1. | Orbital | $n$ | $l$ | number of nodes | number of nodal planes | number of spherical nodes |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$2s$</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$2p$</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$3s$</td>
<td>3</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>$3p$</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

(a) The number of nodes = $n - 1$

(b) The number of nodal planes = $l$

2. A $3d$ orbital has $n = 3$ and $l = 2$ and hence:

(a) number of nodes = $3 - 1 = 2$

(b) number of nodal planes = 2

A $4f$ orbital has $n = 4$ and $l = 3$ and hence:

(a) number of nodes = $4 - 1 = 3$

(b) number of nodal planes = 3

3. 

4. This question is about spotting patterns in the orbital shapes – you are not expected to know the shape of these orbitals!

Consider the sequence, in increasing value of $l$:

(i) A $1s$ orbital has 0 nodal planes and is made from one lobe

(ii) A $2p$ orbital has 1 nodal plane and is made from two lobes

(iii) A $3d$ orbital has 2 nodal planes and is made from four lobes

* The last orbital has a different shape with nodal cones – you do not need to be able to draw these: see CHEM2!
A 4f orbital has 3 nodal planes and is made from eight lobes. Passing through a nodal plane changes the phase of the orbital – represented by a change in the colour of the lobe. One possible 4f orbital is pictured below. From the centre of a cube, imagine lobes directed towards the eight corners with each of the three nodal planes cutting through four edges.

Other representations are possible – see the URL below for rotatable, virtually reality representations of atomic and hybrid orbitals:

www.chm.davidson.edu/ChemistryApplets/AtomicOrbitals/AtomicOrbitals.html

5. Neon has filled \( n = 1 \) and \( n = 2 \) shells. Sodium has one extra proton and one extra electron. The extra nuclear charge acts to contract the orbitals but the extra electron has to occupy the next shell, \( n = 3 \), because of the Pauli principle. The \( n = 3 \) shell is significantly larger than the \( n = 2 \) shell so that, despite the increase in nuclear charge, sodium is larger than neon.

6. The energy of the electrons is:

\[
30 \text{ keV} = 30 \times 10^3 \text{ eV} = (30 \times 10^3) \times 1.602 \times 10^{-19} = 4.806 \times 10^{-15} \text{ J}
\]

The shortest wavelength of light emitted corresponds to this energy. The wavelength is related to the energy by Planck’s equation:

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

The shortest wavelength of the emitted X-rays is therefore:

\[
\lambda = \frac{hc}{E} = \frac{(6.626 \times 10^{-34})(2.998 \times 10^8)}{4.806 \times 10^{-15}} = 4.13 \times 10^{-11} \text{ m or } 41.3 \text{ pm}
\]
7. (a) A qualitative MO diagram for H\(_2\) is shown below.

(b) See below.

<table>
<thead>
<tr>
<th></th>
<th>bond length (Å)</th>
<th>bond energy (kJ mol(^{-1}))</th>
<th>bond order</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_2)</td>
<td>0.74</td>
<td>458</td>
<td>1</td>
</tr>
<tr>
<td>H(_2^+)</td>
<td>~1.06</td>
<td>~269</td>
<td>(\frac{1}{2} (1 - 0) = \frac{1}{2})</td>
</tr>
<tr>
<td>H(_2^-)</td>
<td>~1.22</td>
<td>~150</td>
<td>(\frac{1}{2} (2 - 1) = \frac{1}{2})</td>
</tr>
<tr>
<td>He(_2)</td>
<td>-</td>
<td>0</td>
<td>(\frac{1}{2} (2 - 2) = \frac{1}{2})</td>
</tr>
<tr>
<td>He(_2^+)</td>
<td>~1.04</td>
<td>~350</td>
<td>(\frac{1}{2} (2 - 1) = \frac{1}{2})</td>
</tr>
<tr>
<td>He(_2^{2+})</td>
<td>~0.70</td>
<td>~800</td>
<td>(\frac{1}{2} (2 - 0) = 1)</td>
</tr>
</tbody>
</table>

(c) The bond order is clearly related to the bond length and strength – the larger the bond order, the shorter and stronger the bond. The bond order reflects the relative number of bonding and antibonding electrons. Bonding electrons act to bind the atoms more strongly and so reduce the bond length and strength the bond. Antibonding electrons act to weaken and hence lengthen the bond.

Closer inspection shows that H\(_2^-\) has a longer and weaker bond than H\(_2^+\), despite these two species having the same bond order. The presence of e\(^-\)/e\(^-\) repulsion in the latter acts to weaken the bond. The bond order suggests a simple cancellation of bonding and antibonding electrons. In fact, the antibonding electrons destabilize the bond more than this simple measure recognizes (see Optional Question below and the article in the problem book).

The electron density in the bonding orbital is increased between the atoms and is stabilized by attraction to both nuclei. In He\(_2^{2+}\), the two bonding electrons are more stabilized than they are in H\(_2\), due to the higher nuclear
charge of He. As a result, this ion has a stronger bond than that for \( \text{H}_2 \) even though they have the same number of electrons.

Optional question

The energies of the bonding \( 1\sigma \) and antibonding \( 1\sigma^* \) orbitals are not symmetrical with respect to the atomic orbitals. Overlap of the atomic orbitals in fact causes the antibonding level to be raised more than the bonding level is lowered in energy, as shown in the diagram below.

Although the simple definition of bond order leads to a net zero bond order for \( \text{He}_2 \), in fact the molecule is less stable than \( 2\text{He} \) as a result of this.

For more information see http://firstyear.chem.usyd.edu.au/calculators/mo_diagrams.shtml