

MOLECULAR ORBITALS PROBLEM SET

1. (a) Write the ground state molecular orbital configurations for:
(1) N_2^+ (2) N_2^{2+} (3) N_2 (4) N_2^- (5) N_2^{2-}
(b) Deduce the bond order for each case
(c) Arrange in order of decreasing bond length (*longest* bond **first**)
(d) Arrange in order of decreasing bond energy (*strongest* bond **first**)
(e) In each case, say if the species is paramagnetic or diamagnetic. Explain.

2. Using the Molecular Orbital Theory, show the electronic configurations of the species (1) to (9) and match each with one of the statements (a) to (i).

| | |
|-------------|---|
| (1) F_2^- | (a) bond order = 2.5 |
| (2) Be_2 | (b) two unpaired antibonding electrons |
| (3) H_2 | (c) largest bond energy |
| (4) BN | (d) two π bonds and non-polar |
| (5) C_2 | (e) two π bonds and slightly polar |
| (6) O_2^+ | (f) unstable in its ground state |
| (7) NF | (g) two paired bonding electrons |
| (8) OF^- | (h) bond order = 0.5 |
| (9) CO | (i) no. of electrons in π_p orbitals = no. of electrons in π^*_p orbitals |

3. Complete the following by filling in the blanks.
(a) A triple bond consists of ___ σ and ___ π bonds.
(b) Ethylene (ethene) has a total of ___ σ and ___ π bonds.
(c) In ethylene, the hybridization on each carbon is ____ .
(d) In benzene, there are ___ electrons in π bonds.

4. What kind of intermolecular forces are present in the following compounds?
(a) CCl_4 (b) CH_2Cl_2 (c) CH_3OH (d) CO_2 (e) SCl_4 (f) SCl_6