Question 1
MC101

How many nodes does the antibonding $\sigma^*$ orbital have in the N–H bond in the following molecule?

A : 0 nodes  
B : 1 node  
C : 2 nodes  
D : 3 nodes

the colors blue and green signify changes in phase of the wavefunction, i.e. are equivalent to shading and non-shading
Question 2
MCvsepr2

How many sp, sp² and sp³ CARBONS ATOMS (ignore the oxygens) are there in the estrogen Mestranol (line-angle structure provided)?

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td># of sp</td>
<td>2</td>
<td>3</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td># of sp²</td>
<td>8</td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td># of sp³</td>
<td>11</td>
<td>12</td>
<td>13</td>
<td>14</td>
</tr>
</tbody>
</table>

13 sp³ hybridized CARBONS
6 sp² hybridized CARBONS
2 sp hybridized CARBONS
The three Lewis structures shown below, I, II, and III, are incomplete since some of the atoms should have been assigned a formal charge. How many atoms for these structures IN TOTAL are missing a formal charge (add the number of missing charges in structure I to those in structure II to those in structure III)? All non-bonding pairs of electron are shown.

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>3 atoms total (over all 3 structures) are missing a formal charge</td>
</tr>
<tr>
<td>B</td>
<td>4 atoms total (over all 3 structures) are missing a formal charge</td>
</tr>
<tr>
<td>C</td>
<td>5 atoms total (over all 3 structures) are missing a formal charge</td>
</tr>
<tr>
<td>D</td>
<td>6 atoms total (over all 3 structures) are missing a formal charge</td>
</tr>
</tbody>
</table>

C "sees" 8, "owns" 5 electrons, needs 4 to be neutral  
N "sees" 8, "owns" 4 electrons, needs 5 to be neutral  
O "sees" 8, "owns" 7 electrons, needs 6 to be neutral  
C "sees" only 6 electrons, but still "owns" 4 electrons, needs 4 to be neutral, so there is no formal charge, even though this particular carbon does not obey the normal rules of valence. A carbon with 2 bonds and a pair of non-bonding electrons like this is called a carbene. Carbenes are very reactive for the obvious reason that the carbon has 2 electrons that are not in a bond that want to get into a bond. So, not all atoms without a full octet of electrons must also have a formal charge.  
C "sees" 8, "owns" 5 electrons, needs 4 to be neutral  
C "sees" only 6, "owns" 3 electrons, needs 4 to be neutral
Question 4
MC10za

For the C-H bonds in methane, which best represents a plot of the magnitude of the wavefunction of the localized C-H σ*-anti-bonding molecular orbital along the C-H internuclear axis

(hint, draw a picture of the orbital on the indicated C-H bond and work from there, we did not do an example of this in class, work it out by analogy to similar plots we made for the atomic orbitals)

(the C and H on the horizontal axes provided represent the positions of the C and the H nuclei in the C-H bond)

A

C

H

H

H

H

Ψ

B

C

H

H

H

node on H instead of C

D

C

H

H

H

too many nodes

this is the bonding M.O.

the correct numbers of, and...

the positive maxima

the negative maxima

and the nodes

all in the correct places
Question 5
MC10q

What would you expect to be the order of INCREASING first ionization potential for the following four related 1-carbon structures? All non-bonding electrons and formal charges are included in all structures. The methyl cation, anion and methylene are all very reactive intermediates, methane itself is stable and represents the major component of natural gas.

\[
\begin{array}{cccc}
\text{1 methyl cation} & \text{2 methane} & \text{3 methyl anion} & \text{4 methylene} \\
\end{array}
\]

*first ionization potential refers to the energy required to remove the first electron from a structure, i.e. the highest energy electron*

A) 4 < 2 < 3 < 1  
B) 2 < 4 < 1 < 3  
C) 3 < 4 < 2 < 1  
D) 1 < 3 < 4 < 2

Remember, electrons that are not in bonds are almost always higher in energy, thus 3 and 4 should have higher energy electrons than 1 and 2, and thus lower IPs.

The overall negative charge in 3 raises the energy of the non-bonding electrons due to electron repulsion that is not compensated for by the nuclear charge, 3 thus has the HIGHEST ENERGY electrons, thus the LOWEST IP.

There are no non-bonding electrons in 1 or 2, and in 1 the overall positive charge stabilizes the bonding electrons more than in 2, the electrons in the bond are “held tighter” as a consequence of the overall positive charge. The electrons in 1 are thus LOWEST IN ENERGY, 1 thus has the HIGHEST IP.
Question 6
MC10zb
Which best represents the $\Psi^2$ for the C-C sigma bond in ethane, shown below? (the colors have no absolute meaning, when different colors are used they merely represent changes in phase that could equally well be represented by shading and non-shading)

- $\Psi^2$ should have NO phase information
- $\Psi^2$ are NOT wavefunctions, they only represent probabilities
- Probabilities can be zero or positive, not negative
Question 7
MC10z
Which best describes the $\Psi$ for the $\pi$-bonding molecular orbital in ethylene?
the colors blue and green have no particular significance, except that changes in a picture color mean the same thing as shading and non-shading

The C=C bond consists of a sigma-bond ($\sigma$-bond) and a pi-bond ($\pi$-bond). The $\sigma$-bonding molecular orbital is "built" from in-phase combination of an sp2 hybrid atomic orbital from each carbon atom, this is answer B. If in-phase combination of the atomic orbitals occurs, then out-of-phase combination MUST occur simultaneously to give the anti-bonding M.O., answer D.

The $\pi$-bonding molecular orbital is "built" from in-phase combination of a pure p atomic orbital from each carbon atom. if the atoms are close enough for the sp2 A.O.s to overlap, then they are also close enough for the p A.O.s to overlap (althoigh not as well), the requested p-M.O. is this aswer A. Again, if in-phase combination of the atomic orbitals occurs, then out-of-phase combination MUST occur simultaneously to give the anti-bonding $\pi$-M.O., answer C.

The final picture of the C=C bond is thus in terms of the bonding M.O.s, $\sigma$- and $\pi$-, shown below as wavefunctions squared, i.e. as the probabilities of finding the electrons in space. The 2 electrons in the $\sigma$-M.O. are directly between the 2 C atoms, and are thus lower in energy than the 2 in the $\pi$-M.O., which "float" above and below the two atoms. The $\sigma$-bond is thus stronger than the $\pi$-bond.
Question 8

MCvserpl

How many sp, sp\(^2\) and sp\(^3\) CARBONS ATOMS are there in Viagra? (look at the carbon atoms ONLY, ignore N, S, O etc) (non-bonding electrons not shown for clarity)

![Chemical Structure]

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td># of sp</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td># of sp(^2)</td>
<td>11</td>
<td>10</td>
<td>12</td>
<td>11</td>
</tr>
<tr>
<td># of sp(^3)</td>
<td>10</td>
<td>12</td>
<td>10</td>
<td>11</td>
</tr>
</tbody>
</table>

there are NO sp hybridized CARBONS

\(\circ\) sp\(^3\) hybridized CARBONS
\(\circ\) sp\(^2\) hybridized CARBONS

there are NO sp hybridized CARBONS