

Overview of Quantum Mechanics for General Chemistry

- Experiments by Thomson and Millikan gave the charge to mass ratio (1.758819×10^8 coulombs per gram) and the charge (1.602177×10^{-19} coulombs) of the electron. These experiments suggested that the electron is a particle and yielded its mass (9.109390×10^{-28} grams)
- It has also been shown that electrons diffract through crystals suggesting that they can also behave as waves.
- De Broglie gave us an expression relating wave and particle character (so called wave particle duality).

$$\text{wavelength} = \frac{h}{(\text{mass})(\text{velocity})}$$

The relationship suggests that wave particle duality is only important for submicroscopic particles such as the electron. We people are far too big to have much wave character!

- Bohr Theory describes atomic structure in terms of a particle theory and mathematics involving algebra. The electron positions are described as circular orbits characterized by one quantum number (n) and the following relationships for radius

$$r = \frac{n^2(0.528 \text{ angstroms})}{Z}$$

$$E = -\frac{Z^2(2.18 \times 10^{-18} \text{ J / atom})}{n^2}$$

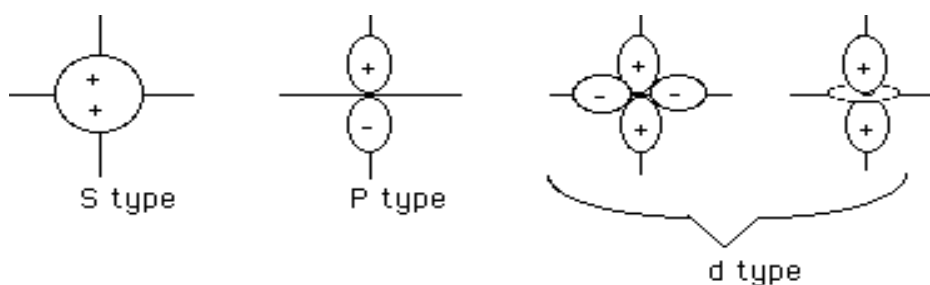
and energy

Where Z is the nuclear charge. The Bohr theory is a perfect description of one electron systems, but can not be extended to multi electron systems.

- The Schrodinger wave mechanical approach assumes that the electron is a wave. The Schrodinger wave equation, therefore, describes the behavior of electrons in atoms as waves. The Schrodinger wave equation is a differential equation meaning that its solutions are mathematical functions. These mathematical functions are called wave

functions. The Schrodinger approach is also a perfect description of one electron systems, and it can be extended in an approximate fashion to multi-electron atoms and ions. The notion of hybridizations also allow a good extension of the Schrodinger atomic orbitals to the description of electrons in molecules.

- The wave functions squared are related to the probability of finding an electron at a point in space. The wave functions also yield the familiar orbital pictures found in most introductory text books.



- There are many wavefunctions that are solutions to the Schrodinger Wave equations. Each wavefunction is identified by a set of three quantum numbers (n , l , & m).
- From the mathematics of the Schrodinger Wave problem, the following relationship between quantum numbers results.

$$n = 1, 2, 3, 4, \dots$$

$$l = n-1, n-2, n-3, \dots 0$$

$$m = -l, -(l-1), -(l-2), \dots 0, \dots (l-2), (l-1), l$$

- If $n=1$ then $l=0$ and $m=0$. The set of quantum numbers $n=1, l=0, m=0$ identify the 1s orbital.

If $n=2$ then $l=1$ or 0. If $l=1$ then $m=-1, 0, 1$. If $l=0$ then $m=0$. So, for $n=2$ the following sets are allowed

$$n = 2, l=1, m = -1$$

2p

$$n=2, l=1, m = 0$$

2p

$$n=2, l=1, m = 1$$

2p

$n=2, l=0, m=0$
2s

If $n=3$ then $l=2,1,0$. If $l=2$ then $m=-2, -1, 0, 1, 2$. If $l=1$ then $m=-1, 0, 1$. If $l=0$ then $m=0$. So, for $n=3$ the following sets are allowed

n	l	m	orbital identified
3	2	-2	3d
3	2	-1	3d
3	2	0	3d
3	2	1	3d
3	2	2	3d
3	1	-1	3p
3	1	0	3p
3	1	1	3p
3	0	0	3s

- So, for $n=1$ there is one place to put electrons, so to speak. That place is the 1s atomic orbital. For $n=2$ there is four places to put electrons; the 2s and three 2p atomic orbitals. For $n=3$ there are 18 places to put electrons; the 3s, three 3p atomic orbitals, and five 3d atomic orbitals. For multi-electron atoms and ions the filling order is related to the structure of the periodic table and is approximately

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

Finally, each AO (atomic orbital) can hold (describes the position probability) two electron providing the spin quantum number are not the same ($s=+1/2$ or $s=-1/2$).

WOW! Neat stuff and it all works pretty well!

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