1260: Types of atomic orbitals

(Atomic orbitals are necessarily derived from the wave nature of electrons. This provides an overview of how atomic orbitals are formed.)

Key words: Cartesian coordinates; polar coordinates; types of quantum numbers correspond to dimensions; principal quantum numbers; azimuthal quantum numbers; magnetic quantum numbers

[Symbol notation of atomic orbitals]

Atomic orbitals are given symbols such as 1*s*, 2*s*, 2*p*, etc. This indicates that there are that many types of orbitals. The symbols of atomic orbitals represent the type and number of quantum numbers.

[Polar coordinates]

The shape of a one-dimensional wave function (for example, the vibration of a string) is expanded on a one-dimensional coordinate axis (for example, the x-axis) and is determined by one type of quantum number and its value. A two-dimensional wave function is determined by the number of coordinates (x-axis and y-axis), that is, two types of quantum numbers and their values.

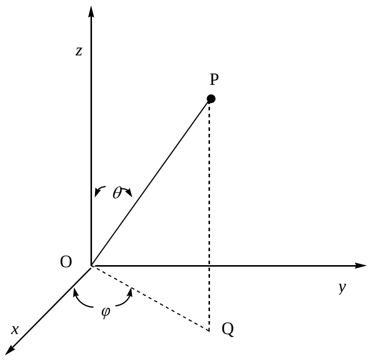
The wave function of an electron confined by an atomic nucleus (atomic orbital) is three-dimensional. Coordinates that represent three-dimensional space are usually expressed using the x, y, and z axes (Cartesian (rectangular) coordinates), but the Schrödinger equation for a hydrogen atom expressed in this coordinate system cannot be solved. Therefore, it is converted to a polar coordinate system and solved (this method of solving difficult mathematical equations in quantum mechanics by coordinate transformation is often used).

A polar coordinate system is a coordinate system that expresses the position of a point **P** in space by its distance from the origin **O** (r), the angle (θ) between OP and the z-axis, and the angle (φ) between OQ and the y-axis when a perpendicular line is drawn from P to the xy plane, and its foot is **Q.**

[Types of atomic orbitals correspond to polar coordinates]

The type of atomic orbital is determined by the principal quantum number, azimuthal quantum number, and magnetic quantum number described below.

The quantum number related to the coordinate r is called the principal quantum number and is represented by n. n can take the value of 1, 2, ... a natural number. It is almost certain that the nucleus is at the origin **O**[1)], so the principal quantum number can be thought of as an indicator of the approximate distance of the electron from the nucleus.



$$z = r\,cos\,\theta$$
$$x = r\,sin\,\theta\,cos\,\varphi$$
$$y = r\,sin\,\theta\,sin\,\varphi$$

Figure 1. Polar coordinate representation of space. The Cartesian coordinate system (x, y, z) and r, θ, φ have the above relationship.

The quantum number related to the coordinate θ is called the azimuthal quantum number and is represented by l. l depends on the value of n and can take the value of 1, 2, ... up to n-1 for n. l represents the general shape of the atomic orbital, but the detailed shape is determined by the magnetic quantum number, which is described below.

The quantum number related to the coordinate φ is the magnetic quantum number, denoted by the symbol m. m depends on the value of l, and for a given value of l, it can take on a total of 2l+1 values: -l, -l+l, -l+2, ... -1, 0, 1, ... l-2, l-1, l. For example, when l=2, m can take on five values: -2, -1, 0, 1, 2.

The magnetic quantum number is a quantum number that functions with motion around the z-axis (φ coordinate). Electrons have a negative charge, so they generate a magnetic field due to their motion. When an external magnetic field is applied, it interacts with the magnetic field caused by the electron's motion, giving it a different energy state according to l, hence the name (magnetic quantum number).

1) The origin is the center of mass, but since the mass of the nucleus is much larger than that of the electron, the position of the nucleus can be the same as the center of mass.