ORBITALS

Quantum Mechanics

With the advent of quantum mechanics, our understanding of the atom has changed dramatically. An important precursor to the field of quantum mechanics was the atomic theory of Max Planck. He figured out that electromagnetic energy is quantized. That is, for a given frequency of radiation (or light), all possible energies are multiples of a certain unit of energy, called a quantum. So, energy changes do not occur smoothly but rather in small but specific steps. Neils Bohr took this quantum theory and predicted that in atoms the electrons orbit the nucleus just as planets orbit the sun. He proposed the Bohr model of the atom, which was later proved to be incorrect. For the SAT Chemistry Subject Test, you have to know that electrons do not circle the nucleus as planets circle the sun. Electrons do not orbit. Instead, they exist in things called orbitals.

Just as a room is a region in a house in which a person may be found, an orbital is a region in an atom where an electron may be found. Rooms come in a variety of sizes and shapes and so do orbitals. A collection of orbitals with roughly similar sizes constitutes an energy shell. Electrons that are farther from the nucleus have greater energy than those that are closer, so electrons in the orbitals of larger energy shells have greater energy than those in the orbitals of smaller energy shells. Each energy shell is designated by a whole number, so we have the 1st (smallest energy shell), 2nd, 3rd, and so on.

Shape is another important characteristic of orbitals. There are four significant types of orbital shapes. Orbitals that have the same shape in a given energy shell comprise a subshell. An s subshell always consists of one spherical orbital; a p subshell always consists of three dumbbell-shaped orbitals, and the d and f subshells contain five and seven oddly shaped orbitals, respectively. Any orbital, regardless of size and shape, can hold a maximum of two electrons.

Quantum Numbers

To find the location of an electron around an atom utilizing quantum theory, a set of numbers is assigned to each electron of an atom. These numbers, called the quantum numbers for that electron, are essentially an electron address—they give us an idea of approximately where the electron is located relative to the nucleus of the atom. Each electron has four primary quantum numbers:

Principal quantum number (n) The first quantum number describes how far an electron is from the nucleus. This is consistent with previous models of the atoms, with the first energy shell (n = 1) being the one closest to the nucleus.

- Azimuthal quantum number (1) Each of the subshells is assigned a different quantum number. An s-subshell = 0, p-subshell = 1, d-subshell = 2, and f-subshell = 3. The subshell describes the shape of the orbital within which the electron can be found.
- Magnetic quantum number (ml) Each of the subshell types has a different number of orbitals, and each of those orbitals is represented with a different quantum number. An s-subshell has one orbital that is always represented with a 0. The three orbitals in a p-subshell are represented with -1, 0, and +1. The five d-orbitals are represented with -2, -1, 0, +1, and +2. Finally, the seven f-orbitals are represented with -3, -2, -1, 0, +1, +2, and +3.
- Spin projection quantum number (ms) Every orbital can contain exactly two electrons, and these two electrons must have opposing spins. One will spin clockwise, and the other will spin counterclockwise. These two spins are represented by $+\frac{1}{2}$ and $-\frac{1}{2}$.

Putting it all together, if you were asked to assign a set of quantum numbers to an electron in a 3p subshell, you have the following six sets of quantum numbers (written as n, l, ml, ms):

$$(3, 1, -1, +\frac{1}{2})$$
 $(3, 1, -1, -\frac{1}{2})$ $(3, 1, 0, +\frac{1}{2})$

$$(3, 1, -1, -\frac{1}{2})$$

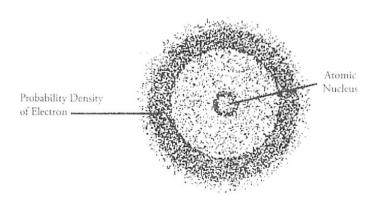
$$(3, 1, 0, +\frac{1}{2})$$

$$(3, 1, 0, -\frac{1}{2})$$

$$(3, 1, 0, -\frac{1}{2})$$
 $(3, 1, +1, +\frac{1}{2})$ $(3, 1, +1, -\frac{1}{2})$

$$(3, 1, +1, -\frac{1}{2})$$

A total of six electrons can fit in the 3p subshell, and those six quantum number sets each represent one possibility. The s-subshells contain a maximum of two electrons and thus would have two potential sets of quantum numbers, d-orbitals would have ten potential sets, and f-orbitals would have fourteen potential sets.



The Heisenberg Principle and De Broglie's Hypothesis

But what's an orbital? The test writers expect you to associate the word orbital with something called a "probability function." An orbital describes the "likelihood that an electron will be found in a particular location." Another important concept to know for the test is the Heisenberg principle. What's the Heisenberg principle? Well, simply put, it means this: It is impossible to know both the position and the momentum of an electron at the same time.

For this test, all you need to know about Louis De Broglie is that he postulated that matter could have the properties of a wave. He extended this to say that electrons can be thought of as behaving similarly to waves of electromagnetic radiation.

Important Facts to Know and Connections to Make

Electron orbitals:

defined by the probability function

· quantum theory

• Heisenberg principle

Bohr model:

 the incorrect idea that electrons orbit the nucleus in true orbits as planets orbit the

Heisenberg principle:

electrons are located in orbitals, not orbits

· one cannot know an electron's position and momentum at the same time

De Broglie's hypothesis:

· matter (including electrons) can be thought of as having properties of both a particle and a wave

DRILL 1

Question Type A

Ouestions 1-3 refer to the following.

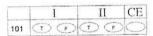
- (A) Bohr model
- (B) De Broglie's hypothesis
- (C) Heisenberg principle
- (D) Quantum theory
- (E) Atomic theory
- 1. Provides that all matter may be considered as a wave
- 2. Views electrons in true orbits around the nucleus
- 3. Considers that one cannot know the position and velocity of an electron at the same moment

Question Type B

II

The Bohr model of the BECAUSE 101. atom is inaccurate

an element may exist as several isotopes, each with a different number of neutrons in the nucleus.



102. Krypton is an extremely unstable atom

BECAUSE

an atom with 8 electrons in its outermost shell tends toward great stability.

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