Chemistry 230–002 First Examination
September 23, 2003

Name (please PRINT LEGIBLY) ________________________________
(last) (first)

<table>
<thead>
<tr>
<th>Problem</th>
<th>Score</th>
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<tbody>
<tr>
<td>1. (a-e)</td>
<td>/28</td>
</tr>
<tr>
<td>2. (a-c)</td>
<td>/14</td>
</tr>
<tr>
<td>3. (a-b)</td>
<td>/16</td>
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<td>4. (a-f)</td>
<td>/24</td>
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<tr>
<td>5. (a-c)</td>
<td>/18</td>
</tr>
<tr>
<td>Total</td>
<td>/100</td>
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Please, please, PLEASE observe the following.

1) Write LARGE and LEGIBLY. If I can’t read what you write, I can’t give you full or partial credit.

2) Read each question carefully before answering. If you don’t answer the question I posed, you won’t get credit.

3) For questions with multiple parts, be consistent. Your answer to a later part will be graded based on the earlier part being correct, whether or not it actually is. For example, suppose I asked the following questions:
   (a) What is the hybridization of the C atom in methane? (5 pts)
   (b) What is the H–C–H bond angle? (5 pts)

Three students gave the following answers:

<table>
<thead>
<tr>
<th></th>
<th>Student 1</th>
<th>Student 2</th>
<th>Student 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>sp²</td>
<td>sp²</td>
<td>sp³</td>
</tr>
<tr>
<td>(b)</td>
<td>120°</td>
<td>109°</td>
<td>109°</td>
</tr>
<tr>
<td>Score</td>
<td>0 pts + 5 pts</td>
<td>0 pts + 0 pts</td>
<td>5 pts + 5 pts</td>
</tr>
</tbody>
</table>

Student 1 correctly answered (b) given her answer for (a). Student 2 incorrectly answered (b) given his answer for (a), even though (b) is formally correct. Student 3 correctly answered both (a) and (b) and got full credit for the question.
(1) (28 pts. total.) Methyl isocyanate, a compound that killed thousands and blinded tens of thousands of people in Bhopal, India, in 1984, has the formula C_2H_3NO.

(a) (4 pts.) How many total valence electrons does methyl isocyanate have?

(b) (6 pts.) The σ-bond network (atom-to-atom connectivity) of methyl isocyanate is sketched below. Fill in the remainder of electrons to draw the BEST resonance structure for methyl isocyanate. Include all unshared pairs of electrons and any formal charges.

(c) (6 pts.) What are the hybridizations of:
   1. the terminal C atom? ________________
   2. the N atom? ________________
   3. the internal C atom? ________________

(d) (4 pts.) What are the bond angles about:
   1. the N atom? ________________
   2. the internal C atom? ________________
(e) (8 pts.) Draw a diagram showing all of the atomic orbitals in CH$_3$N=C=O. Indicate which atomic orbitals overlap to form $\sigma$ bonds, which ones overlap to form $\pi$ bonds, and which ones hold unshared electrons. I’ve drawn out the orbitals around O to get you started. (Note: For sake of clarity, please don’t draw the small back lobes of the hybrid orbitals.)
(2) (14 pts. total.) Consider the vinyl cation, whose structure is shown below.

\[ \text{H}_2\text{C} \equiv \text{CH}^+ \]

(a) (5 pts.) What is the hybridization of the electron-deficient carbon in the vinyl cation?

(b) (4 pts.) Based on your answer to (a), what are the ideal bond angles about the electron-deficient carbon in the vinyl cation?

(c) (5 pts.) The phenyl cation, shown below, is much higher in energy than the vinyl cation. Why? (Think about the optimum bond angles about the electron-deficient carbon.)
(3) (16 pts. total.) Consider the compound with the formula \( \text{C}_5\text{H}_8\text{F}_2 \). A compound with this formula has either one ring or one \( \pi \) bond.

(a) (8 pts.) Draw two skeletal isomers of \( \text{C}_5\text{H}_8\text{F}_2 \). (There are many correct answers.)

(b) (8 pts.) Draw two stereoisomers of \( \text{C}_5\text{H}_8\text{F}_2 \). (There are many correct answers.)
(4) (4 pts. each, 24 pts. total.) For each pair of compounds, indicate the relationship of the first compound to the second by circling the correct answer.

(a)

\[
\begin{array}{c}
\text{is a skeletal isomer of} \\
\text{is a configurational diastereomer of} \\
\text{is a conformational diastereomer of} \\
\text{is an enantiomer of} \\
\text{is a resonance structure of} \\
\text{is the same compound as} \\
\text{has none of the above relationships to}
\end{array}
\]

(b)

\[
\begin{array}{c}
\text{is a skeletal isomer of} \\
\text{is a configurational diastereomer of} \\
\text{is a conformational diastereomer of} \\
\text{is an enantiomer of} \\
\text{is a resonance structure of} \\
\text{is the same compound as} \\
\text{has none of the above relationships to}
\end{array}
\]

(c)

\[
\begin{array}{c}
\text{is a skeletal isomer of} \\
\text{is a configurational diastereomer of} \\
\text{is a conformational diastereomer of} \\
\text{is an enantiomer of} \\
\text{is a resonance structure of} \\
\text{is the same compound as} \\
\text{has none of the above relationships to}
\end{array}
\]
(d) is a skeletal isomer of is a configurational diastereomer of is a conformational diastereomer of is an enantiomer of is a resonance structure of is the same compound as has none of the above relationships to

(e) is a skeletal isomer of is a configurational diastereomer of is a conformational diastereomer of is an enantiomer of is a resonance structure of is the same compound as has none of the above relationships to

(f) is a skeletal isomer of is a configurational diastereomer of is a conformational diastereomer of is an enantiomer of is a resonance structure of is the same compound as has none of the above relationships to
(5) (6 pts. each, 18 pts. total.) Using the curved arrow formalism, draw the best resonance structure of each of the following compounds.

(a) 
\[
\begin{align*}
&\text{H}_3\text{C} \\
&\text{N} \\
&\text{CH}_2 \\
&\text{CH}_3
\end{align*}
\]

(b) 
\[
\begin{align*}
&\text{H}_3\text{C} \\
&\text{N} \\
&\text{CH}_3
\end{align*}
\]

(c) 
\[
\begin{align*}
&\text{H}_2\text{C} \\
&\text{CH}_3 \\
&\text{CH}_3
\end{align*}
\]