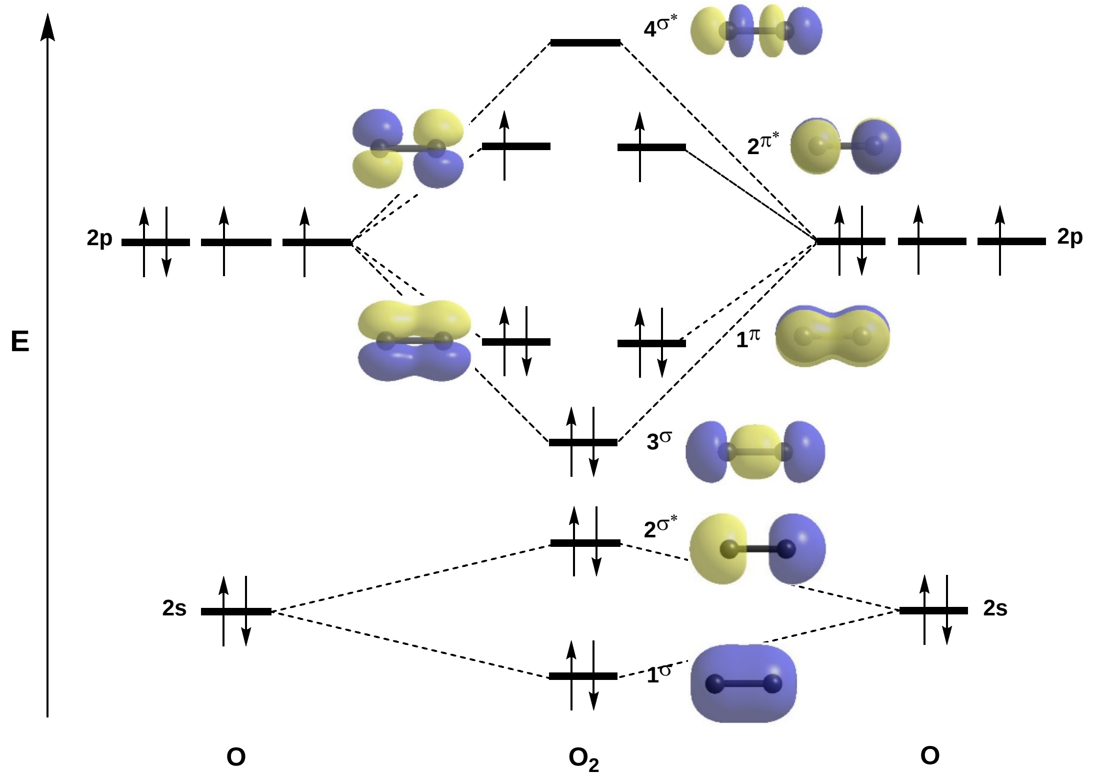
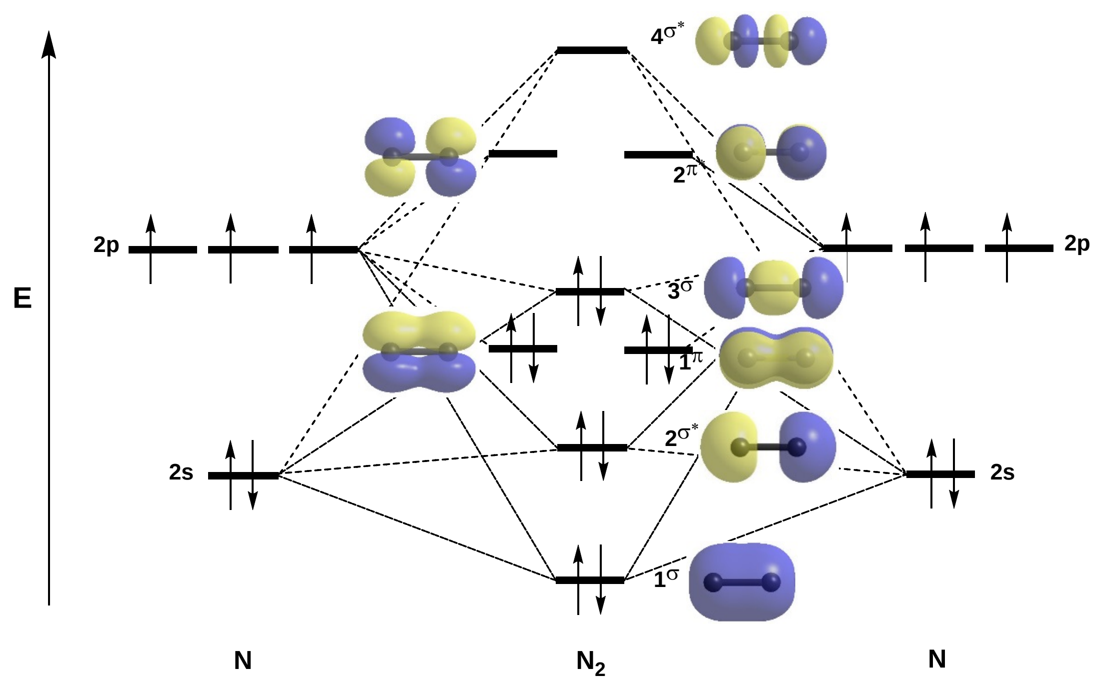
Answers to Exercise 2.4
Molecular Orbital Energy Level Diagrams: Homonuclear Diatomics

