5.6 Wave Functions & Quantum Numbers

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Schrödinger's "wave functions" (Ψ)
Bohr's orbitals (Ψ^2)

Wave equation → wave f(x) or orbital (Ψ) → Probability of finding e^- in region of space

3 Parameters

* Principal Quantum # (n)
  - size & E of orbital (defines E level)
  - called a shell
  - simple (+) integers (1, 2, 3 ...)
* Angular Quantum # (ℓ)
  - defines shape
  - 3D shape of orbital
  - subshells
  - "n" different shapes
    - > s, p, d, f, g (0, 1, 2, 3, 4)
* Magnetic Quantum #
  - define spatial orientation of suborbitals
  - $2\ell+1$ values (can be (-))

eigenvalues (e^- overlap)

TABLE 5.1 Allowed Combinations of Quantum Numbers n, l, and m_l for the First Four Shells

n	l	m_l	Orbital Notation	Number of Orbitals in Subshell	Number of Orbitals in Shell
1	0	0	1s	1	1
2	0	0	2s	1	4
	1	−1, 0, +1	2p	3	
3	0	0	3s	1	9
	1	−1, 0, +1	3p	3	
	2	−2, −1, 0, +1, +2	3d	5	
4	0	0	4s	1	16
	1	−1, 0, +1	4p	3	
	2	−2, −1, 0, +1, +2	4d	5	
	3	−3, −2, −1, 0, +1, +2, +3	4f	7	

Using Quantum # for orbital notation

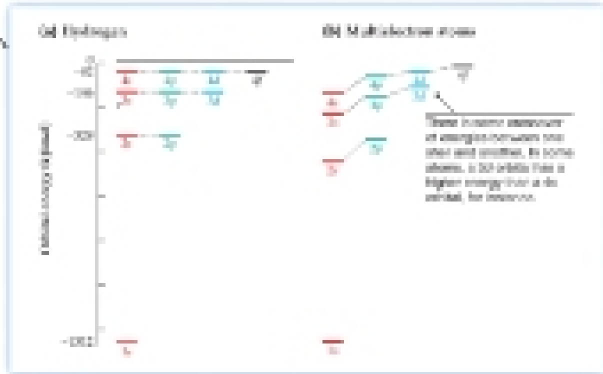
n=3 ℓ=1 m=1

orbital → 3p

your "n" value gives the shell number (3)

p determined using ℓ value (0=s, 1=p, 2=d, 3=f, ..)

Unoccupied Orbitals



→ excited states

← lowest E is "ground state"

5.7 — Shapes of Orbitals

1 "s" orbital is spherical

3 "p" orbitals 2-lobed & dumbbell shaped

5.8 Atomic Line Spectra

Energy Quantanization

- e^- in occupied orbitals excited into unoccupied e^- levels
- Outer shells = ↑ energy
  - > more E required to reach

Spectral Lines

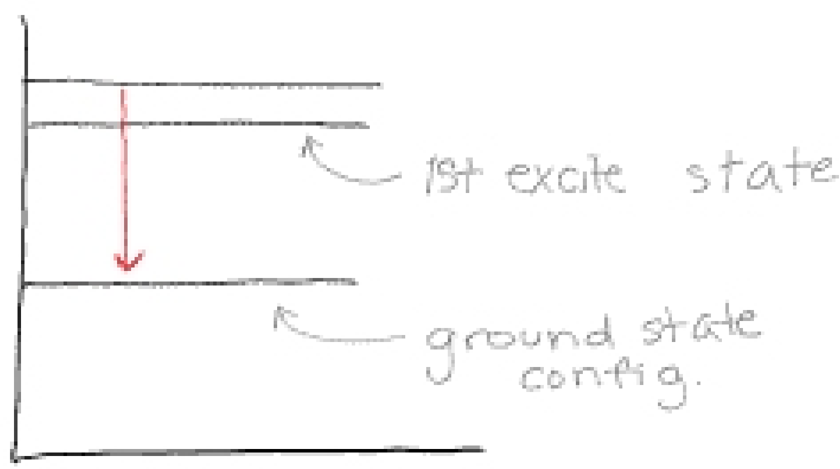
- Separations b/w orbitals (E)

m – shell transferring to (inner)

n – shell transferring from (outer)

$$\frac{1}{\lambda} = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

gap b/w is quantized Energy (E)



d

5.9 E^- Spin & the Pauli Exclusion Principle

Fermions (p^+, n^0, e^-)

↳ · Half integer spins ($+\frac{1}{2}$, $-\frac{1}{2}$)

· Cannot superimpose ↳

Bosons (photons)

↳ · Integer spins

· Can superimpose

What does a half spin mean?

↳ 2 e^- can be in same orbital, if opposite spins

Spin Quantum # (m_s) → e^- spin have tiny magnetic fields

Pauli Exclusion Principle

> No 2 e^- in atom can have same 4 quantum number

1s orbital has 2 e^-

2p orbital has 6 e^-

⋮

5.10 Orbital E levels in Multielectron Atoms

> ↑ the elements get (more protons), orbitals get more strength

> Hydrogen orbitals are degenerate

(1s / 2p separation same as 1s/2s)

· larger elements, E in subshells are ≠

(1s/2p ≠ 1s/2s)

> Radius is relative to stability