The following relate to the electronic structure of the $O_2^+$ molecular ion.

How many valence electrons are there in $O_2^+$?

$6e^-$ on each O, minus 1 for the $+ve$ charge: $11e^-$

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 $O_2^+$?

There are 8 electrons in bonding orbitals (two in $\sigma$ and four in $\pi$) and 3 electrons in antibonding orbitals (two in $\sigma^*$ and one in $\pi^*$):

bond order = $\frac{1}{2} (8-3) = \frac{5}{2}$

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

It has an unpaired electron (in the $\pi^*$ level) so will be paramagnetic

Sketch the following wave functions as lobe representations.

(a) a $2p$ atomic orbital

(b) a $\sigma^*$ molecular orbital
• C₂ is a reaction intermediate observed in flames, comets and circumstellar shells.

How many valence electrons are there in C₂?

4 from each C hence 8 overall

Complete the calculated MO diagram for the ground state of C₂ by inserting the appropriate number of valence electrons into the appropriate orbitals.

What is the bond order of C₂?

There are 6 bonding electrons (in σ and π) and 2 antibonding electrons (in σ*). Hence the bond order = \( \frac{1}{2} (6 - 2) = 2 \)

What is the longest wavelength of light that the ground state C₂⁺ ion will absorb? Show working.

The longest wavelength corresponds to the lowest energy transition that is possible. This is from the highest occupied orbital (π) to the lowest unoccupied (σ). From the diagram, the energies of these orbitals are approximately -12.5 eV and -2.5 eV respectively. The transition energy is therefore ~10 eV.

10 eV corresponds to \( 10 \times (1.602 \times 10^{-19} \text{ J}) = 1.602 \times 10^{-18} \text{ J} \).

From Planck’s equation, the energy is related to the wavelength:

\[ E = \frac{hc}{\lambda} \text{ or } \lambda = \frac{hc}{E} \]

so

\[ \lambda = \frac{(6.626 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m s}^{-1})}{(1.602 \times 10^{-18} \text{ J})} = 1.2 \times 10^{-7} \text{ m or } 120 \text{ nm} \]

Answer: \( 1.2 \times 10^{-7} \text{ m or } 120 \text{ nm} \)