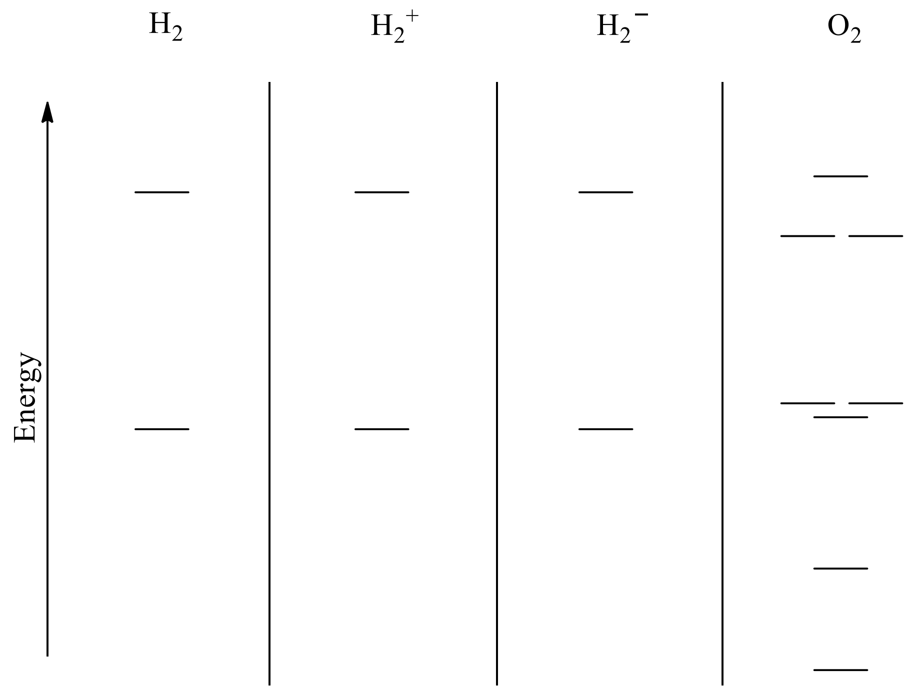
Marks 6

- 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.

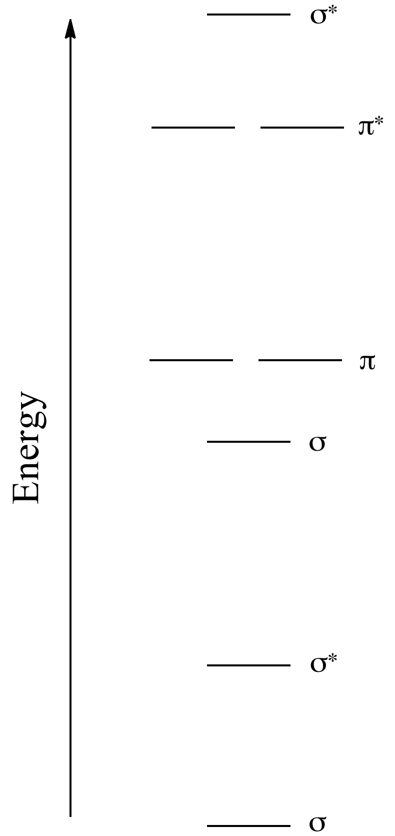
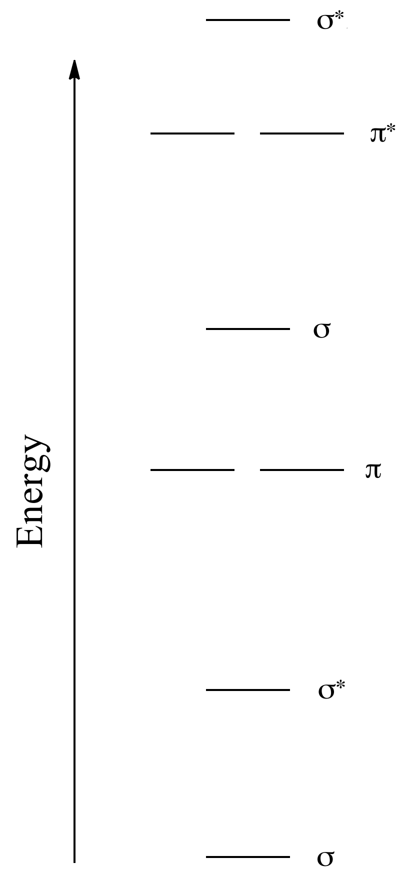
H_2:	H_2^+:	H_2^-:	O_2:

Which of the four species are paramagnetic?