1.





…and that's why the pictures weren't on the diagrams in the explanation! Too cluttered!

2.

(a) $(1\sigma)^2(2\sigma^*)^2(3\sigma)^2(1\pi)^4(2\pi^*)^2$

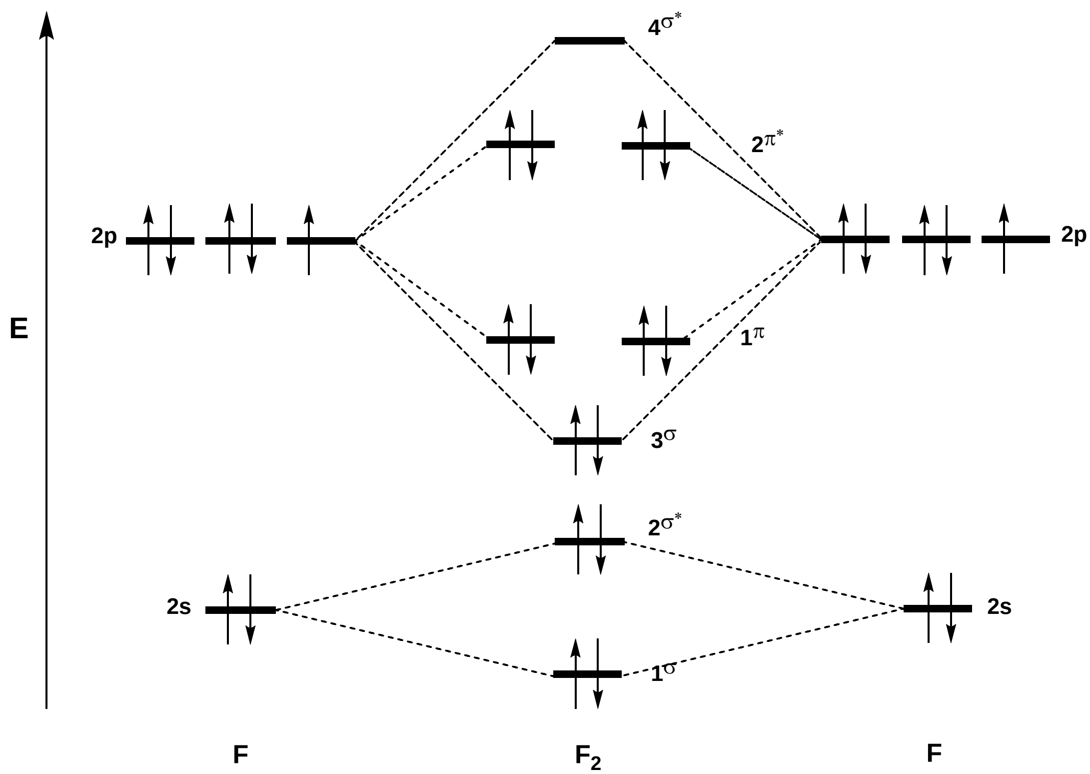
(b) $(1\sigma)^2(2\sigma^*)^2(1\pi)^4(3\sigma)^2$

