This exam consists of 8 pages. When the exam begins make sure you have one of each. Print your name at the top of each page now. Show your work on calculations, this is the only way partial credit can be given. Be sure to include units on calculations, and give answer to the correct number of significant figures. When a blank is not provided make sure you place a box around the correct answer. You may not use a programmable calculator. The exam is 100 points and 50 minutes.

If anything confuses you or is not clear, raise your hand and ask!

Useful Formula: \( \Delta H = \Sigma \text{D(bonds broken)} - \Sigma \text{D(bonds formed)} \)
Points

30  1) For the following compounds draw the Lewis dot structure for each compound. Also determine the geometric structure (give the name) and make a sketch of each compound. Determine the hybridization around the central atom. Also determine if there is a dipole moment. Give the approximate bond angle for the smallest angle formed by the atoms indicated.

A) BeF$_2$

\[
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{SN = 2} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{LP = 0} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Geometric shape = } \text{linear} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Be hybridization = } \text{sp} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Dipole moment (circle one)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Yes } \quad \text{No} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{F – Be – F bond angle = } 180^\circ \\
\cdot
\end{array}
\end{array}
\]

B) NH$_3$

\[
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{SN = 4} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{LP = 1} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Geometric shape = } \text{trigonal pyramidal} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{N hybridization = } \text{sp}^3 \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Dipole moment (circle one)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Yes } \quad \text{No} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{H – N – H bond angle = } < 109.5^\circ \\
\cdot
\end{array}
\end{array}
\]

C) SF$_4$

\[
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{SN = 5} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{LP = 1} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Geometric shape = } \text{see saw (saw horse)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{S hybridization = } \text{dsp}^3 \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Dipole moment (circle one)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Yes } \quad \text{No} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{H – N – H bond angle = } < 90^\circ \\
\cdot
\end{array}
\end{array}
\]

D) XeF$_2$

\[
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{SN = 5} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{LP = 3} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Geometric shape = } \text{linear} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Xe hybridization = } \text{dsp}^3 \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Dipole moment (circle one)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Yes } \quad \text{No} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{F – Xe – F bond angle = } 180^\circ \\
\cdot
\end{array}
\end{array}
\]

E) IF$_5$

\[
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{SN = 6} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{LP = 1} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Geometric shape = } \text{square pyramidal} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{I hybridization = } \text{d}^2\text{sp}^3 \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Dipole moment (circle one)} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{Yes } \quad \text{No} \\
\cdot
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\cdot \\
\cdot \quad \text{F – I – F bond angle = } < 90^\circ \\
\cdot
\end{array}
\end{array}
\]
2) The nitrite ion, \( \text{NO}_2^- \), results when nitrous acid is dissolved in water. The possible connections are N – O – O or O – N – O. Draw two resonance structures for each indicating formal charge. Indicate which connection is most likely and briefly describe how you made your choice.

\[
\begin{align*}
\text{N – O – O connection} & \quad \leftrightarrow \quad \text{O – N – O connection} \\
\begin{array}{c}
\text{N} \\
\text{O} \\
\text{O}
\end{array} & \quad \leftrightarrow \quad \\
\begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array} & \quad \leftrightarrow \quad \\
\begin{array}{c}
\text{N} \\
\text{O} \\
\text{O}
\end{array}
\end{align*}
\]

The O – N – O connection is most likely due to the more favorable formal charges, i.e., smaller number of formal charges and smaller absolute values of formal charge.

3) The molecule SCNCH\(_3\), the skeletal structure of which is shown below, is used as a pesticide.

\[
\begin{align*}
\text{S} & \quad \text{C}_1 \quad \text{N} \quad \text{C}_2 \quad \text{H} \\
& \quad \text{H}
\end{align*}
\]

a) Write down the Lewis dot structure for this molecule.

\[
\begin{align*}
\text{H} & \quad \text{S} = \text{C}_1 = \text{N} \quad \text{C}_2 \quad \text{H} \\
& \quad \text{H}
\end{align*}
\]

b) What is the hybridization around

\[
\begin{align*}
\text{C}_1 & : \quad \text{sp} \\
\text{N} & : \quad \text{sp}^3 \\
\text{C}_2 & : \quad \text{sp}^3
\end{align*}
\]

c) What are the following bond angles

\[
\begin{align*}
\text{S} – \text{C}_1 – \text{N} & : \quad 180^\circ \\
\text{C}_1 – \text{N} – \text{C}_2 & : \quad 120^\circ
\end{align*}
\]

d) The S – C\(_1\) – N – C\(_2\) framework is planar. Assume these atoms lie in the plane of the paper, and that this plane is identified as the x-y plane. Now consider the orbitals (2s, 2p\(_x\), 2p\(_y\) and 2p\(_z\)) on carbon atom 1. Which of these orbitals are involved in hybrid orbital formation? Which of these orbitals are used in \( \sigma \) and \( \pi \) bond formation with the neighboring S and N atoms?

