1300: Diagram of atomic orbital energy levels

(In hydrogen atoms, the energy levels of s, p, d, etc. are determined only by the principal quantum number, but in multi-electron atoms, they are separate)

Key words: Energy levels of atomic orbitals of hydrogen atoms; energy levels and electron shells of atomic orbitals of multi-electron atoms

[Energy levels of hydrogen atoms]

The energy levels of the atomic orbitals of a hydrogen atom are given by the following formula:

$$E_n = -R\left(\frac{Z^2}{n^2}\right)$$
 $Z = 1$, $R = 13.6$ eV or 1312.2kJ/mol

The energy levels are determined solely by the principal quantum number (n). This is shown in Figure 1 (circles represent atomic orbitals).

	<i>l</i> =0	<i>l</i> =1	<i>l</i> =2	<i>l</i> =3
		1	000004 <i>d</i> 00003 <i>d</i>	00000004f
-328.0	$\bigcirc 2s$	$\bigcirc \bigcirc \bigcirc 2p$		

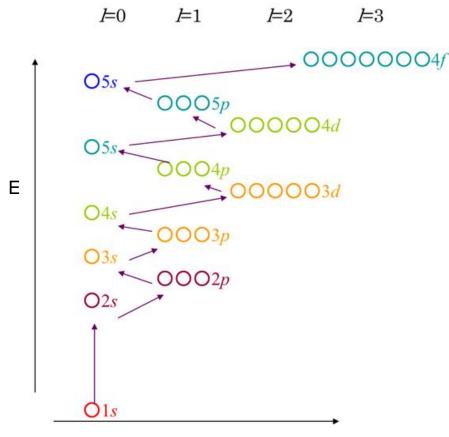
-1312.2 O1s

Figure 1. Energy levels of the atomic orbitals of a hydrogen atom. The unit is kJ.

[Energy levels of multi-electron atoms]

As you can see, the azimuthal quantum number and magnetic quantum number are not related to the energy levels. However, in multi-electron atoms, the energy levels change depending on the azimuthal quantum number, and if the principal quantum number is the same, they are approximately separated into s ... But actually they are, <math>1s < 2s < 2p < 3s < 3p < 4s < 3d < f

 $4p < 5s < \dots$ Note that the 3d and 4s levels are reversed. This is shown in the following diagram.



Azimuthal quantum number

Figure 2. Overview of the energy levels of atomic orbitals of a multi-electron atom.

[Electron shell]

As shown in Figure 1, the energy levels of electrons are layered according to the number of principal quantum numbers. These layers are called electron shells. In multi-electron atoms, the energy levels of electrons in a layer are separated by the azimuthal quantum number, but the atomic orbitals belonging to the principal quantum number n are collectively called shells, and for values of n=1, 2, 3, ..., they are given alphabetical letters starting with K, such as K, L, M, ..., and are called the K shell, L shell, etc. It is said that the reason why the letters starting with K were given is because, at the time the shells were discovered, it was considered that there might be states with lower energy than the K shell that had not yet been discovered. The concept of shells is also obscured by the fact that there are crossings in the energy of atomic orbitals that violate the principal quantum number, and for these reasons the concept of shells is no longer given much importance.