Worksheet 5 – Answers to Critical Thinking Questions

The worksheets are available in the tutorials and form an integral part of the learning outcomes and experience for this unit.

Model 1: Single, Double and Triple Bonds

1. Single bonds: O-H, C-H and C-C
   Double bonds: C=C, C=O and O=O
   Triple bonds: C≡C and N≡N

2. The bond order is the same as the designation of the bond as single, double or triple.

3. In order of increasing strength:
   single < double < triple

Model 2: Molecular Orbitals

1. See below.

2. See below.

![σ, π*, σ*](image)

Model 3: Molecular Orbital Diagrams

1. See overleaf.

2. See overleaf.
   Bond order = \( \frac{1}{2} (8 - 2) = 3 \)

3. See overleaf.
   Bond order = \( \frac{1}{2} (8 - 4) = 2 \)

5. See overleaf.
   Bond order = \( \frac{1}{2} (8 - 3) = 2.5 \)
6. See below.

$p_x$ orbitals overlap above and below the plane of the bond to form a $\pi$-bond

$p_y$ orbitals overlap in front and behind the plane of the bond to form a $\pi$-bond

$p_z$ orbitals overlap end on to form a $\sigma$-bond – this third $p$-orbital overlap prohibits a third $\pi$-bond from forming

\[ \text{N}_2 \]

\[ \text{O}_2 \]

\[ \text{NO} \]
7. (a) See below.

(b) The bond order is an indication of the bond strength and bond length. A higher bond order leads to a strong and shorter bond. It can be calculated as:

\[
\text{bond order} = \frac{1}{2} (\text{number of bonding electrons} - \text{number of antibonding electrons})
\]

The upper state in the violet system has 8 bonding electrons (\(2 \times \sigma, 4 \times \sigma^*\) and \(2 \times \sigma\)) and 1 antibonding electron (\(1 \times \sigma^*\)):

\[
\text{bond order} = \frac{1}{2} (8 - 1) = \frac{7}{2}
\]

The upper state in the red system has 7 bonding electrons (\(2 \times \sigma, 3 \times \sigma^*\) and \(2 \times \sigma\)) and 2 antibonding electrons (\(2 \times \sigma^*\)):

\[
\text{bond order} = \frac{1}{2} (7 - 2) = \frac{5}{2}
\]

The upper state in the violet system has a higher bond order and this is consistent with it having a shorter bond (i.e. it has more bonding and fewer antibonding electrons).

(c) The feature occurs at 41 nm. This corresponds to an energy of:

\[
E = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \text{ J s} \times 2.998 \times 10^8 \text{ m s}^{-1}}{41 \times 10^{-8} \text{ m}}
= 4.85 \times 10^{-19} \text{ J}
\]

The energy of a level in hydrogen is given by \(E_n = -\frac{E_R}{n^2}\). The transition energy is the difference in the energies of the two levels involved:

\[
\Delta E = -\frac{E_R}{n_f^2} - \frac{E_R}{n_i^2} = E_R \left[ \frac{1}{n_i^2} - \frac{1}{n_f^2} \right]
\]

where \(E_R\) is the Rydberg constant.
As \( n_i = 2 \),

\[
\Delta E = (2.18 \times 10^{-18} \text{ J}) \left[ \frac{1}{2^2} - \frac{1}{n_f^2} \right] = 4.85 \times 10^{-19} \text{ J}
\]

which gives \( n_f = 6 \).