Practice Test Questions 2
Molecular Orbital Theory: Homonuclear Diatomic Molecules

1. Draw the potential energy curve for a diatomic molecule. Clearly label the bond dissociation energy and equilibrium bond length on your drawing.

2. Two 3*d* orbitals can overlap in either a σ fashion or in a π fashion.

(a) Show how two 3*d* orbitals can have σ overlap. Draw the resulting molecular orbitals.

(b) Show how two 3*d* orbitals can have π overlap. Draw the resulting molecular orbitals.

3. For a molecule of diatomic boron (B_2), we define the bond as lying along the *z* axis.

(a) Which valence atomic orbitals combine to form σ MOs in B_2? *Be specific.*

(b) Which valence atomic orbitals combine to form π MOs in B_2? *Be specific.*

(c) Draw a valence molecular orbital energy level diagram for B_2. *Label all orbitals.*

(d) Write the valence orbital occupancy for B_2.

(e) Is B_2 diamagnetic or paramagnetic? What does this mean?

(f) What is the net σ bond order for B_2?

(g) What is the net π bond order for B_2?

(h) What is the overall bond order for B_2?

4. The bond dissociation enthalpies for N_2 and N_2^- are 945 kJ/mol and 765 kJ/mol respectively. There is only a small difference between the values for bond dissociation enthalpy and bond dissociation energy.

Using an argument based on molecular orbital theory, explain why N_2^- has a smaller bond dissociation energy than N_2.

5.

(a) Draw Lewis diagrams for N_2^+ and N_2^-. What bond orders would you predict from the Lewis diagrams?

(b) Determine the bond orders for these two ions using molecular orbital theory. Do they agree with the values obtained for your Lewis diagrams?

6. When drawing Lewis diagrams, we ignore the core electrons and focus only on the valence electrons. Discuss how molecular orbital theory provides support for this practice.

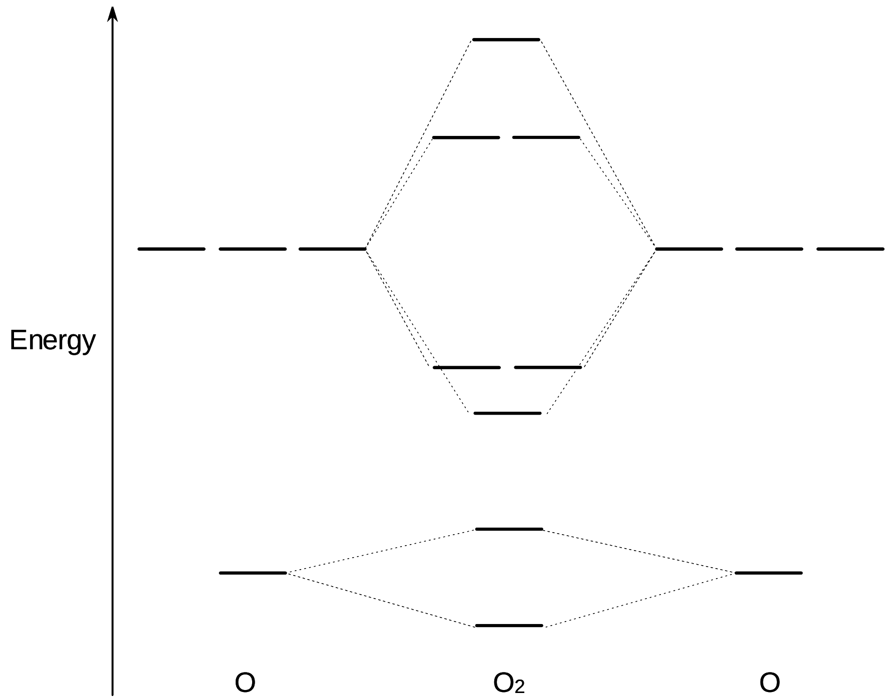
7. Use molecular orbital theory to describe the bonding in diatomic oxygen (O_2).

(a) Complete the valence molecular orbital energy level diagram below by:

i. drawing ***and*** naming the atomic orbitals,

ii. drawing ***and*** naming the molecular orbitals, and

iii. adding electrons to the atomic ***and*** molecular orbitals



(b) Write the valence orbital occupancy (i.e. electron configuration) for O_2

(c) Draw a Lewis diagram for O_2.

(d) What property of oxygen is clearly shown by the molecular orbital energy level diagram but not by the Lewis diagram?

(e) When O_2 reacts with sodium metal, the peroxide anion is generated (O_2^{2-}):

$$2Na(s) + O_2(g) \rightarrow Na_2O_2(s)$$

Draw a Lewis diagram for the peroxide anion (O_2^{2-}) and use your MO diagram to help you describe what is happening in the above reaction. Make sure you rationalize the main difference(s) between your Lewis diagram for O_2 and your Lewis diagram for O_2^{2-}.

