Use the HMO theory web site (http://www.chem.ucalgary.ca/SHMO/) to respond to the following problems.

1. Determine whether it should be easier to reduce 1,3,5-hexatriene or 1,3,5,7-octatetraene.

2. Determine the eigenfunctions and eigenvalues for benzene. Show how they are in accord with the pairing theorem for both functions (viz., the MO’s) and energies.

3. Determine what happens to the energy of the LUMO of ethylene when
   [a] in place of a terminal hydrogen, one substitutes an oxygen (e.g., the oxygen of an ether);
   [b] in place of a terminal hydrogen, one substitutes a carbonyl (e.g., CHO)

NOTE: In the first case, choose the $h_x$ value corresponding to O2 when you add the oxygen; in the second instance, choose the $h_x$ value for O1.

4. The rate of many Diels-Alder reactions can be correlated with the energy gap between the diene HOMO and the dienophile LUMO (the smaller the gap, the faster the reaction). Assuming that 1,3-butadiene is the diene,
   [a] determine that energy gap for the three cases outlined in the previous problem,
   [b] the smallest gap
   [c] the fastest of the three reactions.

5. Imagine treating bromocyclopropene with tributyltin hydride and AIBN in refluxing benzene.
   [a] What are the products of the transformation?
   [b] Determine the unpaired spin density at C$_b$ in the SOMO of the C$_3$H$_3$ adduct.
   [b] Determine the hyperfine coupling constant between the odd electron and C$_a$.
   Assume that Q = 23 Gauss.
   [c] Determine the multiplicity of the observed coupling.

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\begin{align*}
\text{Br} & \quad + \quad (\text{n-Bu}_3\text{Sn})\text{H} & \quad + \quad \text{AIBN}
\end{align*}
\]