I. (20 points)

A. Ozone (O₃) is a molecule which is often in the news because there doesn't seem to be enough of it in the stratosphere. Write all possible closed shell resonance structures for ozone. Note, ozone has the connectivity shown.

- 2 pts each (more than 2 wrong = zero total)

connectivity of ozone

resonance structures of ozone with all closed shell atoms

- 4 pts

B. Using the resonance drawings of ozone above, and knowing that ozone has a dipole moment, provide a proper three-dimensional drawing of ozone. Show the direction of all lone pairs, and bonds, using sticks, dashes, wedges and p orbitals. What can you say about the three dimensional shape of ozone?

- 6 pts

C. An isomer of ozone has no dipole moment. Provide its complete Lewis structure.

- 3 pts

D. Several structural isomers can be drawn which have the molecular formula C₂H₂F₂. Provide two of these isomers (containing only uncharged atoms), one with no overall dipole moment and one containing a dipole which is clearly indicated.

A: Isomer with no dipole moment

B: Isomer with dipole moment indicated

- 4 pts

E. For isomer B, on the right above, draw a picture illustrating the strongest type of intermolecular interaction that the molecule will make that reflects the boiling point of the compound.

- 3 pts
II. (18 points)

A. The structure of beta-hydroxytyrosine, an unusual amino acid produced by bacteria which are used in antibiotic production, is shown at the right. Identify the three most acidic protons by drawing arrows to each, and assigning an approximate pKa.

1 pt for choice of 3 most acidic
1 pt for assignment

B. Rank each of the following sets of molecules according to the criterion listed. (no partial credit)

\[
\begin{align*}
\text{A} & \quad \text{B} & \quad \text{C} \\
\text{OH} & \quad \text{OH} & \quad \text{CH}_3 \\
\text{CH}_2\text{OH} & \quad \text{CH}_2\text{CH}_3 & \quad \text{CH}_2\text{CH}_3 \\
\end{align*}
\]

Boiling point

\[
\begin{align*}
\text{A} & \quad \text{B} & \quad \text{C} \\
\text{C} & \quad \text{C} & \quad \text{C} \\
\text{A} & \quad \text{B} & \quad \text{C} \\
\end{align*}
\]

Dipole moment

\[
\begin{align*}
\text{A} & \quad \text{B} & \quad \text{C} \\
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH} & \quad \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 & \quad \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\
\end{align*}
\]

Water solubility

\[
\begin{align*}
\text{A} & \quad \text{B} & \quad \text{C} \\
\text{Br} & \quad \text{H} & \quad \text{F} \\
\end{align*}
\]

pKa of the most acidic proton
III. (26 points)

A. Two major resonance contributors can be drawn in addition to the structure of urea shown below. Provide these resonance contributors, which contain all closed shell atoms.

\[
\begin{align*}
\text{Urea} & \quad \text{Lewis structure \#1} \\
H_2N & \text{-} C & \text{-} C & \text{-} NH_2
\end{align*}
\]

B. Taking these resonance structures into account and using the hybridization model, provide a proper three-dimensional drawing of Lewis structure \#1. Show directionality of all lone pairs and bonds using lines, dashes, wedges, and p orbitals/pi bonds.

\[
\text{Urea must be } sp^2 \text{ and hold lone pair} \quad 2 \text{pts}
\]

C. Urea is also a valuable biological molecule because of its extensive acid/base properties. Urea can be protonated if it is reacted with a strong acid. There are two possible conjugate acids which could form as a result of this protonation. Draw both possible products as complete Lewis structures.

\[
\begin{align*}
\text{Conjugate acid of Urea \#1} & \quad \text{Conjugate acid of Urea \#2}
\end{align*}
\]

D. Which of the above conjugate acids is more stable and would be predicted to form in the greatest amount? Use drawings and a few words to explain your answer.

\[
\text{protonated at } \text{ because of delocalization} \\
\text{(Also } S^+ \text{ on } N \text{ would not lead to protonation)}
\]

E. Urea can also act as a Bronsted acid. Provide the product(s) for the following reaction. Also, clearly indicate the direction of the reaction equilibrium by providing arrow(s) in the box.

\[
\begin{align*}
\text{Urea} & \quad \text{equilibrium arrows} & \quad \text{H}^+\text{ transfer is shown!}
\end{align*}
\]

No pts for arrows unless products formed

Products formed
IV. (16 points)

A. Using the hybridization model for bonding (with sticks, dashes, wedges and unhybridized p orbitals to show direction of everything), provide a proper three-dimensional representation for the highly reactive molecule X, whose condensed formula is \([C(CH_3)_3]^+\).

\(X\) is a strong Bronsted acid which will react strongly with bases (+B) to form the alkene shown. In your 3-D drawing of \(X\) provide the curved arrows for the one step mechanism which forms this alkene. Show any other products which form in this reaction.

B. The above compound, \(X\), is also a strong Lewis acid which reacts readily with Lewis bases like methylamine, \(CH_3NH_2\). Provide the curved arrow mechanism and the product(s) which would result when compound \(X\) reacts with methylamine to form a Lewis complex.

Compound \(X\) and curved arrow(s) for Lewis complexation reaction
V. (20 points)
Dopa is a natural amino acid found in the seedlings, pods and beans of a broad bean. Dopa’s structure is shown in the first box below. When dopa is given to patients with Parkinson’s disease, it is immediately converted to dopamine by a series of reactions which are catalyzed enzymatically. These reactions include proton transfers and a decarboxylation step, with the use and regeneration of water. In the steps below, this transformation from dopa to dopamine is shown. Provide the curved arrow mechanism for each step of the transformation. Clearly indicate the direction of the equilibrium for the first and last step in the transformation (as specified).

1. [Diagram of dopa structure with labels]
2. [Diagram of dopamine structure with labels]
3. [Diagram of intermediate structure with labels]
4. [Diagram of final dopamine structure with labels]

List the bonds (indicated by letters) in order from longest to shortest in length.

A > E > D > B > C