

## *Modern Theory of Atomic Structure, Page 2*

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### **Magnetic Quantum Number**

The Magnetic Quantum Number is the third quantum number. It is symbolized with the letter "m" and has values that are integers including zero ranging from negative the value of the [Azimuthal quantum](#) number to positive the value of the Azimuthal quantum number. In other words, if  $l = 2$ , then the allowed values of m will be -2, -1, 0, +1, +2. The Magnetic quantum number is used to designate the number of orientations of the various types of orbitals on the three-dimensional axis system. The number of possible values of m associated with a specific value of l will indicate the number of different orientations of the particular orbital type. In the case of  $l = 2$ , there are 5 m values. Therefore, this set of orbitals associated with  $l = 2$ , the d orbitals, will consist of 5 d orbitals, all arranged differently on the axis system.

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### **Nodes (or nodal surfaces)**

Nodes are points in space that have zero probability for locating an electron there. A good example of a node is the nucleus. A nodal surface is usually a spherical surface with infinitely small thickness. Nodal surfaces appear as concentric spheres around the nucleus of an atom. These are also positions around an atom where there is zero probability of locating an electron.

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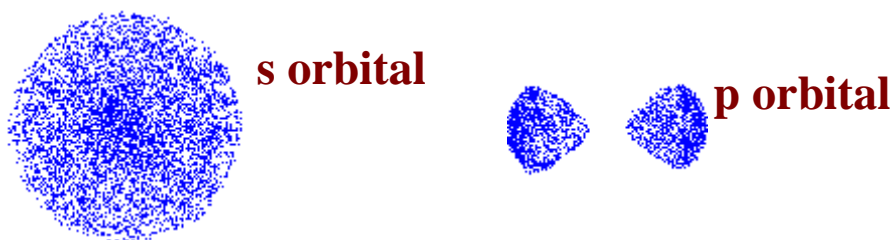
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### **Orbitals**

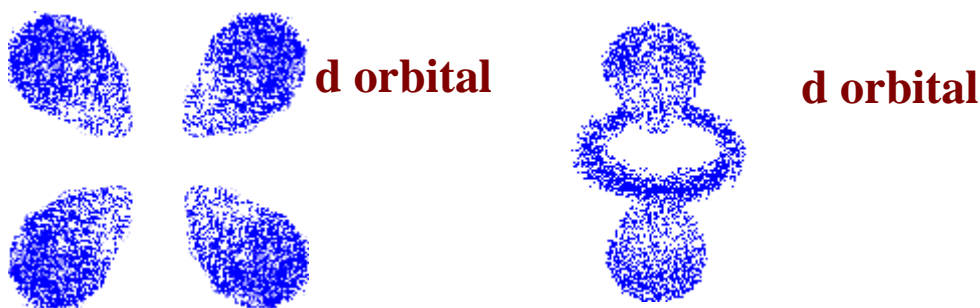
Orbitals are probability diagrams. Specifically, an orbital describes a region in space where there is a 90% chance of finding an electron. The electron is never restricted to an orbital as it travels around a nucleus, but it seems to keep returning to this particular region even though its behavior is random. The concept of the orbital differs from Bohr's concept of the orbit. Bohr considered an orbit to be a path that the electron always followed much like a train stays on a track. The concept of the orbital was developed in Schrodinger's work to avoid violating the Heisenberg Uncertainty Principle. In the Modern Theory of Atomic Structures a picture of an orbital is also called a Probability Diagram. By agreement among chemists, the orbital is a 90% Probability Diagram. This idea allows the electron to be found anywhere and still indicates where the electron spends most of its time.

As a result of applying the Quantum Numbers to Schrodinger's work a series of graphs of orbitals can be drawn. Each different orbital picture is a result of the value of the Quantum Numbers that are applied to a specific electron. Ultimately, all different graphs of orbitals are rendered down to four types, by name. Their names, and shapes, are based on the value of the Azimuthal Quantum Number.

- $l = 0$ , the orbital is called "s".
- $l = 1$ , the orbital is called "p".
- $l = 2$ , the orbital is called "d".
- $l = 3$ , the orbital is called "f".



There are two shapes for d orbitals, even though both occur when  $l = 2$ .



## [Additional Orbital Information](#)

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## Orbital Overlap

Orbital Overlap refers to some of the orbitals at a given value of  $n$  being located above some of the orbitals that are located at a higher value of  $n$ , when plotted on an energy level diagram. Because of the



differing sizes of orbitals, the electrons in various orbitals will experience different relationships with the nucleus. Electrons located at the same value of  $n$  can have different effective nuclear charges because of the way orbitals are constructed. These different relationships the electrons have with the nucleus cause orbitals at a given value of  $n$  to split, or lose their degeneracy. Sometimes, the highest energy orbitals at a given value of  $n$  will move so far up the diagram that they will actually be above the lowest energy orbitals at the next value of  $n$ .

In other words, orbitals at one value of  $n$  overlap into the next value of  $n$ . In the example shown here, the 3d orbital has overlapped into the  $n = 4$  level.

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## Pauli Exclusion Principle



Named after Wolfgang Pauli, the Pauli Exclusion Principle says that no two electrons on a given atom can be described with the same set of four quantum numbers. This is based upon the idea that it would be impossible for two electrons to be at the exact same location at the exact same time. While two electrons may exist together in the same orbital they must have axial spins in the opposite directions. As a result of the Pauli Exclusion Principle, an orbital is limited to a maximum of two electrons.

Electrons are always described by the quantum number sets,  $(n, l, m, s)$ . If an electron was located at  $(4, 1, 0, +1/2)$ , then another electron can be located in that orbital provided that it is spinning in the opposite direction. That second electron will have the quantum numbers  $(4, 1, 0, -1/2)$ . This combination of two sets of quantum numbers describes two electrons, both in the same orbital, but spinning in opposite directions.

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## Principal Quantum Number

The Principal Quantum Number is the first quantum number. It is the single most important quantum number. It establishes the energy level for an electron and indicates the approximate distance of the electron from the nucleus. It is symbolized with the letter "n" and can have any integer value from one up to infinity.

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## Probability Diagrams

Probability Diagrams are graphs that describe the probability of locating an electron around a nucleus a defined percentage of the time. Generally, probability diagrams are drawn as 90% regions. When set at that standard the probability diagram is then referred to as an orbital. Probability diagrams were devised as a method of avoiding problems associated with violating the Heisenberg Uncertainty Principle.

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## Quantum Numbers

Quantum Numbers are terms which were developed to aid in describing electron behavior according to the Schrodinger Wave Equation. Schrodinger found that three variables, called quantum numbers, would help establish specific aspects of electron behavior. These quantum numbers are usually designated as  $n$ ,  $l$  and  $m$ . Together they will specify the energy level, type of orbital and orientation of the orbital that an electron will occupy. A fourth quantum number was eventually added to the electron's description. This number is the spin quantum number and is symbolized as  $s$ . It indicates the direction of the electron's spin on its own axis. This number did not come directly from Schrodinger's work.

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## Schrodinger Wave Equation

The Schrodinger Wave Equation is the foundation of the Modern Theory of Atomic Structure. It is known as a wave-mechanical equation because it treats the electron as both a wave and a particle. The original ideas for this work came from de Broglie who considered an electron to have wave characteristics. From the Schrodinger Wave Equation the basic information about quantum numbers and overall electron behavior have been derived.

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