These valence orbital occupancies do not include the core electrons. Both O_2 and N_2 have an additional four core electrons.

*Make sure you list the orbitals from lowest energy to highest energy, and that the number of electrons in each is written as a superscript. It is essential to include the * for antibonding orbitals and/or the $_{nb}$ for nonbonding orbitals. If you don't, people can't use your orbital occupancy to deduce bond order.*

3.

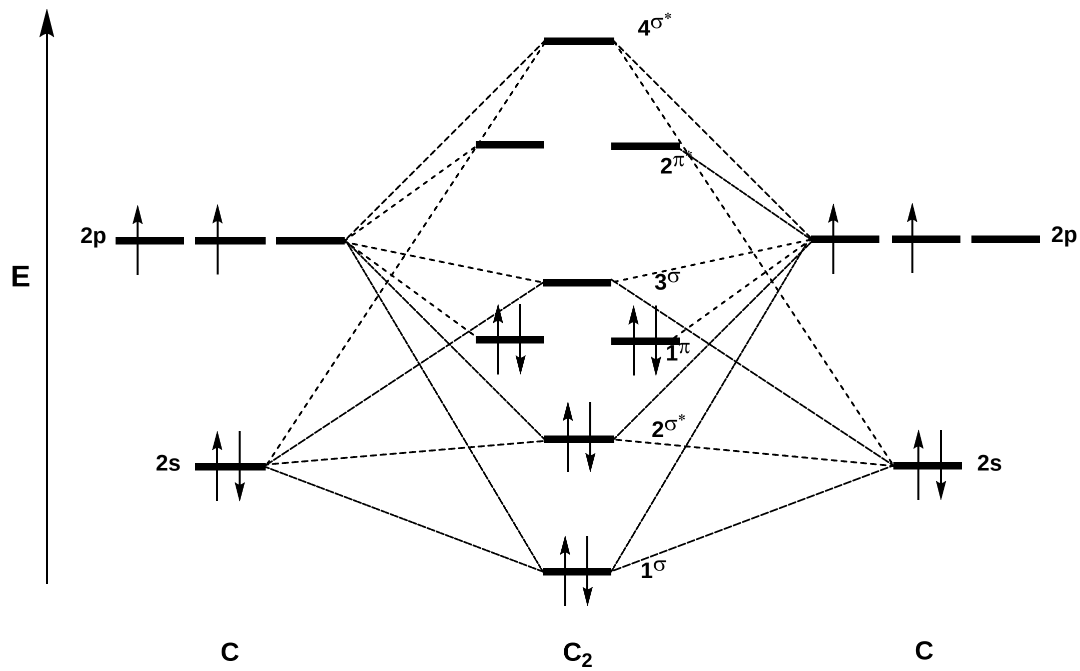
(a) The electron configuration for F is $1s^2 2s^2 2p^5$, so each F has 7 valence electrons and F_2 has 14 valence electrons.



(b) If two electrons are added, they go into $4\sigma^*$ which is an antibonding orbital. This decreases the F-F bond order from 1 to 0. As such, when two electrons are added to F_2, the F-F bond breaks and two F^- anions are formed.

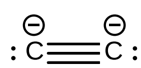
4.

(a) The electron configuration for C is $1s^2 2s^2 2p^2$, so each C has 4 valence electrons and C_2 has 8 valence electrons.



(b) If two electrons are added, they go into 3σ which is a bonding orbital. This increases the C-C bond order from 2 to 3.