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

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.

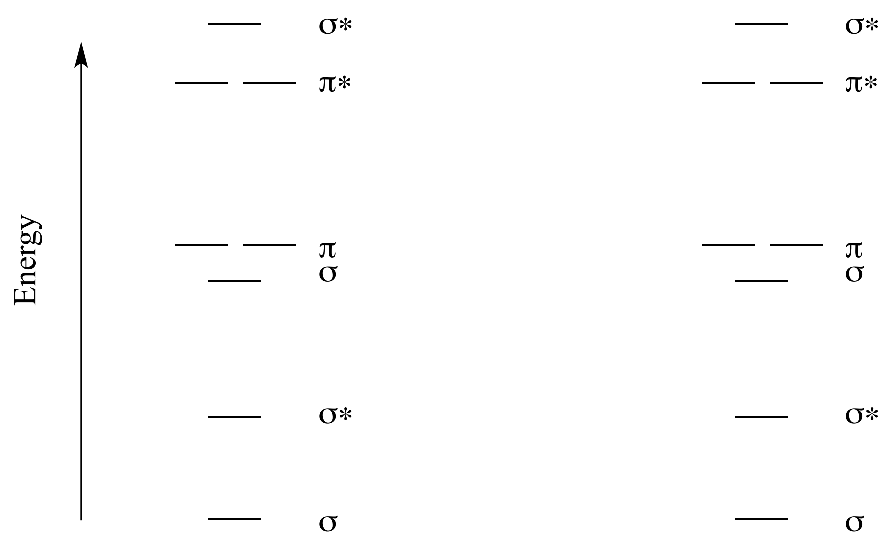
	F_2	B_2
		
Bond order		
Paramagnetic or diamagnetic		

Marks
8

- Oxygen exists in the troposphere as a diatomic molecule.

  How many valence electrons in the O_2 molecule?

  The molecular orbital energy levels for O_2 are shown below. On the left-hand diagram, fill in the **valence** electrons for oxygen, O_2, in the ground state.



(a) What is the bond order for O_2?

(b) Clearly label a bonding orbital and an anti-bonding orbital on the left-hand diagram.

(c) Clearly label the HOMO of O_2 on the left-hand diagram.

(d) On the right-hand diagram, indicate the lowest energy electronic configuration for O_2 which has no unpaired electrons.

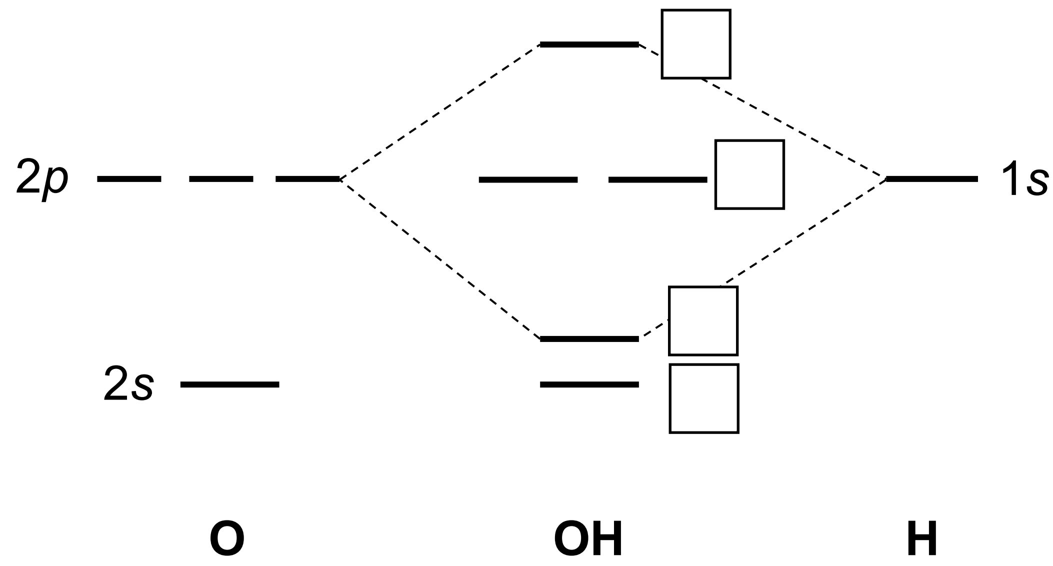
The blue colour of liquid O_2 arises from an electronic transition whereby one 635 nm photon excites two molecules to the state indicated by the configuration in (d) *at the same time*. What wavelength photon would be emitted by one molecule returning from this state to the ground state?

