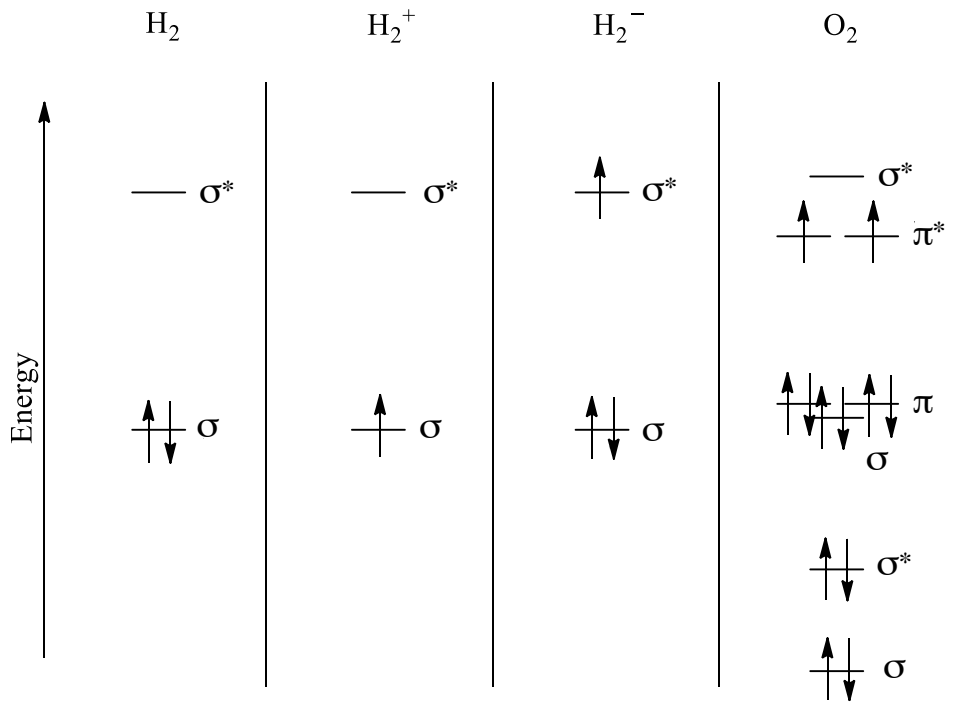
Marks 6

- The molecular orbital energy level diagrams for H_2, H_2^+, H_2^- and O_2 are shown below. Fill in the valence electrons for each species in its ground state and label the types of orbitals (σ, σ*, π, π*).



Give the bond order of each species.

H_2: **½ (2 - 0) = 1**	H_2^+: **½ (1 - 0) = ½**	H_2^-: **½ (2 - 1) = ½**	O_2: **½ (8 - 4) = 2**

Which of the four species are paramagnetic?

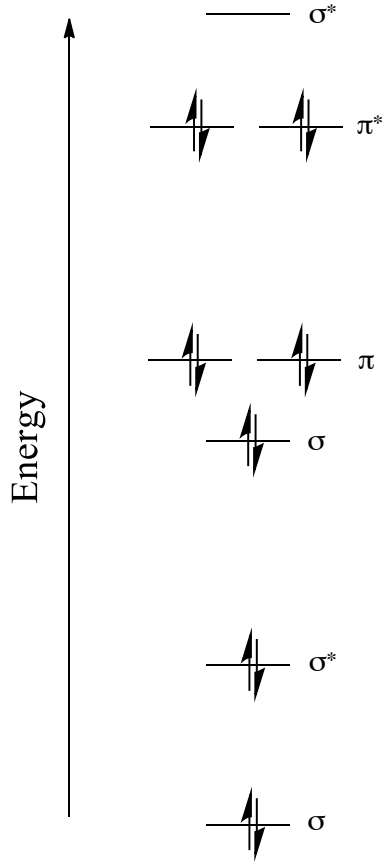
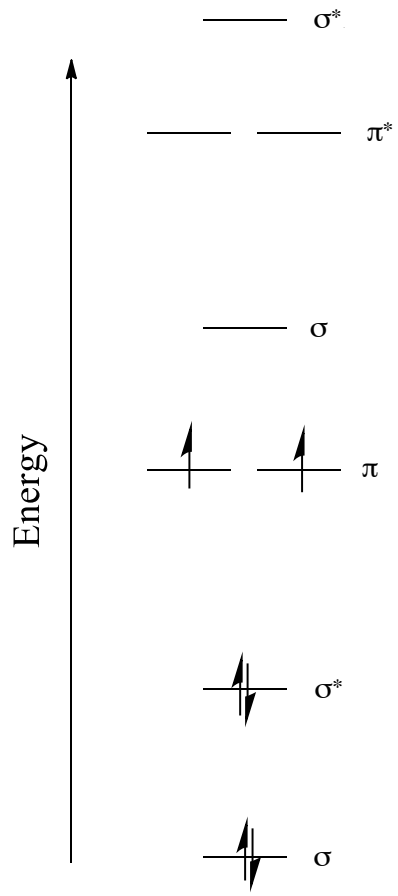
H_2^+, H_2^- and O_2

The bond lengths of H_2^+ and H_2^- are different. Which do you expect to be longer? Explain your answer.