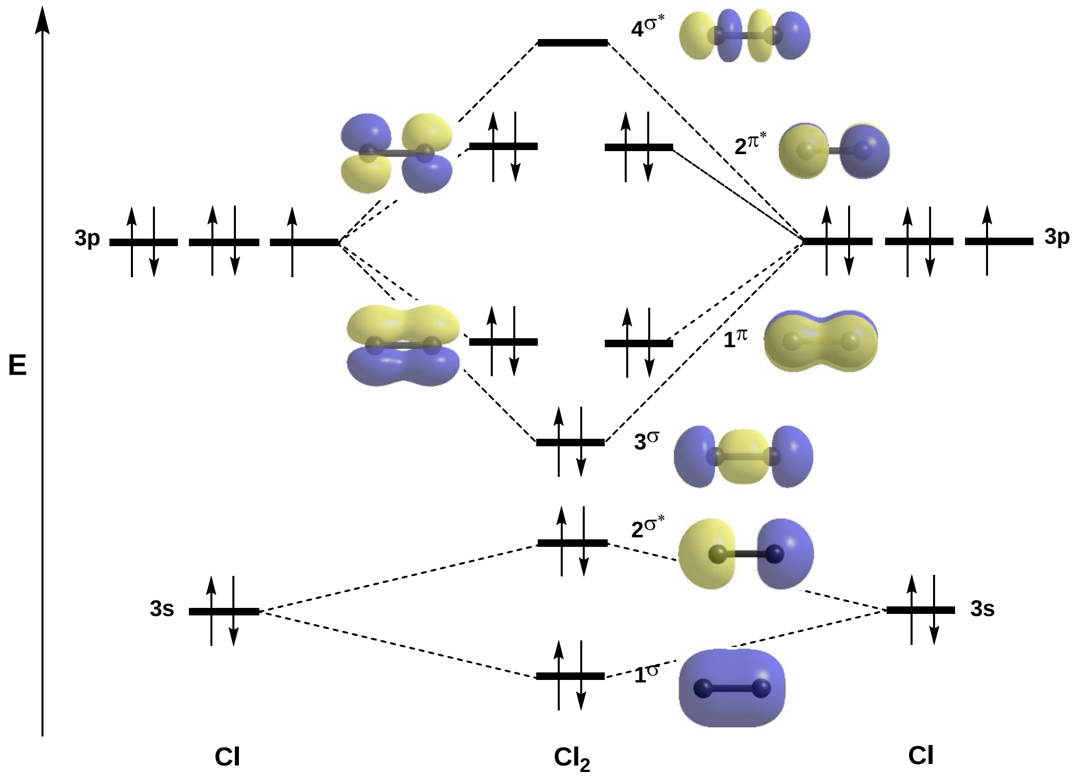
If you drew a Lewis diagram of the C_2^{2-} anion, you would get:



This is consistent with what is the molecular orbital energy level diagram tells us.

Some chemists would argue that the orbitals we have labeled $2\sigma^*$ and 3σ are actually both nonbonding in C_2. That would increase the bond order of C_2 to 3, though the bond order of C_2^{2-} would remain 3. What sort of experiment could you do to measure the bond order of C_2 in order to see who is right (or if the true picture is somewhere between those two extremes)?

5. The electron configuration for Cl is $1s^2 2s^2 2p^6 3s^2 3p^5$, so each Cl has 7 valence electrons and Cl_2 has 14 valence electrons.



This diagram is almost identical to the molecular orbital energy level diagram for F_2. This is to be expected given that fluorine and chlorine are both halogens (both Group 17 elements) and have the same number of valence electrons.

The main difference is that the valence atomic orbitals in the chlorine atoms are in the $n = 3$ shell rather than the $n = 2$ shell. The exact energies of the orbitals will also be different, but we'd need a computer to calculate those for us anyway. There are, of course, more core electrons in Cl_2 but we don't show core electrons on a valence molecular orbital energy level diagram.