INSTRUCTIONS:
PRINT YOUR NAME ———> NAME

WORK all 4 problems

USE THE CORRECT NUMBER OF SIGNIFICANT FIGURES

YOUR SUPPLEMENTAL MATERIALS CONTAIN:

A PERIODIC TABLE
Water MO diagram
C\textsubscript{2v} and D\textsubscript{3h} POINT GROUP CHARACTER TABLEs

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Quiz 4

1 ___ (30)

R = 0.08206 \text{lit-atm/mol-K} 

R = 8.3145 \text{J/mol-K} 

3 ___ (20)

4 ___ (20)

30

\[ R = 8.3145 \text{ J/mol-K} \]

\[ R = 0.08206 \text{ lit-atm/mol-K} \]

\[ c = 2.9979 \times 10^8 \text{ m/s} \]

\[ h = 6.626 \times 10^{-34} \text{ J-s} \]

TOTAL(100) ___
1. Give a short answer or explanation for the following.

(a) Explain why s-p mixing must be considered for early second row diatomics such as B₂ and C₂, but s-p mixing is ignored for late second row diatomics such as O₂ and F₂.

(b) Give at least two reasons how the use of symmetry helps in molecular orbital construction.

The molecular orbital diagram for water is included in the quiz. Refer to it for (c) – (e)

(c) Using the diagram explain why a proton attached to oxygen instead of hydrogen

(d) The 1 b₂ orbital is called a pure non-bonding orbital. Explain what this means.

(e) How does the molecular orbital diagram differ from the valence bond (Lewis structure) description of water.
2. Consider the species, NO⁺, NO (neutral), and NO⁻. (these species have s-p mixing)

(a) Sketch the energy levels of the molecular orbitals (just draw one diagram and populate it with the electrons for neutral NO).

(b) Calculate the bond order of each species.

(c) Rank the species in order of increasing bond length

___________ < __________ < __________

(d) Rank the species in order of increasing bond strength.

___________ < __________ < __________

(e) Which if any of the species is paramagnetic? __________________

(f) Sketch the lowest energy orbital’s shape. Sketch the shape of one of the π* antibonding orbitals.
3. This problem runs over two pages. You will construct the symmetry adapted orbitals for BrF$_3$.

Point group C$_2$v

(a) Construct reducible representations for the group orbitals by applying the symmetry operations.

\[
\begin{array}{ccc}
\text{E} & \text{C}_2(z) & \sigma_v(xz) & \sigma_v(yz) \\
\Gamma = 3 & 1 & 3 & 1 \\
\end{array}
\]

\[
\begin{array}{ccc}
\text{E} & \text{C}_2(z) & \sigma_v(xz) & \sigma_v(yz) \\
\Gamma = 3 & 1 & 3 & 1 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{E} & \text{C}_2(z) & \sigma_v(xz) & \sigma_v(yz) \\
\Gamma = \_\_\_ & \_\_\_ & \_\_\_ & \_\_\_ \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{E} & \text{C}_2(z) & \sigma_v(xz) & \sigma_v(yz) \\
\Gamma = \_\_\_ & \_\_\_ & \_\_\_ & \_\_\_ \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{E} & \text{C}_2(z) & \sigma_v(xz) & \sigma_v(yz) \\
\Gamma = \_\_\_ & \_\_\_ & \_\_\_ & \_\_\_ \\
\end{array}
\]

(continue on next page)
(b) Reduce your representation to a sum of irreducible representations, and identify the central atom orbitals that interacts with the orbital. (I did the first two)

\[ s \text{ or } p \sigma \]

\[ \Gamma = 2 \quad A_1 = s, \text{pz} + B_1 \]

<table>
<thead>
<tr>
<th>Central Atom Orbitals</th>
<th>s, pz</th>
<th>px</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p(\pi\text{-bond(1)}) )</td>
<td>E</td>
<td>C_2(z)</td>
</tr>
</tbody>
</table>

From previous page: \( \Gamma = \text{______} \quad \text{______} \quad \text{______} \quad \text{______} \)

Reduce and identify the central atom orbitals.

\( \#A1 = \)

\( \#A2 = \)

\( \#B1 = \)

\( \#B2 = \)

<table>
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From previous page: \( \Gamma = \text{______} \quad \text{______} \quad \text{______} \quad \text{______} \)

Reduce and identify the central atom orbitals.

\( \#A1 = \)

\( \#A2 = \)

\( \#B1 = \)

\( \#B2 = \)

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<tr>
<td>( p(\pi\text{-bond(1)}) )</td>
<td>E</td>
<td>C_2(z)</td>
</tr>
</tbody>
</table>
3. A ion of $\text{UO}_2\text{F}_5^{5-}$ has pentagonal bipyramidal geometry. The point group of the ion is $D_{5h}$.

(b) The group orbitals for the O atoms (using the s orbitals) are shown below with their symmetries. To the right of the figures indicate which U orbital will interact with the group orbital to form a molecular orbital. Consider the s, p, and d orbitals on U. Sketch the shape of the bonding molecular orbital formed by this interaction.