If we choose the x-axis to go from left to right on this page, then the 2s and 2p\(_x\) orbitals are involved in the formation of the two hybrid sp-orbitals on C\(_1\). The sp-orbitals form the sigma bonds. The 2p\(_y\) and 2p\(_z\) orbitals form the pi bonds in plane of the page and perpendicular to the page, respectively.
e) Sketch the $\sigma$ and $\pi$ bonds formed between C$_1$ and N identifying the orbitals used on each atom.

$$\begin{align*}
\text{sp} & \quad \text{sp}^2 \\
2p & \quad 2p
\end{align*}$$

sp and $\text{sp}^2$ orbitals form the $\sigma$ bond and the 2p orbitals form the $\pi$ bond

4) The $\Delta H^0_{\text{rxn}}$ for the following reaction is $-511.2$ kJ.

$$\text{CH}_2\text{Cl}_2(\text{l}) + \frac{3}{2} \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + \text{H}_2\text{O}(\text{g}) + \text{Cl}_2(\text{g})$$

<table>
<thead>
<tr>
<th>Bond Type</th>
<th>D, Average Bond Energy (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-H</td>
<td>432</td>
</tr>
<tr>
<td>C-H</td>
<td>413</td>
</tr>
<tr>
<td>C-C</td>
<td>347</td>
</tr>
<tr>
<td>C-O</td>
<td>358</td>
</tr>
<tr>
<td>C=O (in CO$_2$)</td>
<td>799</td>
</tr>
<tr>
<td>Cl-Cl</td>
<td>239</td>
</tr>
<tr>
<td>O-H</td>
<td>467</td>
</tr>
<tr>
<td>O-O</td>
<td>146</td>
</tr>
<tr>
<td>O=O</td>
<td>495</td>
</tr>
</tbody>
</table>

a) Using the values given in the table above determine the average C – Cl bond energy.

$$\Delta H^0_{\text{rxn}} = 2(D \text{ of C–H}) + 2(D \text{ of C-Cl}) + 1.5(D \text{ of O=O}) - 2(D \text{ of C=O}) - 2(D \text{ of O-H}) - (D \text{ of Cl-Cl})$$

Rearrange and solve for (D of C-Cl)

$$\begin{align*}
(D \text{ of C-Cl}) &= \frac{1}{2} [\Delta H^0_{\text{rxn}} - 2(D \text{ of C–H}) - 1.5(D \text{ of O=O}) + 2(D \text{ of C=O}) + 2(D \text{ of O-H}) + (D \text{ of Cl-Cl})] \\
&= \frac{1}{2} [-511.2 - 2(413) - 1.5(495) + 2(799) + 2(467) + 239] \text{ kJ} \\
&= 346 \text{ kJ}
\end{align*}$$

b) The actual value for the average C – Cl bond energy is 339 kJ/mol. Why is the value calculated in a) different from this value?

The average C – Cl bond is just that, an average of all different types of C – Cl bonds not just the C – Cl bonds in CH$_2$Cl$_2$. Thus, there is a difference.
Draw a molecular energy diagram, give the electronic configuration, determine the bond order, and the magnetic properties of each of the following diatomics: \( \text{N}_2^+ \), \( \text{N}_2 \), and \( \text{N}_2^- \).

\[
\begin{array}{ccc}
\text{Electronic Configuration:} & (\sigma_{\text{1s}})^2(\sigma_{\text{1s}}^*)^2(\sigma_{\text{2s}})^2 & (\sigma_{\text{1s}})^2(\sigma_{\text{1s}}^*)^2(\sigma_{\text{2s}})^2 & (\sigma_{\text{1s}})^2(\sigma_{\text{1s}}^*)^2(\sigma_{\text{2s}})^2 \\
\text{Bond Order:} & 2.5 & 3.0 & 2.5 \\
\text{Magnetic Property:} & \text{paramagnetic} & \text{diamagnetic} & \text{paramagnetic}
\end{array}
\]

Arrange the above diatomics in the order of increasing bond strength and increasing bond length in the space provided below.

Bond Strength: \( \text{N}_2^- \) \( \leq \) \( \text{N}_2^+ \) \(<\) \( \text{N}_2 \)

Bond Length: \( \text{N}_2^- \) < \( \text{N}_2^+ \) \( \leq \) \( \text{N}_2 \)

Note: Full credit will be given if \( \text{N}_2^- \) and \( \text{N}_2^+ \) are switched in the bond strength and length ordering or if they are assumed to be the same.
Points

5 6) Diethyl ether has a boiling point of 34.5 °C and 1-butanol has a boiling point of 117 °C.

\[
\begin{align*}
\text{Diethyl Ether} & : \text{H} \quad \text{H} & \quad \text{H} \quad \text{H} \\
& : \text{H} - \text{C} - \text{C} - \text{O} - \text{C} - \text{C} - \text{H} & \quad \text{H} - \text{C} - \text{C} - \text{C} - \text{C} - \text{O} - \text{H} \\
& : \text{H} \quad \text{H} & \quad \text{H} \quad \text{H} \\
\text{1-Butanol} & : \text{H} \quad \text{H} \quad \text{H} \\
\end{align*}
\]

Both of these compounds have the same number and type of atoms. List all of the intermolecular forces present in each liquid. Explain the difference in their boiling points.

**Diethyl Ether**: dipole-dipole, London dispersion forces

**1-Butanol**: dipole-dipole, hydrogen bonding, London dispersion forces

Since 1-Butanol has the additional intermolecular force of H-bonding it should have the higher boiling point.