H_2^- will be longer. Both have bond order of 0.5, but H_2^- is a multi-electron system so is destabilised by electron-electron repulsion. H_2^+ is single electron system so has no electron-electron repulsion.

Marks 3

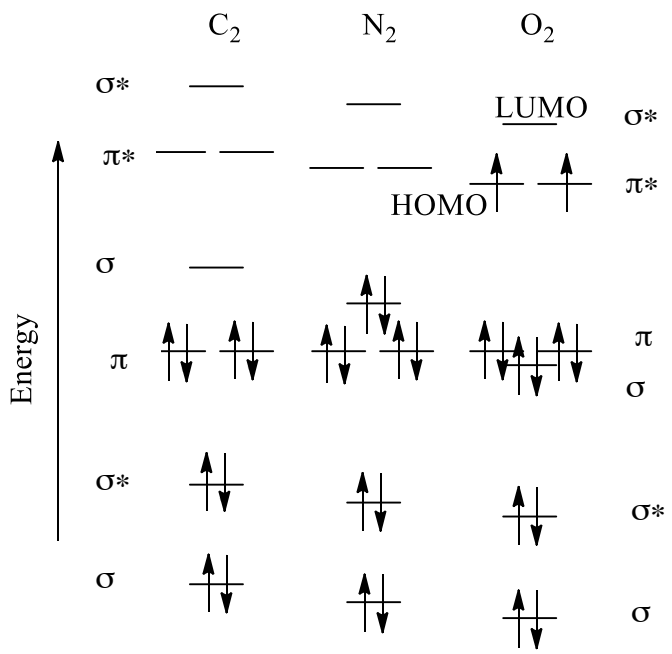
- The molecular orbital energy level diagrams for F_2 and B_2 are shown below. Fill in the valence electrons for each species in its ground state. Hence calculate the bond order for F_2 and B_2 and indicate whether these molecules are paramagnetic or diamagnetic.

	F_2	B_2
		
Bond order	**½ (8 – 6) = 1**	**½ (4 – 2) = 1**
Paramagnetic or diamagnetic	**diamagnetic**	**paramagnetic**

Marks 6

- The following diagram shows the molecular orbital energy level diagrams for the valence electrons in the homonuclear diatomic molecules C_2, N_2 and O_2.

  Complete the diagram by filling in the remaining *valence* electrons for each molecule and determining its bond order.



Bond order:	**2**	**3**	**2**

Explain why the energy of the lowest energy σ orbital shown above gets lower from left to right across the periodic table.

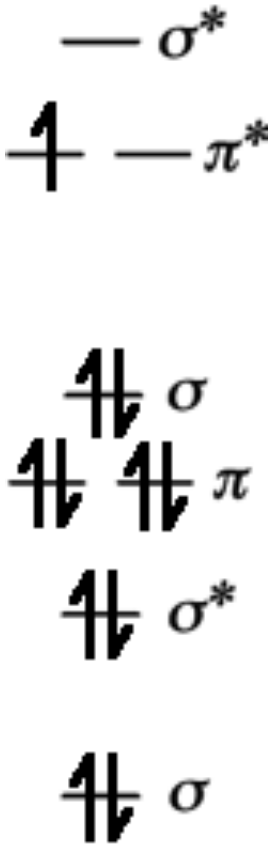
The atomic number of the elements increase moving across a period, reflecting an increase in the number of protons. This results in an increasing effective nuclear charge which pulls the electrons closer to the nucleus and lowers the energy of their orbitals.

Clearly label the HOMO and LUMO of O_2 on the diagram above.

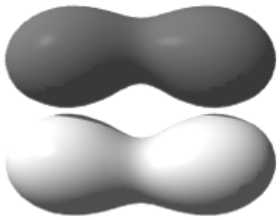
f) The NO molecule formed in the reaction in part d) is also formed in its ground electronic state. Complete the molecular orbital diagram for NO by filling in the valence electrons in the occupied orbitals. Sketch the shape of the π and π* orbitals, clearly showing all nodes. Determine the bond order of NO and whether it is paramagnetic or diamagnetic.