<table>
<thead>
<tr>
<th>Group Orbital</th>
<th>U Orbital</th>
<th>Bonding Orbital</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1'$</td>
<td>s orbital</td>
<td>Molecular orbital (s)</td>
</tr>
<tr>
<td>$A_2''$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Continues on next page.
(b) The group orbitals for the F atoms (using the s orbitals) are shown below with their symmetries. The ion has been rotated to show the view perpendicular to the xy plane. To the right of the figures indicate which U orbital will interact with the group orbital to form a molecular orbital. Consider the s, p, and d orbitals on U. Sketch the shape of the bonding molecular orbital formed by this interaction.

<table>
<thead>
<tr>
<th>Group Orbital</th>
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<th>Bonding Molecular orbital</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \text{Group Orbital} \quad \text{U Orbital} \quad \text{Bonding Molecular orbital} \]

\[ (b) \quad \text{The group orbitals for the F atoms (using the s orbitals) are shown below with their symmetries. The ion has been rotated to show the view perpendicular to the xy plane. To the right of the figures indicate which U orbital will interact with the group orbital to form a molecular orbital. Consider the s, p, and d orbitals on U. Sketch the shape of the bonding molecular orbital formed by this interaction.} \]
### Character table for $D_{5h}$

<table>
<thead>
<tr>
<th>$C_{2v}$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_v(xz)$</th>
<th>$\sigma_v'(yz)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$z$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

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### Character table for point group $D_{5h}$ (x axis coincident with $C'_2$ axis)

<table>
<thead>
<tr>
<th>$D_{5h}$</th>
<th>$E$</th>
<th>$2C_5$</th>
<th>$2(C_5)^2$</th>
<th>$5C'_2$</th>
<th>$\sigma_h$</th>
<th>$2S_5$</th>
<th>$2(S_5)^3$</th>
<th>$5\sigma_v$</th>
<th>Linear functions, rotations</th>
<th>Quadratic functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A'_{1}$</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-</td>
<td>-</td>
<td>$x^2+y^2, z^2$</td>
</tr>
<tr>
<td>$A'_{2}$</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>$R_z$</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$E'_{1}$</td>
<td>+2</td>
<td>+2cos(2 $\pi$/5)</td>
<td>+2cos(4 $\pi$/5)</td>
<td>0</td>
<td>+2</td>
<td>+2cos(2 $\pi$/5)</td>
<td>+2cos(4 $\pi$/5)</td>
<td>0</td>
<td>(x, y)</td>
<td>-</td>
</tr>
<tr>
<td>$E'_{2}$</td>
<td>+2</td>
<td>+2cos(4 $\pi$/5)</td>
<td>+2cos(2 $\pi$/5)</td>
<td>0</td>
<td>+2</td>
<td>+2cos(4 $\pi$/5)</td>
<td>+2cos(2 $\pi$/5)</td>
<td>0</td>
<td>-</td>
<td>$(x^2-y^2, \text{xy})$</td>
</tr>
<tr>
<td>$A''_{1}$</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$A''_{2}$</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
<td>z</td>
<td>-</td>
</tr>
<tr>
<td>$E''_{1}$</td>
<td>+2</td>
<td>+2cos(2 $\pi$/5)</td>
<td>+2cos(4 $\pi$/5)</td>
<td>0</td>
<td>-2</td>
<td>-2cos(2 $\pi$/5)</td>
<td>-2cos(4 $\pi$/5)</td>
<td>0</td>
<td>$(R_x, R_y)$</td>
<td>(xz, yz)</td>
</tr>
<tr>
<td>$E''_{2}$</td>
<td>+2</td>
<td>+2cos(4 $\pi$/5)</td>
<td>+2cos(2 $\pi$/5)</td>
<td>0</td>
<td>-2</td>
<td>-2cos(4 $\pi$/5)</td>
<td>-2cos(2 $\pi$/5)</td>
<td>0</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
3. This problem runs over two pages. You will construct the symmetry adapted $\sigma$ group orbitals for BrF$_5$. Point group $C_{4v}$

(a) Construct reducible representations for the group orbitals by applying the symmetry operations. Hint: they are all odd numbers.

$$\Gamma = \begin{array}{cccc}
E & 2 C_4(z) & C_2(z) & 2 \sigma_v(xz) & 2\sigma_d(bisectror of xz and yz) \\
\end{array}$$

*When you finish bring it to me to grade so you can do the next part.*
Reproduce your representation here and reduce it.

\[ \Gamma = E \quad 2 \text{C}_4(z) \quad C_2(z) \quad 2 \sigma_v(xz) \quad 2\sigma_d(\text{bisector of } xz/yz) \]

Reduce and identify the central atom orbitals.

\#A1 = 

\#A2 = 

\#B1 = 

\#B2 = 

\#E =

(s-bond(1)) \quad \Gamma = _____ + _____ + _____ + _____ + _____

Not all blanks may be needed for central atom orbitals (Use s, p, and d)
4. The following involves drawing the pi molecular orbitals for a square planar complex such as XeF$_4$. The group orbital symmetry is as shown. Identify the central atom orbital that interacts, and draw the bonding combination for each set.