Answer:

Suggest a heteronuclear diatomic species, isoelectronic with O_2, that might be expected to have similar spectroscopic behaviour.

Marks
8

- The OH radical is the most important species in the atmosphere for removing pollutants. A molecular orbital diagram of this species is shown below. Core orbitals are omitted.



Using arrows to indicate electrons with their appropriate spin, indicate on the above diagram the ground state occupancy of the atomic orbitals of O and H, and of the molecular orbitals of OH.

In the provided boxes on the above diagram, label the molecular orbitals as *n*, σ, $\sigma*$, π, $\pi*$, etc.

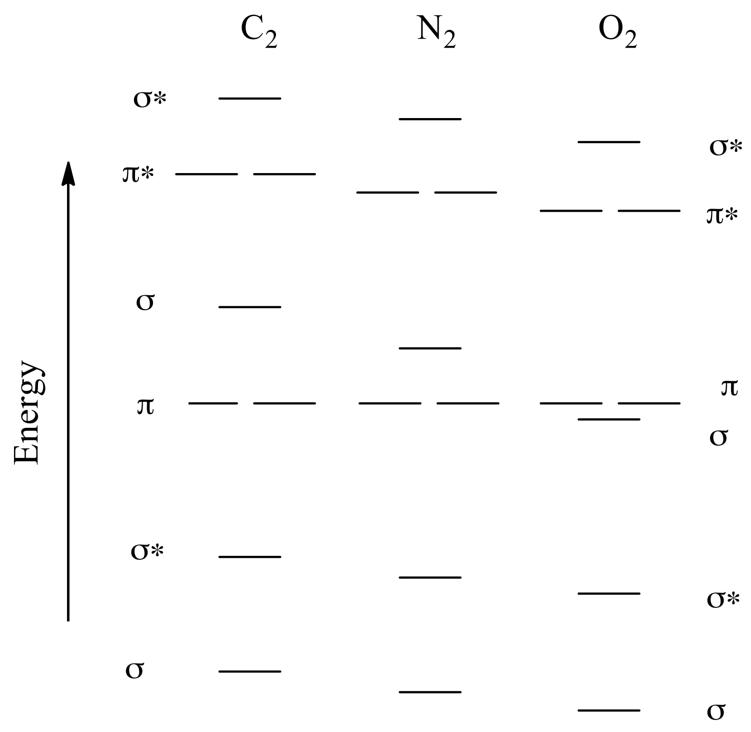
What is the bond order of the O–H bond?

Why do we call OH a "radical"? How does the MO diagram support this?

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.



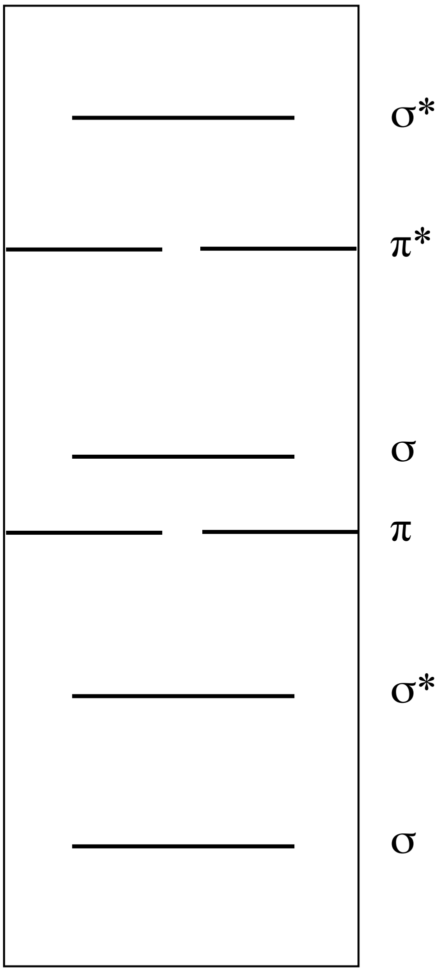
Bond order:			

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

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

Marks
6

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.