Marks 6

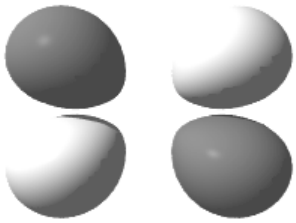
MO orbital energy level diagram for NO



Sketch of the π MO



Sketch of the π* MO



Bond order of NO: **½ (8 – 3) = 2.5**

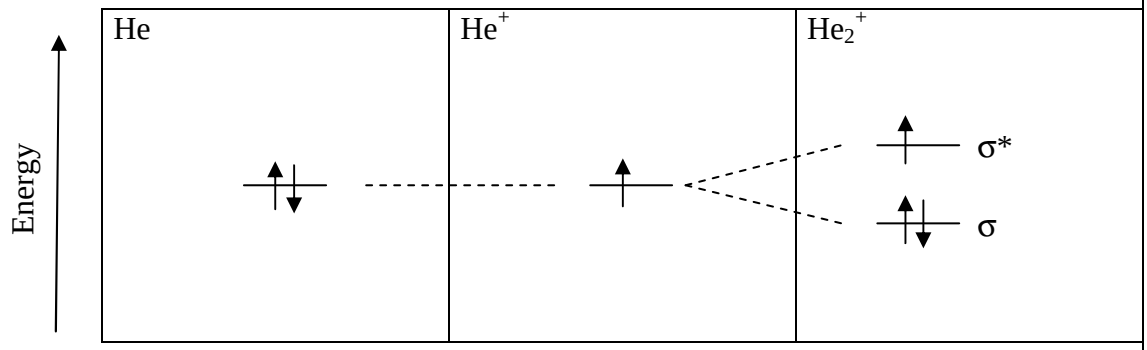
Paramagnetic or diamagnetic? **Paramagnetic (as it has 1 unpaired electron)**

Marks 6

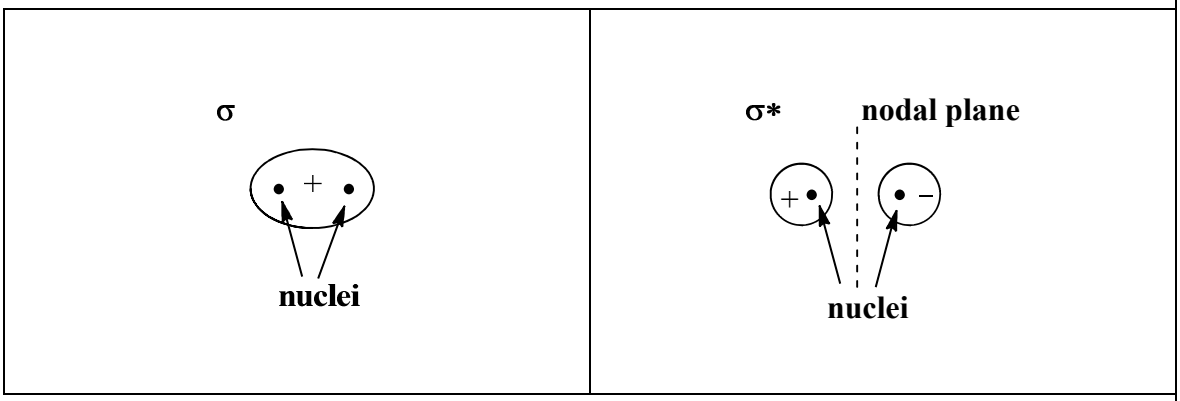
- In order to predict if it is possible to form the He_2^+ cation, complete the following steps.

  In the boxes below, draw an energy level diagram showing labelled electron orbitals and their occupancies for the two reacting species, He and He^+.

  In the other box below, draw an energy level diagram showing labelled electron orbitals and their occupancies in a postulated He_2^+ molecule. Use the same energy scale.



Draw the lobe representation of the two occupied molecular orbitals in this molecule. Show all nuclei and nodal surfaces.



What is the bond order of this molecular ion?

It has 2 bonding (σ) and 1 antibonding (σ*) electron. Hence:

bond order = ½ (number of bonding – number of antibonding electrons)
= ½ (2 – 1) = ½

Make a prediction about the stability of He_2^+ in comparison to the H_2 molecule.

H_2 has a bond order of 1 and He_2^+ has a bond order of ½ so the bond in H_2 is probably stronger.

As the nuclear charge in He is larger than H, the bonding orbital is more stable in He_2^+ than the bonding orbital in H_2 so the ½ bond in He_2^+ is likely to be more than half as strong as the single bond in H_2.