I. Derive an approximate molecular orbital energy level diagram for the aluminum hydride ion, AlH₄⁻, with

1. tetrahedral geometry
2. square planar geometry
3. Based on your MO diagrams, which geometry would be favored? Why?
4. Would the photoelectron spectrum for this ion be able to differentiate between the two possible geometries? Why or why not?

\[
\begin{array}{c|cccc}
\text{Td} & E & 3\gamma & 3\zeta & 6\sigma_v \\
\hline
4 & 1 & 0 & 0 & 2
\end{array}
\quad
\begin{array}{c|cccc}
\text{D}_{4h} & E & 2\gamma & 2\zeta & 2\sigma_v \\
\hline
4 & 0 & 0 & 2 & 0
\end{array}
\]

\[
t_{2g} = A_1 + T_2
\]

\[
t_2(\pi, \pi, \pi) \equiv \pi^*_{a_1}
\]

\[
\pi_s \equiv \pi_{a_1}
\]

\[
t_{2g} = e_u
\]

\[
\psi_{e_u} \equiv e_u
\]

\[
\psi_{a_2g} \rightarrow \psi_{a_2g}
\]

\[
\psi_{a_{1g}} \rightarrow \psi_{a_{1g}}
\]

\[
\frac{1}{2} \psi_{a_{1g}} - \frac{1}{2} \psi_{a_{1g}}
\]

\[
\psi_{e_u} \rightarrow \psi_{e_u}
\]

\[
\psi_{a_{1g}} \rightarrow \psi_{a_{1g}}
\]

\[
\psi_{A_1} \rightarrow \psi_{A_1}
\]

\[
\psi_{T_2} \rightarrow \psi_{T_2}
\]

3. Td would be favored — only 5 bonding orbitals occupied.

4. Photoelectron spectrum for Td — 2 peaks, both with vibrational fine structure.

5. For D₄h — 3 peaks; lowest energy sharp peak (for non-bonding orbital) and 2 peaks with vibrational fine structure.
II. Consider the out-of-plane $\pi$-system for the planar molecule (NH$_2$)$_2$BH, I, where each boron atom and each nitrogen atom contribute an out-of-plane $p$ orbital.

1. Show the relative signs of the $p$-orbitals for each of the $\pi$ molecular orbitals in compound I.
2. Identify HOMO and LUMO.
3. Using the first approximation approach, take linear combinations of the $\pi$-molecular orbitals you derived for compound I to produce the $\pi$-molecular orbitals on compound II. (Only show the relative signs of the $p$-orbitals and the positions of the nodes. It is not necessary to assign symmetry names to the orbitals.)
4. Would the dianion of compound II have a longer or shorter boron-boron bond than neutral compound II? Why?

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**Diagram Notes:**
- Shading for HOMO and LUMO
- Energy levels indicated
- Electron configurations labeled

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**Additional Notes:**
- The dianion would have a weaker B-B bond since it has more B-B bonding interaction.