MO orbital energy level diagram for NO	Sketch of the π MO
	Sketch of the π* MO

Bond order of NO:

Paramagnetic or diamagnetic?

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.

Energy

He	He^+	He_2^+

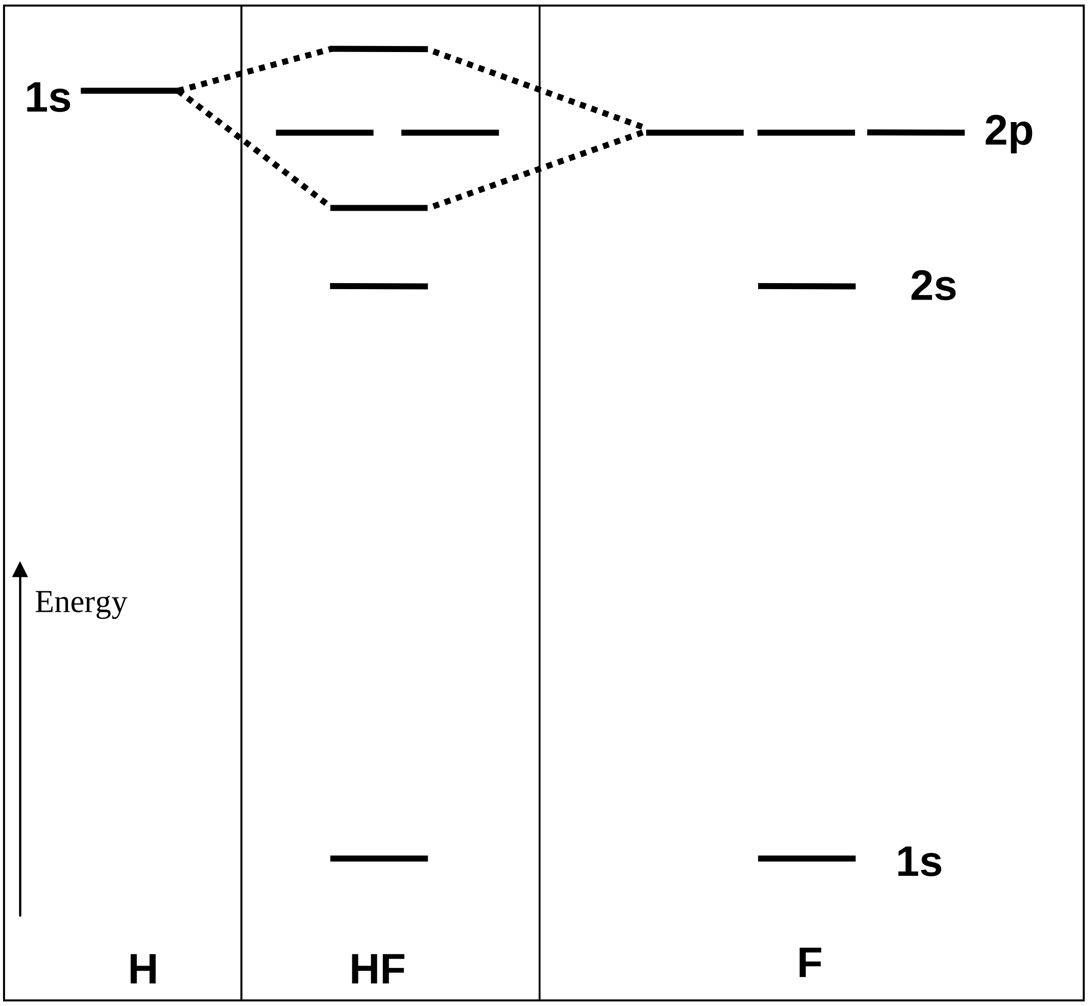
Draw the lobe representation of the two occupied molecular orbitals in this molecule. Show all nuclei and nodal surfaces.

What is the bond order of this molecular ion?

