Quantum Chemistry
Exercises 11

1. Predict the relative stability of the species N_2^+, N_2, and N_2^-.

2. Determine the ground-state electron configurations of NO^+ and NO. Compare the bond order of these two species.

3. Determine the bond order in a cyanide ion.

4. Determine the ground-state molecular term symbols of O_2 and O_2^+.

5. The highest occupied molecular orbitals for an excited electronic configuration of the oxygen molecule are

$$[1\pi_\gamma]^1[3\sigma_\upsilon]^1$$

What are the molecular term symbols for oxygen with this electronic configuration?

6. In class I derived the expressions for the three sp^2 orbitals of carbon:

$$\xi_1 = \frac{1}{\sqrt{3}}2s + \sqrt{\frac{2}{3}}2p_z$$

$$\xi_2 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_z + \frac{1}{\sqrt{2}}2p_x$$

$$\xi_3 = \frac{1}{\sqrt{3}}2s - \frac{1}{\sqrt{6}}2p_z - \frac{1}{\sqrt{2}}2p_x$$

Using the angular parts of the *p* orbitals (*i.e.*, the spherical harmonics), show that ξ_1 and ξ_2 are directed 120° from each other.