

Chapter 7 - Quantum Numbers, Orbitals, and Electron Configurations

Quantum Mechanics and the H Atom

Bohr theory (1914) ran into problems when it was applied to atoms other than H, and was soon replaced by quantum mechanics (1926). When quantum mechanics was applied to the H atom, the same energies were calculated for the H atom energy levels as in the Bohr model,

$$E_n = -R_H \left(\frac{1}{n^2} \right) \quad \text{for } n = 1, 2, 3, \dots \quad (\text{Applies only to H atom!!}) \quad (1)$$

but the method by which they were calculated was entirely different.

Quantum mechanics assumes the electron is wave-like, and the planetary orbits of Bohr theory (which views the electron as a particle) are discarded. Orbitals, which give us a picture of the most probable locations for the electron in a particular energy state, replace the Bohr orbits. Since the electron is viewed as a wave, it is impossible to describe its precise location: an averaged picture is the best we can do! Another change is that while the quantum number n still plays the prominent role, it is augmented by the quantum numbers l , m_l , and m_s . The allowed quantum numbers for the H atom are given in the tables below.

Table 1.

Quantum Number	Allowed Values	Name and Meaning
n	$n = 1, 2, 3, \dots$	<i>Principal quantum number</i> : orbital energy and size.
l	$l = (n-1), (n-2), \dots, 0$	<i>Azimuthal (or orbital) quantum number</i> : orbital shape (and energy in a multi-electron atom), letter name for subshell (s, p, d, f)
m_l	$m_l = l, (l-1), \dots, 0, \dots, (-l+1), -l$	<i>Magnetic quantum number</i> : orbital orientation
m_s	$m_s = 1/2, -1/2$	<i>Electron spin quantum number</i> : spin up (\uparrow) or spin down (\downarrow).

Table 2

l Value	Letter Equivalent to l Value	No. of Orbitals in Set	Approximate Shape of Orbitals with Specific l Values
0	s	1	spherical
1	p	3	p_x, p_y, p_z are dumbbells along x, y, and z axes
2	d	5	mostly cloverleaf shapes
3	f	7	very complicated shapes!

Table 3

Shell (n)	Subshell (l)	Orbital Name (nl)	Orientations (m_l)	No. of Orbitals	Maximum Occupancy
$n = 1$	$l = 0$	1s	$m_l = 0$	1	2 e ⁻
$n = 2$	$l = 0$	2s	$m_l = 0$	1	2 e ⁻
	$l = 1$	2p	$m_l = 1, 0, -1$ (or p_x, p_y, p_z)	3	6 e ⁻
$n = 3$	$l = 0$	3s	$m_l = 0$	1	2 e ⁻
	$l = 1$	3p	$m_l = 1, 0, -1$ (or p_x, p_y, p_z)	3	6 e ⁻
	$l = 2$	3d	$m_l = 2, 1, 0, -1, -2$ (or $d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$)	5	10 e ⁻

Orbital Energies and Electron Configurations of Multi-Electron Atoms

For the H atom the orbital energy depends only on n , so all orbitals with the same value of n have the same energy. This is not true, however, for any other atom!

The H atom orbitals may be used to approximate the orbitals for multi-electron atoms. But since these atoms have more than one electron, electrons in the outer orbitals are shielded somewhat from the nucleus: they do not feel the full nuclear charge. Orbitals with a lower l value *penetrate closer* to the nucleus and are *less shielded* and have a *lower energy* than those with a higher l value. The result is that for a given value of n the energy order is $s < p < d < f$.

Orbitals are filled from *lowest energy to highest energy*. Each orbital holds 2 electrons (Pauli Exclusion Principle), one with spin up (\uparrow) and one with spin down (\downarrow). If more than one orbital has the same energy (e.g., p_x, p_y, p_z), electrons first enter *different* orbitals with *spins parallel* (Hund's Rule); once each orbital in the set contains one electron, additional electrons form pairs.

The order of orbital filling is easily remembered if correlated with the periodic chart. The order is 1s (first row of chart); 2s, 2p (second row); 3s, 3p (third row); 4s, 3d, 4p (fourth row); 5s, 4d, 5p (fifth row); 6s, 4f, 5d, 6p (sixth row); 7s, 5f, 6d. There are a few exceptions to these rules: see Chang, Table 7.3, p. 293 for atomic configurations.

CHM1045/Ch7/Quantum Numbers/ Practice Problems Name: _____

- Which type of electromagnetic radiation has the shortest wavelength?
 - red light
 - x rays
 - microwaves
 - gamma rays
 - blue light
- What is the wavelength of a photon having a frequency of 4.50×10^{14} Hz? ($c = 3.00 \times 10^8$ m/s, $h = 6.63 \times 10^{-34}$ J · s)
 - 667 nm
 - 1.50×10^{-3} nm
 - 4.42×10^{-31} nm
 - 0.0895 nm
 - 2.98×10^{-10} nm
- What is the energy of a photon of electromagnetic radiation with a wavelength of 877.4 nm? ($c = 3.00 \times 10^8$ m/s, $h = 6.63 \times 10^{-34}$ J · s)
 - 2.27×10^{-19} J
 - 5.82×10^{-40} J
 - 2.27×10^{-28} J
 - 3.42×10^{14} J
 - 1.94×10^{-39} J
- Which of the following is/are correct postulates of Bohr's theory of the hydrogen atom?
 - The energy of an electron in an atom is quantized (i.e. only specific energy values are possible).
 - The principal quantum number (n), specifies each unique energy level.
 - An electron transition from a lower energy level to a higher energy level results in an emission of a photon of light.
 - 1 only
 - 2 only
 - 3 only
 - 1 and 2
 - 1, 2, and 3
- List all the orbitals for which $n = 4$. (b) How many orbitals are there in all?

6. Which of the following subshells cannot exist: (a) 1p; (b) 4f; (c) 2d; (d) 5p; (e) 3f? Why not?
7. List all possible values of m_l for each of the indicated subshells. What role does the principal quantum number n play in determining your answer?

<i>Subshell</i>	<i>Values of m_l</i>
(a) 4s	
(b) 2p	
(c) 3d	
(d) 5f	

8. Give the formula that relates the number of possible values of m_l to the value of l .
9. Which of the following sets of quantum numbers (n, l, m_l, m_s) refers to a 3d orbital?
- A) 2 1 0 +1/2
 B) 5 4 3 +1/2
 C) 4 2 1 -1/2
 D) 4 3 1 -1/2
 E) 3 2 1 -1/2
10. An orbital with the quantum numbers $n = 3, l = 2, m_l = -1$, may be found in which subshell?
- A) 3f
 B) 3d
 C) 3p
 D) 3g
 E) 3s