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

Marks
6

- The following diagram shows the energy level diagram for the molecular orbitals in the HF molecule (centre), in comparison to the atomic energy levels of hydrogen (left) and fluorine (right).



Add the ground state electron configuration to the diagrams for all three species using the arrow notation for electron spin.

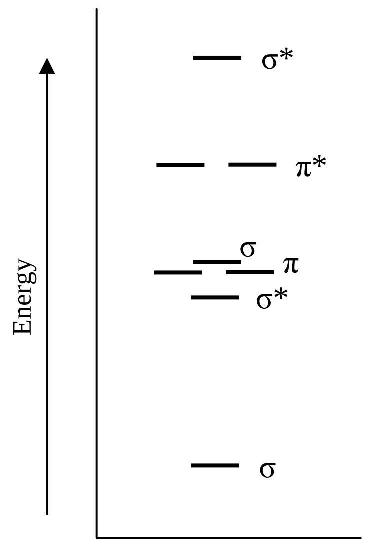
Label the orbitals of HF according to whether they are bonding, non-bonding, or anti-bonding.

Sketch the σ-bonding orbital showing the position of the atomic nuclei.

Marks
6

- Carbon forms a homonuclear diatomic molecule which is observed in comets, flames and interstellar clouds.

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in the C_2 molecule. Indicate on this diagram the ground state electronic configuration of C_2 using the arrow notation for electron spins.



In its ground state, is C_2 paramagnetic or diamagnetic?

The lowest energy excited state of C_2 possesses two electrons with parallel, unpaired spins. What is the bond order of C_2 in this excited state?

Answer:

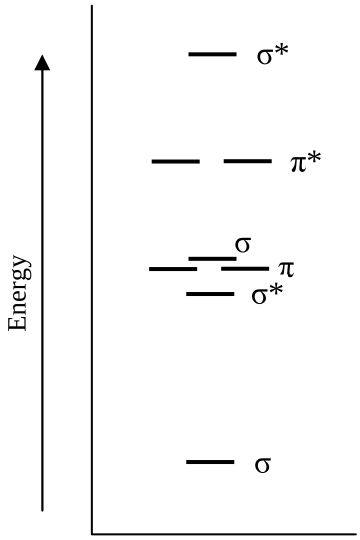
Starting in this excited state, further exciting an electron from the lowest σ* orbital to the next lowest σ orbital brings about the doubly excited state responsible for green emission in flames. What is the bond order of this doubly excited state?

Answer:

Marks
6

- Carbon and nitrogen can combine to form a cyanide ion or a neutral free radical.

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in the free radical CN. Indicate on this diagram the ground state electronic configuration of CN using the arrow notation for electron spins.



How would you expect the magnetic properties of CN to differ from that of CN^{-}?

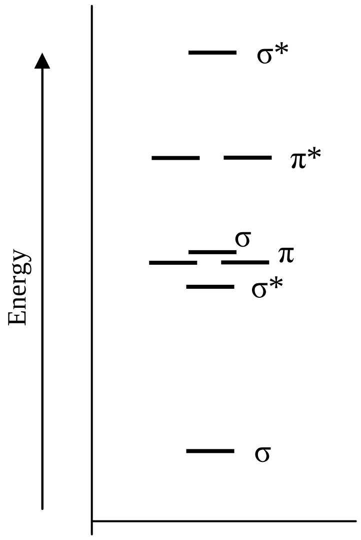
How would adding an electron to CN to form CN^{-} affect the strength of the bond between the two atoms? Explain your answer.

Why do we only need to consider the valence electrons when discussing the bonding of CN?

Marks
6

- Carbon and oxygen can combine to form carbon monoxide, the second most abundant molecule in the universe.

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in CO. Indicate on this diagram the ground state electronic configuration of CO using the arrow notation for electron spins.



What homonuclear diatomic molecule has the same electronic structure as CO? Comment on the bond orders of these two species.

How would adding an electron to CO to form CO^{-} affect the strength of the bond between the two atoms? Explain your answer.