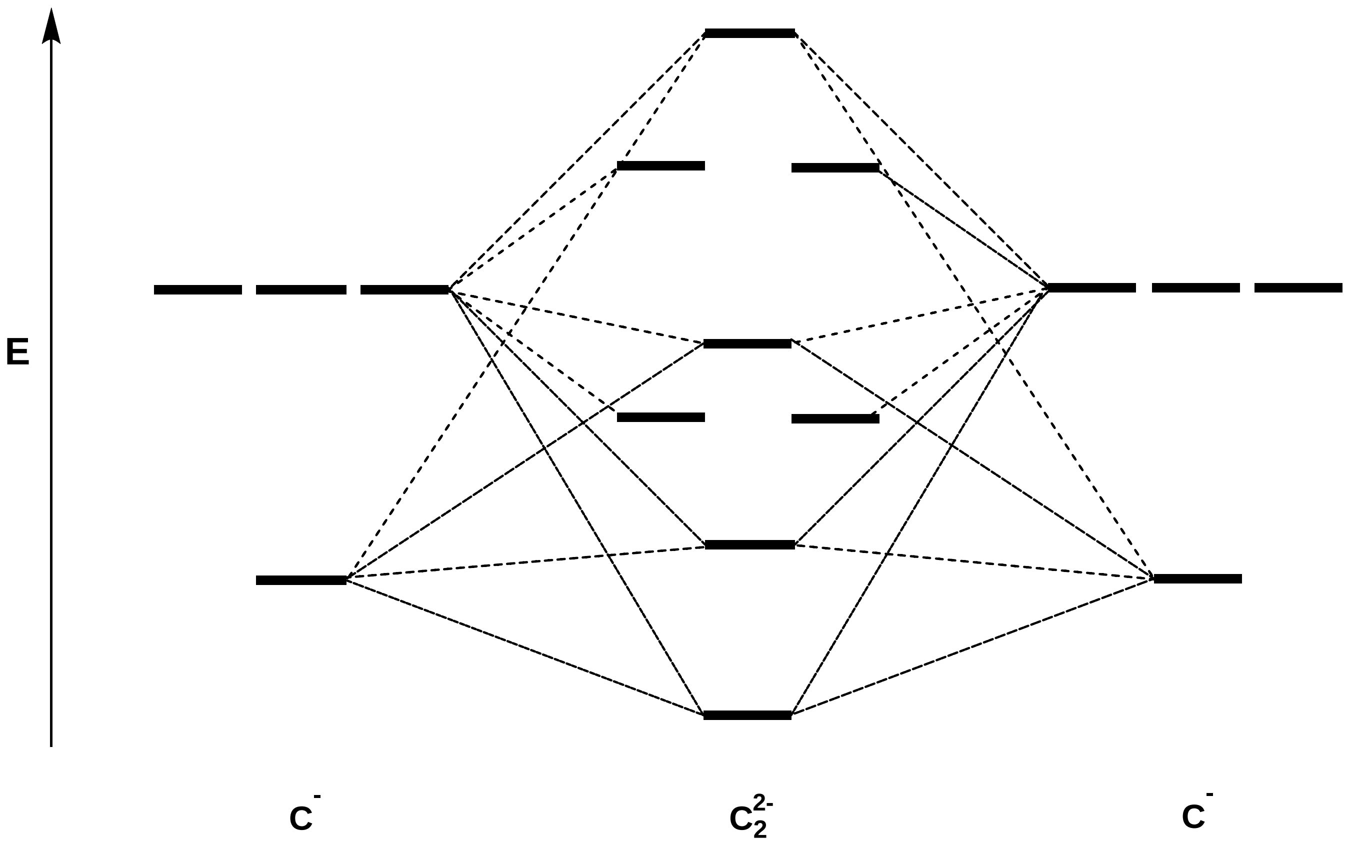
8. Calcium carbide, CaC_2, is a reactive salt used in a number of industrial processes including the production of acetylene. Use molecular orbital theory to describe the bonding of the carbide anion (C_2^{2-}).

(a) Complete the valence molecular orbital energy level diagram below by:

i. drawing ***<u>and</u>*** naming the atomic orbitals,

ii. drawing ***<u>and</u>*** naming the molecular orbitals, and

iii. populating the atomic and molecular orbitals with electrons



(b) Write the valence orbital occupancy (i.e. electron configuration) for C_2^{2-}.

(c) Would you expect the carbide anion to have a larger or smaller bond dissociation energy than C_2? Justify your answer.

(d) Give formulas for two neutral diatomic molecules that are isoelectronic with C_2^{2-}.