# 1 Cognitive reasoning in the chemical sciences 5.4

1. **Constructing MO diagrams:**

   (a) *Use the techniques presented in class to derive the MO diagrams for the following molecules.*

      i. CrH, assume that the only Cr valence orbitals are its $3d$ orbitals. Place the Cr-H bond along the z direction.

      ii. CrH, assume that the only Cr valence orbitals are its $4s$ and $3d$ orbitals. Place the Cr-H bond along the z direction.

      iii. Cr_2, assume that the only Cr valence orbitals are its $3d$ orbitals. Place the Cr-Cr bond along the z direction.

   (b) Based on the above MO diagrams, draw Lewis structures for each molecule.

   (c) Based on the above MO diagrams, calculate the greatest number of energies of photons which each of these MO diagrams can receive, without the emission of any electron.

   (d) Based on these diagrams, calculate the total number of peaks in the PES.

2. **Connecting MO diagrams to graphs**

   (a) In the graph below. please give a qualitative plot of the all three MO energies of the H_3 molecule as a function of r.
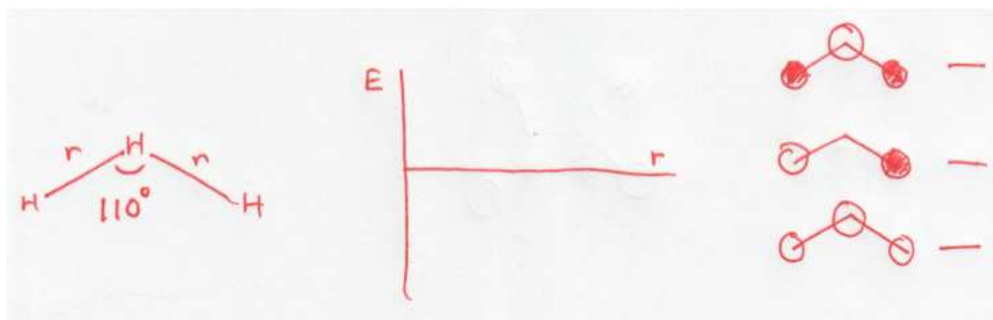
   (b) In the graph below. please give a qualitative plot of the given ethylene MO's energy as a function of both d and l.
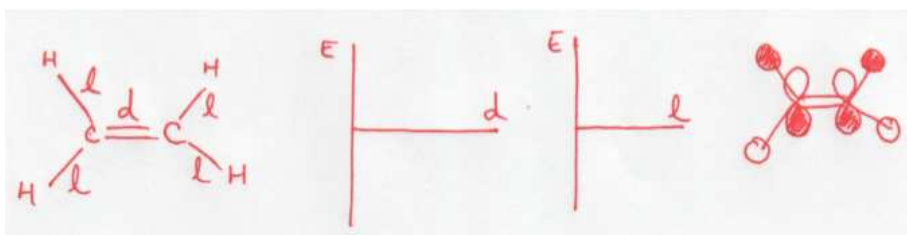
   (c) Plot as a graph the energies of the unhybridized OH MO diagram as a function of O-H bond distance, r. Plot the total bonding energy of the OH molecule for the molecule as a whole using the same energy scale used to display the other orbital energies.