

Answer on the question #68067, Chemistry / Physical Chemistry

Question:

b) Write molecular orbital configuration for the following molecular ions. Comment on the paramagnetic properties of these ions:

(i) N_2^+

(ii) N_2^{2-}

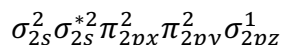
Answer:

Writing the molecular orbital configuration, one should consider only valence electron shell, and core electrons are screened and strongly attached to the nucleus. For the atoms up to nitrogen, the following order of orbitals must be respected:

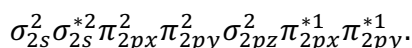
$$\sigma_{2s} < \sigma_{2s}^* < \pi_{2px}, \pi_{2py} < \sigma_{2pz} < \pi_{2px}^*, \pi_{2py}^* < \sigma_{2pz}^* .$$

Then, one should count the valence electrons and fill molecular orbitals:

$$N_2^+: 5+5-1 = 9$$



$$N_2^{2-}: 5+5+2 = 12$$



In regard of the availability of unpaired electrons, our ions can be expected to be para- or diamagnetic, i.e. with or without unpaired electrons, respectively. Thus, N_2^+ ion and N_2^{2-} ion are paramagnetic, as there is one unpaired electron on antibonding sigma orbital of the former and two unpaired electrons on the anti-bonding π orbitals of the latter.