_2$F molecule. (N is the central atom.)
b. Based on your structures, would you expect the N-F bond to be more like a single bond or a
double bond? Why?

\[
\begin{align*}
\text{O} & \quad \text{O} \\
\text{N} & \quad \text{O} \\
\text{F} & \quad \text{O}
\end{align*}
\]

The lowest in energy, \( \text{N} \equiv \text{O} \) will be most like a single bond.

(12) 2. The first ionization energies for O, S, and Se, are 13.62, 10.36, and 9.75 eV respectively.
a. Write the electron configuration for each of the three atoms.
b. Using Slater's rules, determine \( Z^* \) for the highest energy electron for each of the three atoms.
c. Do your results from part b explain the observed trend in ionization potential? Why or why not?

\[
\begin{align*}
\text{O} & : 1s^2 \ 2s^2 \ 2p^4 \\
Z^* & = 8 - \left[ (5 \times 0.35) + (2 \times 0.85) \right] = 8 - 3.45 = 4.55 \\
\text{S} & : 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^4 \\
Z^* & = 16 - \left[ (10 \times 1.0) + (8 \times 0.85) + (5 \times 0.35) \right] = 16 - 10.55 = 5.45 \\
\text{Se} & : 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6 \ 4s^2 \ 3d^{10} \ 4p^4 \\
Z^* & = 34 - \left[ (10 \times 1.0) + (18 \times 0.85) + (5 \times 0.35) \right] = 34 - 27.05 = 6.95
\end{align*}
\]

(10) 3. Answer each of the following:

a. A 2+ ion with two 4d electrons: \( \text{Zr}^{2+} \)
b. A 3+ ion with two 6s electrons: \( \text{Bi}^{3+} \)
c. Two different atoms with five 3d electrons: \( \text{Cr} \) \text{ Mn} 
d. A 3+ ion with fourteen 4f electrons \( \text{Lu}^{3+} \)

(15) 4. a. Draw representations for each of the following orbitals.
b. How many lobes does the orbital have?
c. Describe the location of the angular nodes. (Be precise.)
d. Show the relative signs of the wavefunction for each lobe.

\[
\begin{align*}
a) & \quad \text{p}_x \\
b) & \quad 2 \text{ lobes} \\
c) & \quad \text{yz plane} \\
d) & \quad 4 \text{ lobes}
\end{align*}
\]

\[
\begin{align*}
a) & \quad \text{d}^{2} \ \\
b) & \quad 2 \text{ planes intersecting x-y} \\
c) & \quad \text{and -x, y and z containing basis}
\end{align*}
\]
(32) 5. Answer the following questions for each of the following molecules or ions:
   a. Draw the Lewis dot structure.
   b. What is the shape of the molecule or ion?
   c. To what point group does the molecule belong?
   d. Is the molecule polar or non-polar?

   \[
   \begin{align*}
   &\text{BH}_4^- \quad \text{ClF}_3 \\ &\begin{array}{c}
   \text{C}_3 \text{v} \\
   \begin{array}{c}
   \text{H} \\
   \text{H} \\
   \text{H}
   \end{array}
   \end{array} \\
   &\begin{array}{c}
   \begin{array}{c}
   \text{F} \\
   \text{F}
   \end{array}
   \end{array}
   \end{align*}
   \]

   b) tetrahedral

   c) Td

   d) non-polar

   \[
   \begin{align*}
   &\text{SO}_2 \\ &\begin{array}{c}
   \text{S} \\
   \text{O}
   \end{array} \\
   &\begin{array}{c}
   \begin{array}{c}
   \text{O} \\
   \text{O}
   \end{array}
   \end{array}
   \end{align*}
   \]

   b) bent

   c) C\_2\text{v}

   d) non-polar

   \[
   \begin{align*}
   &\text{N}_3 \\ &\begin{array}{c}
   \text{N} \\
   \text{N}
   \end{array} \\
   &\begin{array}{c}
   \text{N}
   \end{array}
   \end{align*}
   \]

   b) linear

(23) 6. The following are some of the “new” shapes introduced in class. (Assume idealized structures with all atoms at each position the same.)

   a. For each shape, what is the steric number?
   b. What is the point group for each of the idealized shapes?

   \[
   \begin{align*}
   &\text{pentagonal bipyramid} \\ &\quad \begin{array}{c}
   \text{SN} \\
   \text{7}
   \end{array} \\ &\text{D}_{5h}
   \end{align*}
   \]

   \[
   \begin{align*}
   &\text{square antiprism} \\ &\quad \begin{array}{c}
   \text{8}
   \end{array} \\ &\text{D}_{4d}
   \end{align*}
   \]

   \[
   \begin{align*}
   &\text{capped octahedron} \\ &\quad \begin{array}{c}
   \text{7}
   \end{array} \\ &\text{C}_{3v}
   \end{align*}
   \]

   \[
   \begin{align*}
   &\text{trigonal prism} \\ &\quad \begin{array}{c}
   \text{6}
   \end{array} \\ &\text{D}_{3h}
   \end{align*}
   \]

   c. Which, if any, of these four structures could be polar? Why or why not?

   Capped octahedron This is the only shape of the four with only one C\_n axis.

   d. Which, if any, of these four structures are chiral? Why or why not?

   none are chiral All have at least a \(\pi\) reflection. To be chiral, the molecule can have either no symmetry operations or only C\_n rotations.