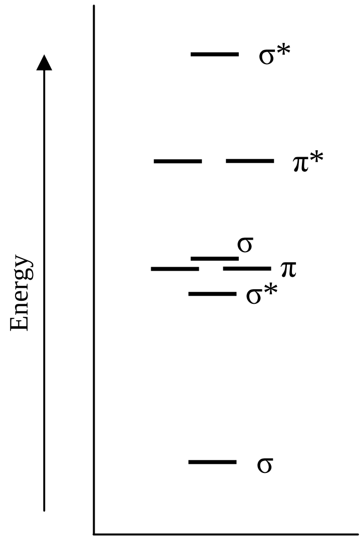
Are the atomic orbital energies of oxygen lower or higher than carbon? Explain your answer and comment on how this may affect the electron density in bonding orbitals of the CO molecule.

Marks
5

- The following relate to the electronic structure of the N_2^- molecular ion.

How many valence electrons are in N_2^-?

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in N_2^-. Indicate on this diagram the ground state electronic configuration of N_2^- using the arrow notation for electron spins.



Calculate the bond order of N_2^-.

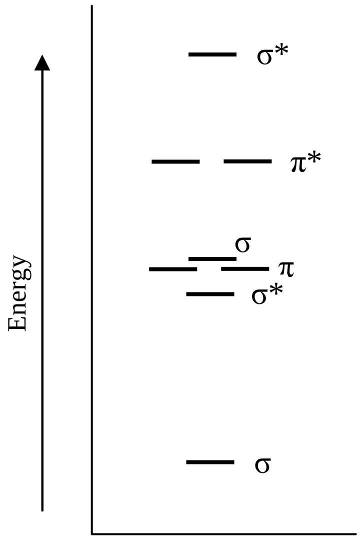
Is the bond strength in N_2^- stronger or weaker than the bond strength in N_2? Why?

Do you expect N_2^- to be paramagnetic? Explain your answer.

Marks
5

- The N_2^+ ion plays a role in the colourful display of the Northern Lights (the *Aurora Borealis*).

The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in the N_2^+ ion. Indicate on this diagram the ground state electronic configuration of N_2^+ using the arrow notation for electron spins.



Calculate the bond order of N_2^+.

Indicate the lowest energy electron excitation in this ion by identifying the initial and final states of the electron undergoing the excitation.

The line at 3914 Å (391.4 nm) in the emission spectrum of the *Aurora Borealis* is due to N_2^+ returning to its ground state. Calculate the energy gap (in eV) between the molecular orbitals involved in this transition.

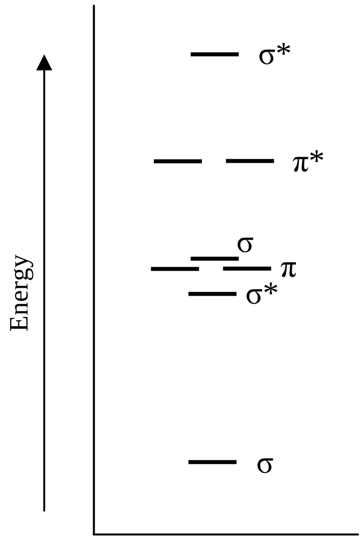
Answer:

Marks
5

- The NO molecule plays an important signalling role in the human body.

  How many valence electrons are in the molecule NO?

  The molecular orbital energy level diagram provided shows the energies of the orbitals for the valence electrons in the NO molecule. Indicate on this diagram the ground state electronic configuration of NO using the arrow notation for electron spins.



  Calculate the bond order of NO.

  Is the NO molecule diamagnetic or paramagnetic? Explain your answer.

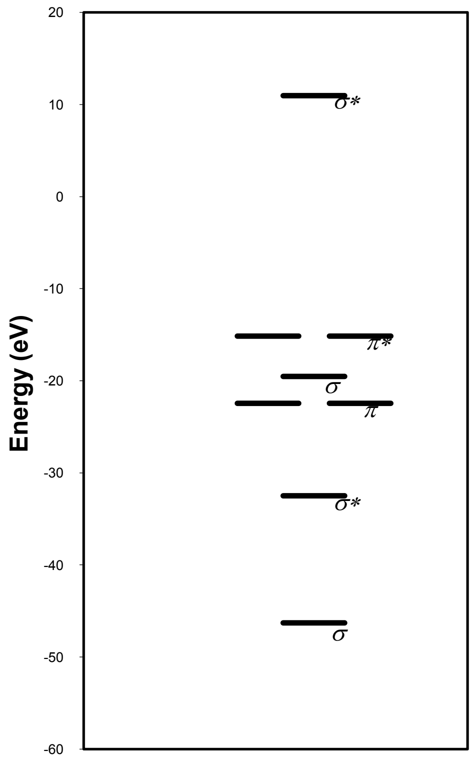
  Would removing an electron from NO to form NO^+ strengthen or weaken the bond between the two atoms? Explain your answer.

