**2.2.2 Full electron configurations**

**Learning objectives**

* Determine the full electron configuration of atoms with up to 36 electrons
* Understand what is meant by an orbital and a subshell (sub-energy level)

**Introduction**

A modification of Bohr’s model could only be achieved at the expense of changing our model of the electron as a particle. Dalton’s atomic model and quantum theory are both examples of such radical changes of understanding, often called paradigm shifts.

The Uncertainty Principle

**What was the major problem with Bohrs atomic model that was modified by the quantum model?**

Another fundamental problem with the Bohr model is that it assumes the electron’s trajectory can be precisely described. This is now known to be impossible, as any attempt to measure an electron’s position will disturb its motion (momentum).

According to Heisenberg’s **Uncertainty Principle** we cannot know where an electron is at any given moment in time – the best we can hope for is a probability picture of where the electron is *likely* to be.

**Schrödinger model of the hydrogen atom**

**What is an atomic orbital? What is the maximum number of electrons in an atomic orbital?**

Erwin Schrödinger (1887–1961) proposed that a wave equation could be used to describe the behaviour of an electron in the same way that a wave equation could be used to describe the behaviour of light.

The equation can be applied to multi-electron systems and its solutions are known as **atomic orbitals**.

*An atomic orbital is a region around an atomic nucleus in which there is a 90% probability of including the electron.*

The shape of the orbitals will depend on the energy of the electron. When an electron is in an orbital of higher energy it will have a higher probability of being found further from the nucleus.

TOK

In our efforts to learn as much as possible about the atom, we have found that certain things can never be known with certainty. Much of our knowledge must always remain uncertain. Some suggest that Heisenberg’s Uncertainty Principle has major implications for *all* areas of knowledge. Does science have the power to inform thinking in other areas of knowledge such as philosophy and religion? To what extent should philosophy and religion take careful note of scientific developments?

**Atomic orbitals**

Each main energy level in an atom is made up of **sub-energy levels** (subshells), s,p,d,and f. The electrons in the outer energy level are mainly responsible for compound formation and are called **valence electrons**.

|  |
| --- |
| An orbital can contain a maximum of two electrons  **What are the shapes of s and p atomic orbitals?** |

The dots in Figure represent locations where the electron is most likely to be found. The denser the arrangement of dots, the higher the probability that the electron occupies this region of space. The electron can be found anywhere within a spherical space surrounding the nucleus.





The first energy level consists of a 1s atomic orbital which is spherical in shape.

The second energy level has a 2s and 2p level

The second energy level of the Bohr model is split into two **sub-levels.** The 2s orbital has the same symmetry as a 1s orbital but extends over a larger volume. 2s atomic orbitals are spherical





2s atomic orbitals 2p atomic orbitals

More at: <http://www.shsu.edu/~chm_tgc/BbAIF/PDBs/applet/PDBorbitals.html>

**How many atomic orbitals are in p sub-energy level?**

The 2p sub-level contains three 2p atomic orbitals of equal energy which are said to be **degenerate**. They all have the same **dumbbell shape**; the only difference is their orientation in space. They are arranged at right angles to each other with the nucleus at the centre.

**d and f orbitals**

The pattern in energy Level and the number of orbitals can be generalized. The *n*th energy level of the Bohr atom is divided into *n* sub-levels. The third energy level is made up from three sub-levels: the 3s, 3p, and 3d. The letters **s**, **p**, **d**, and **f** are used to identify different sub-levels and the atomic orbitals which comprise them.(see the shapes of these orbitals online or in the textbook).

Complete the table of sub-orbitals below

|  |  |  |  |
| --- | --- | --- | --- |
| Level ,n | Sub-level | Maximum no of electrons in sub- level | Maximum no. of electrons in the level |
| 1 | 1s | 2 | 2 |
| 2 | 2s | 2 | 8 |
| 2p | 6 |
| 3 | 3s | 2 |  |
| 3p |  |
|  | 10 |
| 4 | 4s |  |  |
|  |  |
|  |  |
|  | 14 |

**There are three main rules for electron configuration:**

* **Aufbau principle – electrons enter orbitals of lowest energy first. *This gives the lowest possible (potential) energy*.**
* **Pauli exclusion principle – an orbital can only hold 2 electrons with opposite spins.**
* **Hund’s rule (Bus rule) – electrons enter orbitals singly until they have to pair up.**

The **Aufbau principle** is simply the name given to the process of working out the electron configuration of an atom.

The full electron configuration of sodium is therefore 1s2 2s2 2p6 3s1.

