I. Consider a 5-coordinate compound formed when an octahedral $AB_6$ molecule loses a B ligand but does not rearrange.

A. To what point group does this compound belong?

C$_{4v}$

B. What symmetry elements are present?
C$_4$ axis (a), $C_2$ axis (2), 2 vertical planes (x-z and y-z planes),
2 vertical planes (between the other vertical planes — bisecting the dihedral angles)

C. What symmetry operations are present?

E, $C_4$, $C_4^2$, $C_2$, $2V$, $2T_d$

D. What is the order of the group? Why?

$|G| = \text{order} = 8 = \text{number of symmetry operations}$

E. How many irreducible representations are there in this group? Why?

5 irreducible representations = number of symmetry classes

F. What are the dimensions of the irreducible representations?

$1, 1, 1, 1, 2$

$1^2 + 1^2 + 1^2 + 1^2 + 2^2 = 8 = n$

G. How do the $d_{xy}$ and $d_{x^2-y^2}$ orbitals transform under this symmetry? Show the full irreducible representations and name the representations. (To avoid confusion, indicate the position of any vertical planes relative to the x,y axes shown on the diagram above.)
II. The rhenium nonahydrde anion, \([\text{ReH}_9]^2^-\), is a tricapped trigonal prism, with three of the hydrides centered over the three rectangular faces of a trigonal prism. The ion therefore has \(D_{3h}\) symmetry.

A. Draw the \([\text{ReH}_9]^2^-\) ion and put a coordinate system on the central atom.

B. The three hydride ligands over the rectangular faces are, by symmetry, different than the other six hydride ligands. Using the \(D_{3h}\) character table, determine which of the \(s\), \(p\), and \(d\) orbitals on the central rhenium atom can sigma bond with the six outer hydrides and the three equatorial hydrides. Show all work.

C. Specifically indicate which of the rhenium orbitals, if any, can only interact with the six "outer" hydrides. \(p_z \text{ and } (d_{x^2-y^2}, d_{xy})\)

D. Indicate which of the rhenium orbitals, if any, can only interact with the three equatorial hydrides. None

E. Indicate which of the rhenium orbitals, if any, can interact with all nine of the hydrides. \(s, d_{z^2}, (p_x, p_y), (d_{x^2-y^2}, d_{xy})\)

\[\begin{array}{c|cccccc|cc}
D_{3h} & E & 2C_3 & 3C_2 & 2S_3 & 3\sigma_d & \Gamma_{\text{outer}} \\
\hline
A_1' & 1 & 1 & 1 & 1 & 1 & 1 & \Gamma_{\text{outer}} \\
A_2' & 1 & 1 & -1 & 1 & -1 & 1 & \Gamma_{\text{outer}} \\
E' & 2 & -1 & 0 & 2 & -1 & 0 & \Gamma_{\text{outer}} \\
A_1'' & 1 & 1 & 1 & -1 & -1 & 1 & \Gamma_{\text{outer}} \\
A_2'' & 1 & 1 & -1 & -1 & -1 & 1 & \Gamma_{\text{outer}} \\
E'' & 2 & -1 & 0 & -2 & 1 & 0 & \Gamma_{\text{outer}} \\
\end{array}\]

\[\Gamma_{\text{outer}} = 6, 0, 0, 0, 0, 2\]

\[\Gamma_{\text{eq}} = 3, 0, 1, 3, 0, 1\]

For \(\Gamma_{\text{outer}}\):

\[\begin{align*}
\Gamma_{\text{outer}} &= \frac{1}{12} \left( 6 + 0 + 0 + 0 + 0 + 6 \right) = 1 \\
E' &= \frac{1}{12} \left( 12 + 0 + 0 + 0 + 0 + 0 \right) = 1 \\
A_2'' &= \frac{1}{12} \left( 6 + 0 + 0 + 0 + 0 + 6 \right) = 1 \\
E'' &= \frac{1}{12} \left( 12 + 0 + 0 + 0 + 0 + 0 \right) = 1 \\
A_1' &= \frac{1}{12} \left( 3 + 0 + 3 + 3 + 0 + 3 \right) = 1 \\
E' &= \frac{1}{12} \left( 6 + 0 + 0 + 6 + 0 + 0 \right) = 1
\end{align*}\]

For \(\Gamma_{\text{eq}}\):

\[\begin{align*}
\Gamma_{\text{eq}} &= \frac{1}{12} \left( (p_x)^2 \right) = \frac{1}{12} \left( d_{x^2} \right) = \frac{1}{12} \left( d_{x^2-y^2} \right) = \frac{1}{12} \left( d_{xy} \right)
\end{align*}\]