To be able to use Crystal Field Theory (CFT) successfully, it is essential to first determine the electronic configuration of the central metal ion in any complex. This requires being able to recognize all the entities making up the complex and knowing whether the ligands are neutral or anionic, so that you can determine the oxidation number of the metal ion.

In many cases the oxidation number for first row transition metal ions will be either (II) or (III), but in any case you may find it easier to start with the M(II) from which you can easily add or subtract electrons to get the final electronic configuration.

**A simple procedure exists for the M(II) case**

First write out all the first row transition metals with their symbols and atomic numbers:

<table>
<thead>
<tr>
<th>22</th>
<th>23</th>
<th>24</th>
<th>25</th>
<th>26</th>
<th>27</th>
<th>28</th>
<th>29</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
<td>Ni</td>
<td>Cu</td>
</tr>
</tbody>
</table>

To see the number of electrons in the 3d orbitals then cross off the first 2, hence:

| 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |

So, the electronic configuration of Ni(II) is \( d^8 \) and the electronic configuration of Mn(II) is \( d^5 \).

What is the electronic configuration of Fe(III)?

Well, using the above scheme, Fe(II) would be \( d^6 \), by subtracting a further electron to make the ion more positive, the configuration of Fe(III) will be \( d^5 \).

This simple procedure works fine for first row transition metal ions, but sorry it is no good for 2nd or 3rd row elements!

**Oxidation Numbers and their Relative Stabilities**

The transition metals show a wide range of oxidation numbers. The reason for this is the closeness of 3d and 4s energy states as discussed above. The Table below summarizes known oxidation numbers of the first row transition elements. The most prevalent oxidation numbers are shown in **bold** and those in blue are likely to be met in General Chemistry.
A number of important conclusions can be drawn from this Table.

1. There is an increase in the number of oxidation numbers from Sc to Mn. All seven oxidation numbers are exhibited by Mn. The oxidation number of VII represents the formal loss of all seven electrons from 3d and 4s orbitals. In fact all of the elements in the series can utilize all the electrons in their 3d and 4s orbitals.

2. There is a decrease in the number of oxidation states from Mn to Zn. This is because the pairing of d-electrons occurs after Mn (Hund’s rule) which in turn decreases the number of available unpaired electrons and hence, the number of oxidation states.

3. The stability of higher oxidation states decreases in moving from Sc to Zn. Mn(VII) and Fe(VI) are powerful oxidizing agents and the higher oxidation states of Co, Ni and Zn are unknown.

4. The relative stability of the +2 state with respect to higher oxidation states, particularly the +3 state increases in moving from left to right. This is justifiable since it will be increasingly difficult to remove the third electron from the d orbitals.

5. There is a tendency of intermediate oxidation states to disproportionate. For example, \[ \text{Mn(VI)} \rightarrow \text{Mn(IV)} + \text{Mn(VII)} \] \[ \text{Cu(I)} \rightarrow \text{Cu(0)} + \text{Cu(II)} \]

6. The lower oxidation numbers are usually found in ionic compounds and higher oxidation numbers tend to be involved in covalent compounds.

The relative stability of oxidation numbers is an extremely important topic in transition metal chemistry and is usually discussed in terms of the standard reduction potential (E°) values. Thermodynamically E° values are equated to ΔG° values in the form of the well known relationship:

\[ \Delta G^o = -nF\Delta E^o \]
where

- \( n \) is the number of electrons involved (from balanced Redox reaction) and
- \( F \) is Faraday constant

Hence, the \( E^\circ \) values indicate the possibility of spontaneous change from one oxidation state to the other. This value, however, does not give any information about the reaction rate. Predictions regarding the stability of a particular oxidation state of an element can be made from the Tables P1 or P2.

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