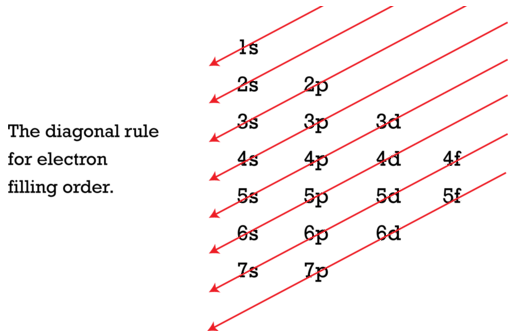
This can also be abbreviated to [Ne]3s1. [1s2 2s2 2p6] 3s1 from neon.

The order of filling sub-orbitals

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7s.

The 3d and 4s levels are very close in energy and their relative separation is very sensitive to inter-electron repulsion. For the elements potassium and calcium, the 4s orbitals are repelled before the 3d sub-level. Electrons are, however, first lost from the 4s sub-level when transitional metals form their ions, as once the 3d sub-level is occupied the 3d electrons push the 4s electrons to higher energy.

**This can be remembered by use of the diagonal rule filling order below**



<https://chem.libretexts.org/Textbook_Maps/Introductory_Chemistry/Map%3A_Introductory_Chemistry_(Tro)/09%3A_Electrons_in_Atoms_and_the_Periodic_Table/9.6%3A_Quantum-Mechanical_Orbitals_and_Electron_Configurations>

When the transition metal atoms form ions they lose electrons from the 4s sub-level before the 3d sub-level.

The full electron configuration of iron (26 electrons) is: 1s2 2s2 2p6 3s2 3p6 4s2 3d6. Note that because the 4s sub-level is lower in energy than the 3d sub-level, it is filled first.

The full electronic configuration of germanium (32 electrons) is: 1s2 2s2 2p6 3s2 3p6 4s2 3d10 4p2.

**Practice questions**

1. Draw the shapes of a 1s orbital and a 2px orbital.
2. Write the full electronic configuration for germanium (32 electrons.
3. State the full electron configuration of vanadium and deduce the number of unpaired electrons.

**Putting electrons into orbitals – the Aufbau principle (part 2)**

As well as moving around in space within an orbital, electrons also have another property called **spin**.

Two rules are followed in placing electrons in orbitals

1. The **Pauli exclusion principle:** the maximum number of electrons in an orbital is two. If there are two electrons in an orbital, they must have opposite spin.



1. **Hund’s rule:** electrons fill orbitals of the same energy (degenerate orbitals) so as to give the maximum number of electrons with the same spin.

3 electrons in p orbital will occupy



The electrons in the different 2p orbitals have parallel spins, as this leads to lower energy.

These diagrams are sometimes described as ‘orbital diagrams’, ‘arrows in boxes’ or ‘electrons in boxes’.

There are a small number of exceptions to the rules for filling sub-levels – i.e. electron configurations that are not quite as expected. Two of these exceptions are **chromium** and **copper**, which, instead of having electron configurations of the form [Ar]3d*n*4s2 have only one electron in the 4s sub-level:

24Cr: [Ar]3d54s1 29Cu: [Ar]3d104s1

1. Draw the orbital diagrams (electron in boxes) for the following elements:
2. Oxygen
3. Silicon
4. Carbon
5. Nitrogen
6. Chromium
7. Copper

Electron configuration of ions

Positive ions are formed by the loss of electrons. These electrons are lost from the outer sub-levels.

When positive ions are formed for transition metals, the outer 4s electrons are removed before the 3d electrons, as discussed earlier.

Examples

1. Al3+ is 1s22s22p6
2. Cr is [Ar]\_3d54s1 and Cr3+ is [Ar]\_3d3

The electron configuration of negative ions is determined by adding the electrons into the next available electron orbital: For sulfur, S is 1s22s22p63s23p4 and S2– is 1s22s22p63s23p6

1. State the ground-state electron configuration of the Fe3+ ion.

Electronic configuration and the Periodic Table

**•** elements whose valence electrons occupy an s sub-level make up the **s block**;

**•** elements with valence electrons in p orbitals make up the **p block**;

**•** the **d block** and the **f block** are similarly made up of elements with outer electrons in d and f orbitals.

The position of an element in the Periodic Table is based on the occupied sub-level of highest energy in the ground-state atom. Conversely, the electron configuration of an element can be deduced directly from its position in the Periodic Table.

Here are some examples.

**•** Caesium is in Group 1 and Period 6 and has the electronic configuration: [Xe]\_6s1.

**•** Iodine is in Group 17 and in Period 5 and has the configuration: [Kr]\_5s24d105p5.

Placing the 4d sub-level before the 5s gives [Kr]\_4d105s25p5.

