KEY
CHE 450G Practical Inorganic Chemistry
Problem Set 3 (HW3) F. Bramwell
October 29, 2007

(2c) 1) How many sigma-bonding orbitals will there be in cyclopropane? How many sigma antibonding orbitals? How many pi-binding orbitals? How many pi-antibonding orbitals? How many lone pairs? Make a diagram showing the relative energies of these orbitals.

7,7,1,1,0. Energy: sigma<pi<pi*<sigma*

(4c) 2) Propose a molecular orbital scheme for the vinyl cation with the geometry below.
   a. Draw the basis atomic orbitals and determine how they transform.
   b. Construct appropriate linear combinations of the basis orbitals to make reasonable molecular orbitals
   c. Order the mo’s by increasing energy as best you can
   d. Place the proper number of electrons in the diagram
Using the coordinate system below, derive the symmetries of the four bridging B
hybrid orbitals and two bridging H (1s) orbitals of diborane (B₂H₆). Construct six
bridging molecular orbitals of diborane and label each with the correct symmetry.
Indicate which are bonding, nonbonding, and antibonding. Which will be
occupied in diborane?

\[
\begin{array}{c|cccc|c}
E & C_2 (z) & C_2 (y) & C_2 (x) & i & x^2 + y^2 + z^2 + xy + xz + yz \\
4 & 0 & 0 & 0 & 0 & a_g + b_{3u} + b_{1u} + b_{1u} \\
2 & 2 & 0 & 0 & 0 & a_2 + 2 \\
& & & & & = a_g + b_{1u}
\end{array}
\]

\[
\begin{array}{cccc}
\sigma_g & \sigma_u \\
ag & b_{1u} \\
b_{3u} & b_{2g} \\
ag & b_{1u} \\
\text{bonding} & \text{non bonding} & \text{antibonding} \\
ag, b_{1u}, b_{3u} & \text{occupied}
\end{array}
\]