STRUCTURE & PROPERTIES OF MATTER



Chapter 3 & 4 in Chemistry 12



Recap!



Exciting Atoms





Spectra of Hydrogen





Quantum Mechanics

- We left off by saying Bohr's model only explained the electron arrangement of Hydrogen...
- A new model was needed.
- Because of observations made regarding ionization energy and line spectra, it was concluded that we needed to take into consideration more than just the energy level of an electron
- Enter QUANTUM MECHANICS!

Ionization energy

- The first ionization energy of an element is the energy required to remove one electron from an atom
- We can see a pattern



© 2007 Encyclopædia Britannica, Inc.

• Why is there a difference between Li and Ne ? Draw a BR diagram of both.

Quantum Mechanics



Schrodinger applied idea of electrons behaving as a wave to the problem of electrons in atoms.

He developed the WAVE EQUATION

Solution gives set of math expressions called WAVE FUNCTIONS, Ψ

1887-1961

E. Schrodinger

The solutions to the Schrodinger wave equation describe the 3D shapes of the atomic orbitals where there is a high probability that electrons are located.



W. Heisenberg

1901-1976

Heisenberg "Uncertainty Principle"

• Electrons behave as both waves and particles.

- Heisenberg determined that it is impossible to know **BOTH** the exact position and momentum of an electron.
- He observed that on cannot simultaneously define the position and momentum (= m•v) of an electron.
 - If we define the energy exactly of an electron precisely we must accept limitation that we do not know exact position.

QUANTUM NUMBERS

The shape, size, and energy of each orbital is a function of 4 quantum numbers which describe the location of an electron within an atom or ion

n (principal) --->

l(orbital) --->

m_l (magnetic) --->

m_s(spin)

Principal Quantum Number, n

Each energy level (think: shell) has a number called the PRINCIPAL QUANTUM NUMBER, n

n can be 1-7 (because there are 7 periods on the periodic table



Secondary Orbital, l

Each energy level (n) has between 1 and 4
 sublevels or subshells, l

Possible values of $\ell = 0$ to n-1

Each sublevel is associated with a particular shape of probability

•4 shapes: s, p, d, and f

SHAPES



TYPES OF ORBITALS: S

When l = 0, the orbital is called s



Types of Orbitals (l)

When $\ell = 1$, the orbital is called p



planar node There is a PLANAR NODE thru the nucleus, which is an area of zero probability of finding an electron

PORBITALS



The p sublevel has 3 orbitals

The three p orbitals lie 90° apart in space

They are designated px, py, pz for the axis

Magnetic (m_l)

- How do we know p orbitals have 3 orbitals?
- Magnetic number represents the orientation





When $\ell = 2$, the orbital is called d



d orbitals



FORBITALS



When $\ell = 3$, the orbital is called f



Table 7.1 • Summary of the Quantum Numbers, Their Interrelationships, and the Orbital Information Conveyed

| Principal Quantum Number | Angular Momentum Quantum Number | Magnetic Quantum Number | Number and Type of Orbitals in the Subshell Number of orbitals in shell = n^2 and number of orbitals in subshell = $2\ell + 1$ | |
|--|--|---|--|--|
| Symbol = n Values = 1, 2, 3, n = number of subshells | $Symbol = \ell$ $Values = 0 \dots n - 1$ | $Symbol = m_{\ell}$ $Values = -\ell \dots 0 \dots + \ell$ | | |
| 1 | 0 | 0 | one 1s orbital (one orbital of one type in the $n = 1$ shell) | |
| 2 | 0 | 0 | one 2s orbital | |
| | 1 | +1, 0, -1 | three 2p orbitals | |
| | | | (four orbitals of two types in the $n = 2$ shell) | |
| 3 | 0 | 0 | one 3s orbital | |
| | 1 | +1, 0, -1 | three 3p orbitals | |
| | 2 | +2, +1, 0, -1, -2 | five 3d orbitals | |
| | | | (nine orbitals of three types in the $n = 3$ shell) | |
| 4 | 0 | 0 | one 4s orbital | |
| | 1 | +1, 0, -1 | three 4p orbitals | |
| | 2 | +2, +1, 0, -1, -2 | five 4d orbitals | |
| | 3 | +3, +2, +1, 0, -1, -2, -3 | seven 4f orbitals | |
| | | | (16 orbitals of four types in the $n = 4$ shell) | |

© 2003 Thomson - Brooks/Cole

RULES TO FOLLOW

Only 2 electrons per orbital!

The <u>Pauli Exclusion Principle</u> says that no two electrons within an atom (or ion) can have the same four quantum numbers.

If two electrons are in the same energy level, the same sublevel, and the same orbital, they must have opposite spins!

So M_s can be either +1/2 or -1/2 (and can be arbitrarily assigned)

Try it!

• Write a set of quantum numbers for an electron in a **1s** orbital

1S

Try some more!

• Write a set of quantum numbers for an electron in a **3p** orbital

3p

You made it!

- Let's try writing some quantum numbers!
- Write a set of 4 quantum numbers for an electron in:

• 2S

• 3d

• 4f

Try it!

- 1. What are the allowed values for *l* in each of the following cases?
 - (a) n = 5 (b) n = 1
- 2. What are the allowed values for m_l, for an electron with the following quantum numbers:
 - (a) l = 4 (b) l = 0
- 3. What are the names, m_l values, and total number of orbitals described by the following quantum numbers?

(a) n = 2, l = 0 (b) n = 4, l = 3

- 4. Determine the n, l, and possible m_l values for an electron in the 2p orbital.
- 5. Which of the following are allowable sets of quantum numbers for an atomic orbital? Explain your answer in each case.

(a) $n = 4, l = 4, m_l = 0$ (c) $n = 2, l = 0, m_l = 0$

(b) $n = 3, l = 2, m_l = 1$ (d) $n = 5, l = 3, m_l = -4$

Try it!

Practice Quantum numbers: p. 184 #3,4,6,7

Summarizing the Four Quantum Numbers for Electrons in Atoms

| Quantum Number Name | Symbol | Allowed Values | Property |
|------------------------|--------|-----------------------------------|-------------------------|
| principal | п | positive integers (1, 2, 3, etc.) | orbital size and energy |
| orbital-shape | 1 | integers from 0 to $(n-1)$ | orbital shape |
| magnetic | m_l | integers from $-l$ to $+l$ | orbital orientation |
| spin | m_s | $+\frac{1}{2}$ or $-\frac{1}{2}$ | electron spin direction |