Marks

- The following relate to the electronic structure of the O_2^+ molecular ion. **4**

How many valence electrons are there in O_2^+?

Complete the MO diagram for the ground state electronic configuration of O_2^+ by inserting an arrow to represent each valence electron.



What is the bond order of O_2^+?

Do you expect O_2^+ to be paramagnetic? Explain your answer.

- Sketch the following wave functions as lobe representations. **2**

(a) a 2*p* atomic orbital	(b) a *σ** molecular orbital

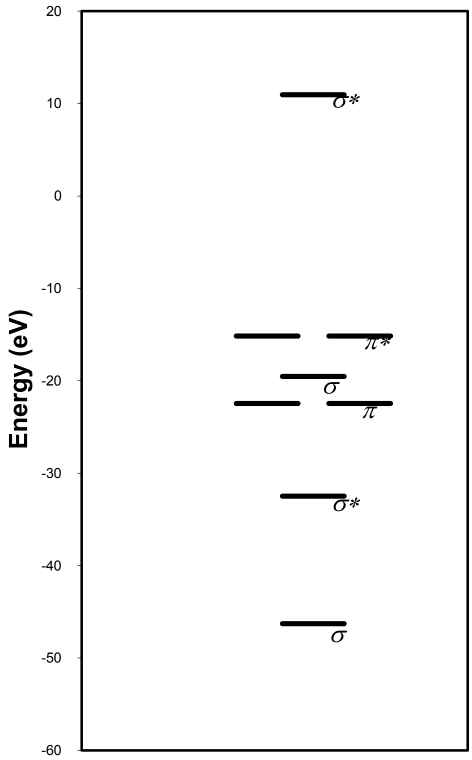
Marks

4

- Oxygen gas, O_2, constitutes about 21% of the Earth's atmosphere.

How many valence electrons are there in O_2?

Complete the MO diagram for the ground state electronic configuration of O_2 by inserting an arrow to represent each valence electron.



What is the bond order of O_2?

Do you expect O_2 to be paramagnetic? Explain your answer.

2

- Sketch the following wave functions as lobe representations.

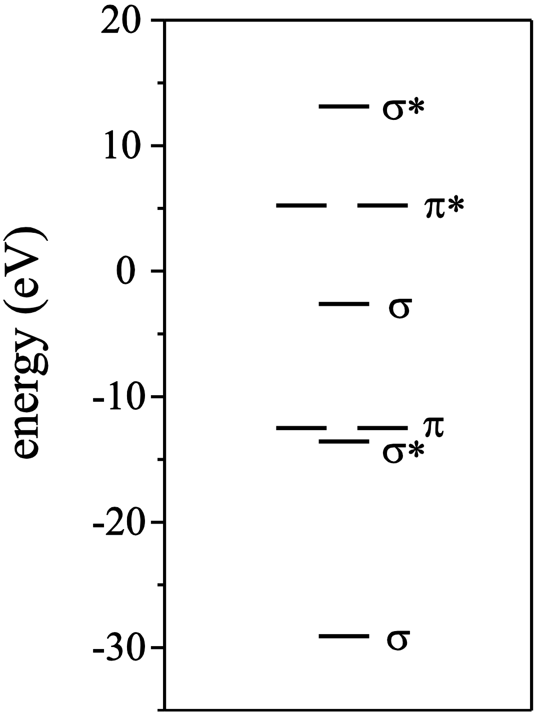
(a) a 2*p* atomic orbital	(b) a *π** molecular orbital

Marks
5

- C_2 is a reaction intermediate observed in flames, comets and circumstellar shells.

How many valence electrons are there in C_2?

Complete the calculated MO diagram for the ground state of C_2 by inserting the appropriate number of valence electrons into the appropriate orbitals.



What is the bond order of C_2?

What is the longest wavelength of light that the ground state C_2^+ ion will absorb? Show working.

Answer: