Atomic Number

- The atomic number is equal to the number of protons in the nucleus.
  - Sometimes given the symbol Z.
  - On the periodic chart Z is the uppermost number in each element's box.
- In 1913 H.G.J. Moseley realized that the atomic number determines the element .
  - The elements differ from each other by the number of protons in the nucleus.
  - The number of electrons in a **neutral** atom is also equal to the atomic number.

Neutrons

- James Chadwick in 1932 analyzed the results of α-particle scattering on thin Be films.
- Chadwick recognized existence of massive neutral particles which he called neutrons.
  - Chadwick discovered the neutron.

Mass Number and Isotopes

- Mass number is given the symbol A.
- A is the sum of the number of protons and neutrons.
  - Z = proton number N = neutron number
  - A = Z + N
- A common symbolism used to show mass and proton numbers is

$$^{A}_{Z}E \text{ for example } ^{12}_{6}C,\ ^{48}_{20}Ca,\ ^{197}_{79}Au$$

- Can be shortened to this symbolism.

$$^{14}N,\ ^{63}Cu,\ ^{107}Ag, \text{ etc.}$$

Mass Number and Isotopes

- **Isotopes** are atoms of the same element but with different neutron numbers.
  - Isotopes have different masses and A values but are the same element.
- One example of an isotopic series is the hydrogen isotopes.

^{1}H or protium: one proton and no neutrons

^{2}H or deuterium: one proton and one neutron

^{3}H or tritium: one proton and two neutrons

Mass Number and Isotopes

- Another example of an isotopic series is the oxygen isotopes.

^{16}O is the most abundant stable O isotope.

8 protons and 8 neutrons

^{17}O is the least abundant stable O isotope.

8 protons and 9 neutrons

^{18}O is the second most abundant stable O isotope.

8 protons and 10 neutrons

The Atomic Weight Scale and Atomic Weights

- If we define the mass of ^{12}C as exactly 12 atomic mass units (amu), then it is possible to establish a relative weight scale for atoms.
  - 1 amu = (1/12) mass of ^{12}C by definition

The Atomic Weight Scale and Atomic Weights

- The atomic weight of an element is the weighted average of the masses of its stable isotopes
- Naturally occurring Cu consists of 2 isotopes. It is 69.1% ^{63}Cu with a mass of 62.9 amu, and 30.9% ^{65}Cu, which has a mass of 64.9 amu. Calculate the atomic weight of Cu to one decimal place.

The Atomic Weight Scale and Atomic Weights

$$\text{atomic weight} = \underbrace{(0.691)(62.9\ \text{amu})}_{^{63}\text{Cu isotope}} + \underbrace{(0.309)(64.9\ \text{amu})}_{^{65}\text{Cu isotope}}$$

$$\text{atomic weight} = 63.5\ \text{amu for copper}$$

The Atomic Weight Scale and Atomic Weights

- Naturally occurring chromium consists of four isotopes. It is 4.31% ${}_{24}^{50}Cr$, mass = 49.946 amu, 83.76% ${}_{24}^{52}Cr$, mass = 51.941 amu, 9.55% ${}_{24}^{53}Cr$, mass = 52.941 amu, and 2.38% ${}_{24}^{54}Cr$, mass = 53.939 amu. Calculate the atomic weight of chromium.

The Atomic Weight Scale and Atomic Weights

$$\begin{aligned}\text{atomic weight} &= (0.0431 \times 49.946\,\text{amu}) + (0.8376 \times 51.941\,\text{amu}) \\ &\quad + (0.0955 \times 52.941\,\text{amu}) + (0.0238 \times 53.939\,\text{amu}) \\ &= \left(2.153 + 43.506 + 5.056 + 1.284\right)\text{amu} \\ &= 51.998\,\text{amu}\end{aligned}$$

The Atomic Weight Scale and Atomic Weights

- The atomic weight of boron is 10.811 amu. The masses of the two naturally occurring isotopes ${}_{5}^{10}B$ and ${}_{5}^{11}B$, are 10.013 and 11.009 amu, respectively. Calculate the fraction and percentage of each isotope.
- This problem requires a little algebra.
  - A hint for this problem is $x + (1-x) = 1$

The Atomic Weight Scale and Atomic Weights

$$10.811\,\text{amu} = \underbrace{x(10.013\,\text{amu})}_{^{10}\text{B isotope}} + \underbrace{(1-x)(11.009\,\text{amu})}_{^{11}\text{B isotope}}$$

$$= (10.013\,x + 11.009 - 11.009\,x)\,\text{amu}$$

$$(10.811 - 11.009)\,\text{amu} = (10.013\,x - 11.009\,x)\,\text{amu}$$

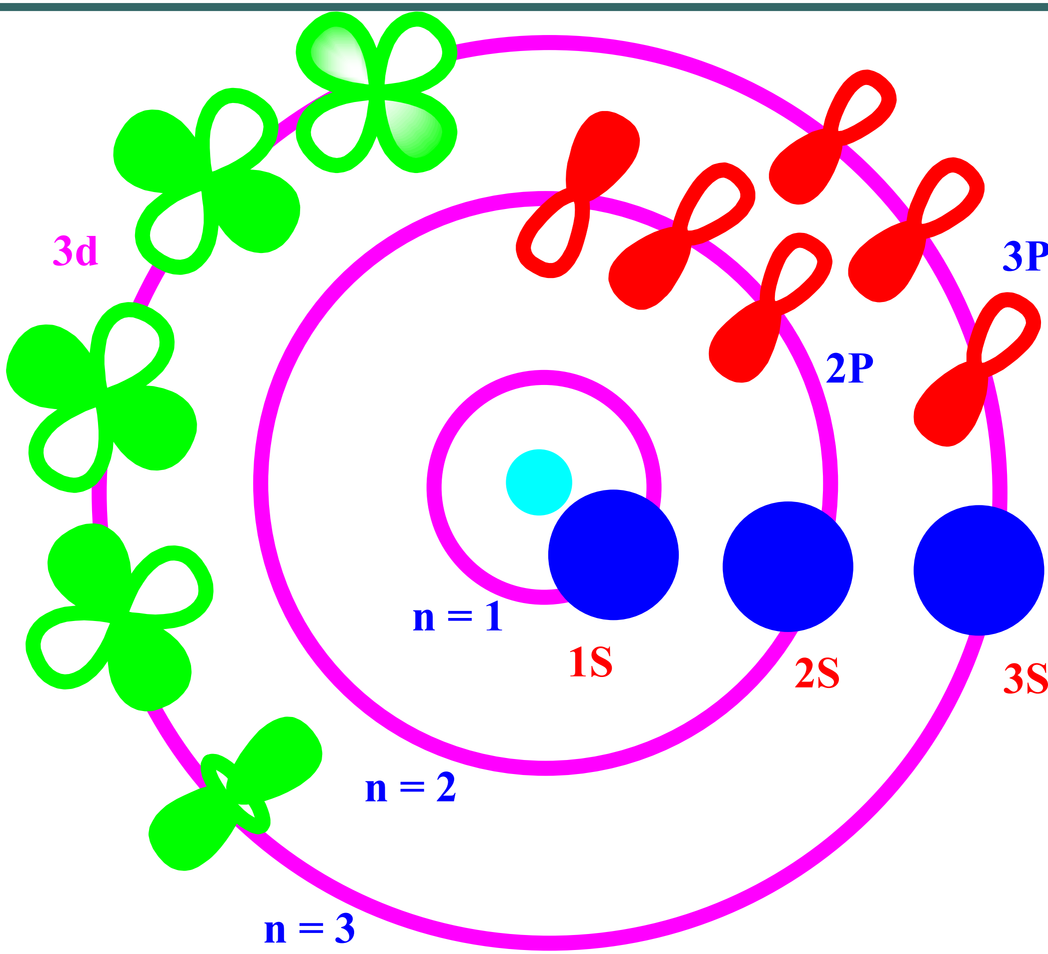
$$-0.198 = -0.996\,x$$

$$0.199 = x$$

The Atomic Weight Scale and Atomic Weights

- Note that because *x* is the multiplier for the ^{10}B isotope, our solution gives us the fraction of natural B that is ^{10}B.
- Fraction of ^{10}B = 0.199 and % abundance of ^{10}B = 19.9%.
- The multiplier for ^{11}B is (1-*x*) thus the fraction of ^{11}B is 1-0.199 = 0.811 and the % abundance of ^{11}B is 81.1%.

Quantum Numbers (n, ℓ, m_ℓ, m_s)



Quantum Numbers

- The principal quantum number has the symbol n.

  n = 1, 2, 3, 4, ... "shells"

  n = K, L, M, N, ...

  The electron's energy depends principally on n .

Quantum Numbers

- The angular momentum quantum number has the symbol ℓ.

  ℓ = 0, 1, 2, 3, 4, 5, ...(n-1)

  ℓ = s, p, d, f, g, h, ...(n-1)
- ℓ tells us the shape of the orbitals.
- These orbitals are the volume around the atom that the electrons occupy 90-95% of the time.

Quantum Numbers

- The symbol for the magnetic quantum number is m_ℓ.
  m_ℓ = - ℓ , (- ℓ + 1), (- ℓ +2), ...0, ..., (ℓ -2), (ℓ -1), ℓ
- If ℓ = 0 (or an s orbital), then m_ℓ = 0.
  - Notice that there is only 1 value of **m_ℓ**.
    Thus there is one s orbital per n value. $n \geq 1$
- If ℓ = 1 (or a p orbital), then m_ℓ = -1,0,+1.
  - There are 3 values of **m_ℓ**.
  - Thus there are 3 p orbitals per n value. $n \geq 2$

Quantum Numbers

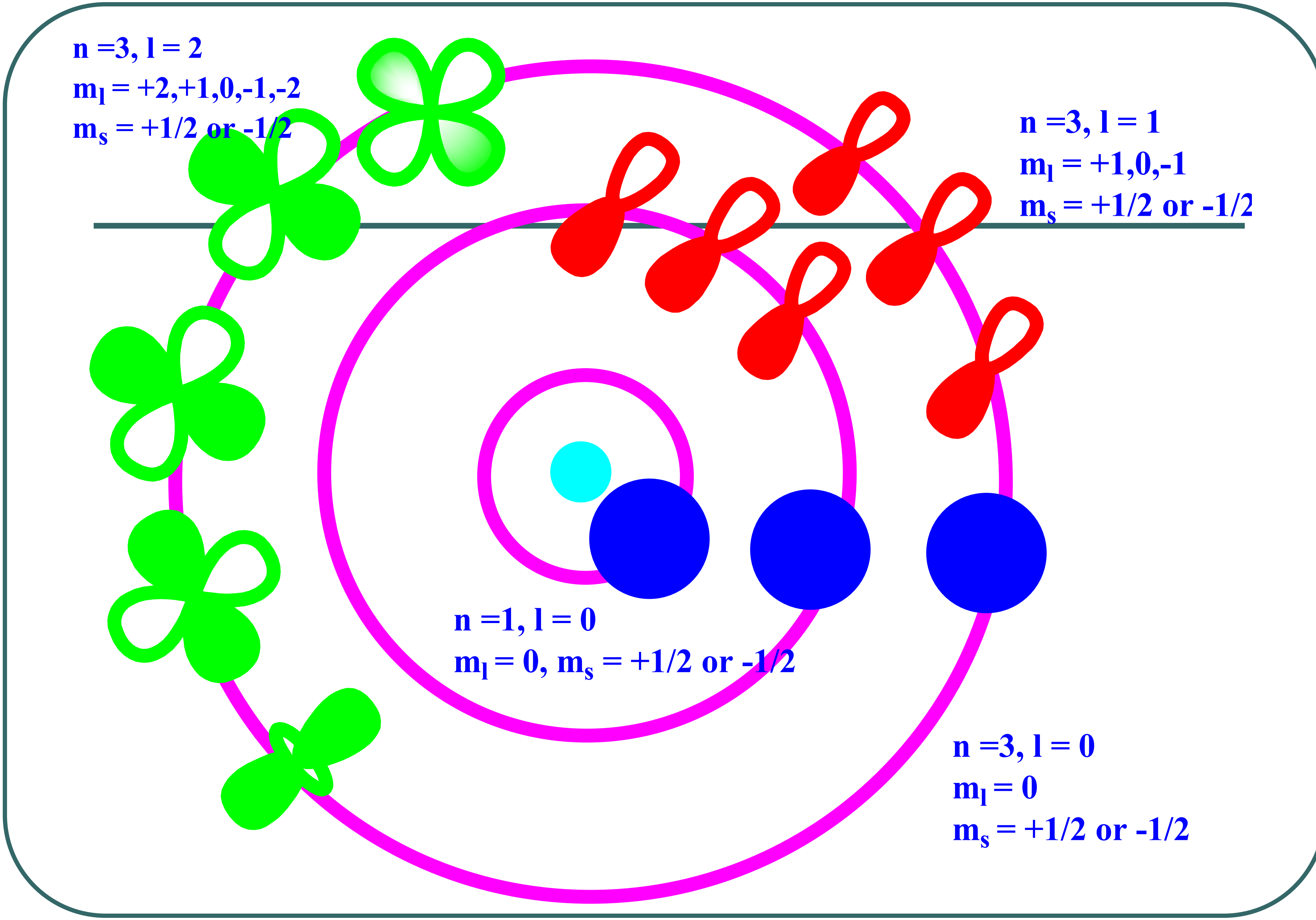
- If ℓ = 2 (or a d orbital), then m_ℓ = -2,-1,0,+1,+2.
  - There are 5 values of $\mathbf{m_\ell}$.

    Thus there are five d orbitals per n value. $n \geq 3$
- If ℓ = 3 (or an f orbital), then m_ℓ = -3,-2,-1,0,+1,+2, +3.
  - There are 7 values of $\mathbf{m_\ell}$.

    Thus there are seven f orbitals per n value, n

Quantum Numbers

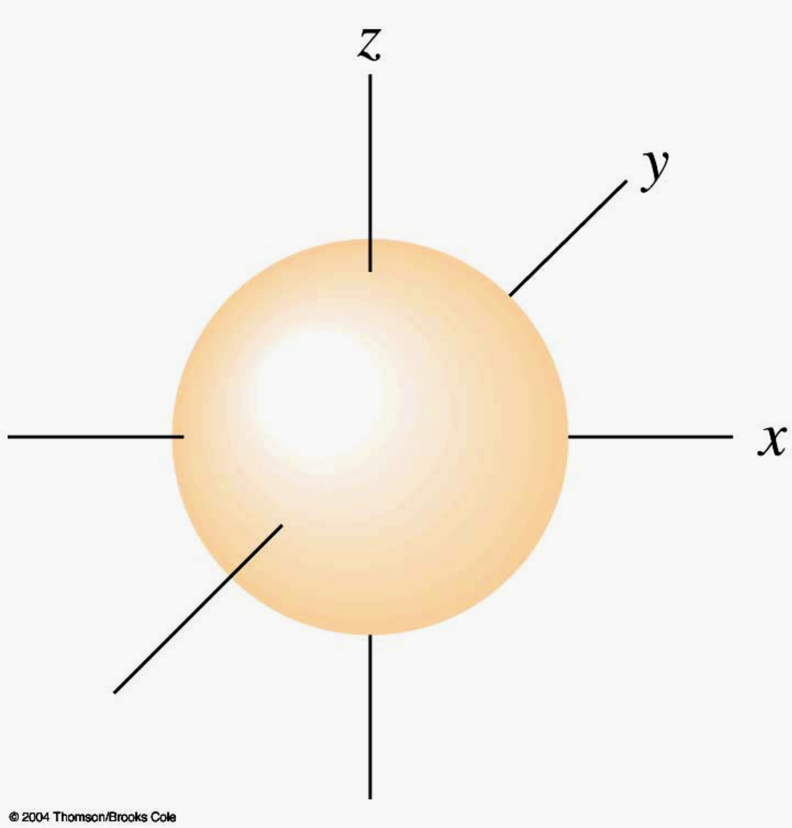
- The last quantum number is the <u>spin quantum number</u> which has the symbol m_s.
- The spin quantum number only has two possible values.
  - $m_s = +1/2$ or $-1/2$
  - $m_s = \pm 1/2$
- This quantum number tells us the spin and orientation of the magnetic field of the electrons.
  - <u>No two electrons in an atom can have the same set of 4 quantum numbers.</u>


n =3, l = 2
m_l = +2,+1,0,-1,-2
m_s = +1/2 or -1/2
n =3, l = 1
m_l = +1,0,-1
m_s = +1/2 or -1/2
n =1, l = 0
m_l = 0, m_s = +1/2 or -1/2
n =3, l = 0
m_l = 0
m_s = +1/2 or -1/2

Atomic Orbitals

- Atomic orbitals are regions of space where the probability of finding an electron about an atom is highest.
- s orbital properties:

  s orbitals are spherically symmetric.
  - There is one s orbital per n level.
  - $\ell = 0$
  - 1 value of m_ℓ

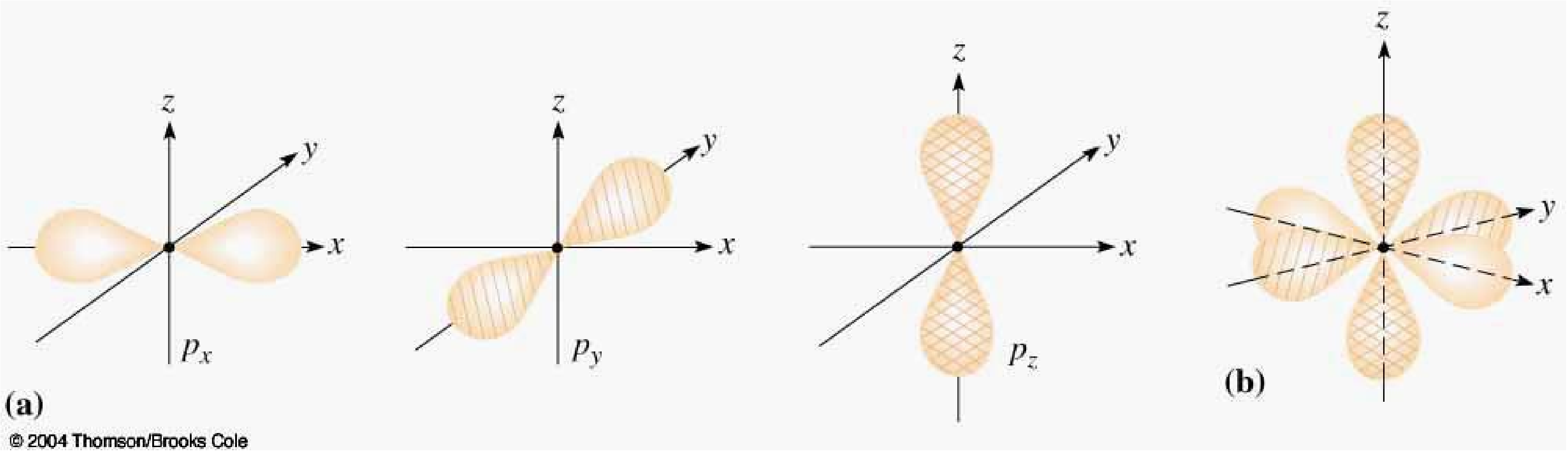


Atomic Orbitals

- p orbital properties:
  - The first p orbitals appear in the n = 2 shell.
- p orbitals are peanut or dumbbell shaped volumes.
  - They are directed along the axes of a Cartesian coordinate system.
- There are 3 p orbitals per n level.
  - The three orbitals are named p_x, p_y, p_z.
  - They have an $\ell = 1$.
  - $m_\ell = -1,0,+1$ 3 values of m_ℓ

Atomic Orbitals

- p orbitals are peanut or dumbbell shaped.

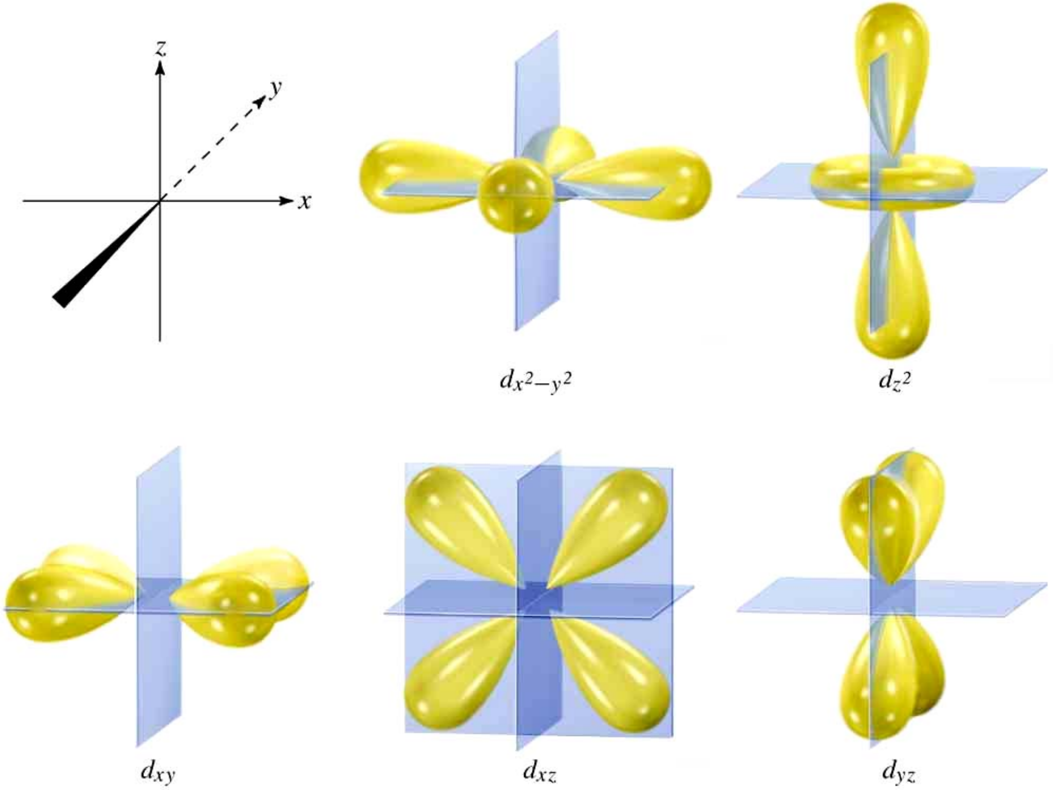


Atomic Orbitals

- d orbital properties:
  - The first d orbitals appear in the n = 3 shell.
- The five d orbitals have two different shapes:
  - 4 are clover leaf shaped.
  - 1 is peanut shaped with a doughnut around it.
  - The orbitals lie directly on the Cartesian axes or are rotated 45° from the axes.
- There are 5 d orbitals per n level.
  - The five orbitals are named $d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$
  - They have an $\ell = 2$.
  - $m_\ell = -2,-1,0,+1,+2$ 5 values of m_ℓ

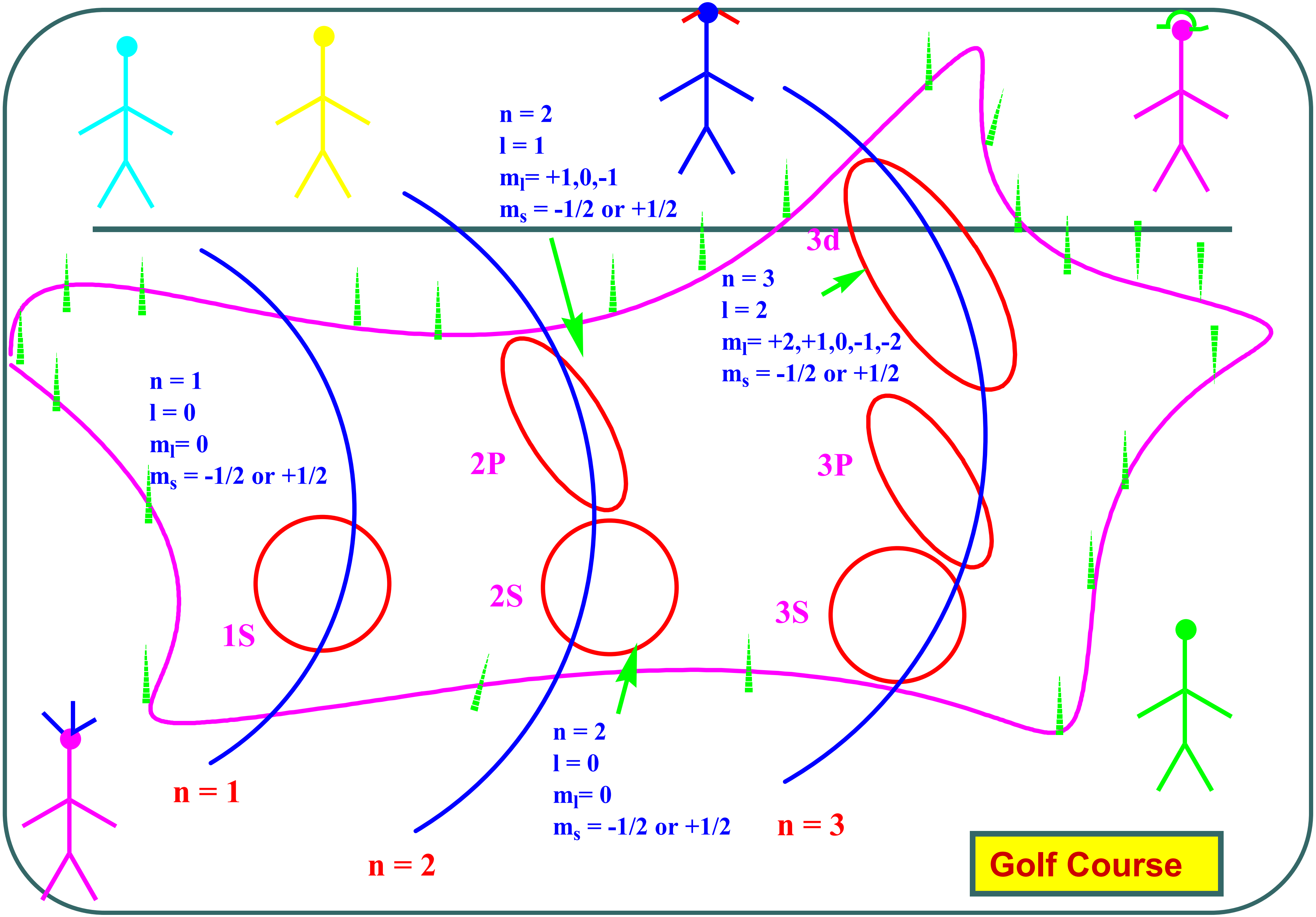
Atomic Orbitals

- d orbital shapes



Atomic Orbitals

- f orbital properties:
  - The first f orbitals appear in the n = 4 shell.
- The f orbitals have the most complex shapes.
- There are seven f orbitals per n level.
  - The f orbitals have complicated names.
  - They have an $\ell = 3$
  - $m_\ell = -3,-2,-1,0,+1,+2, +3$ 7 values of m_ℓ



n = 2
l = 1
m_l= +1,0,-1
m_s = -1/2 or +1/2
3d
n = 3
l = 2
m_l= +2,+1,0,-1,-2
m_s = -1/2 or +1/2
n = 1
l = 0
m_l= 0
m_s = -1/2 or +1/2
2P
3P
2S
3S
1S
n = 2
l = 0
m_l= 0
m_s = -1/2 or +1/2
n = 1
n = 2
n = 3
Golf Course

Atomic Orbitals

- Spin quantum number effects:
  - Every orbital can hold up to two electrons.
    - Consequence of the Pauli Exclusion Principle.
  - The two electrons are designated as having
  - one spin up $\uparrow$ and one spin down $\downarrow$
- Spin describes the direction of the electron's magnetic fields.

Chemistry is fun!