

What is inorganic chemistry?

Organic Chemistry:

the chemistry of life

the chemistry of hydrocarbon compounds

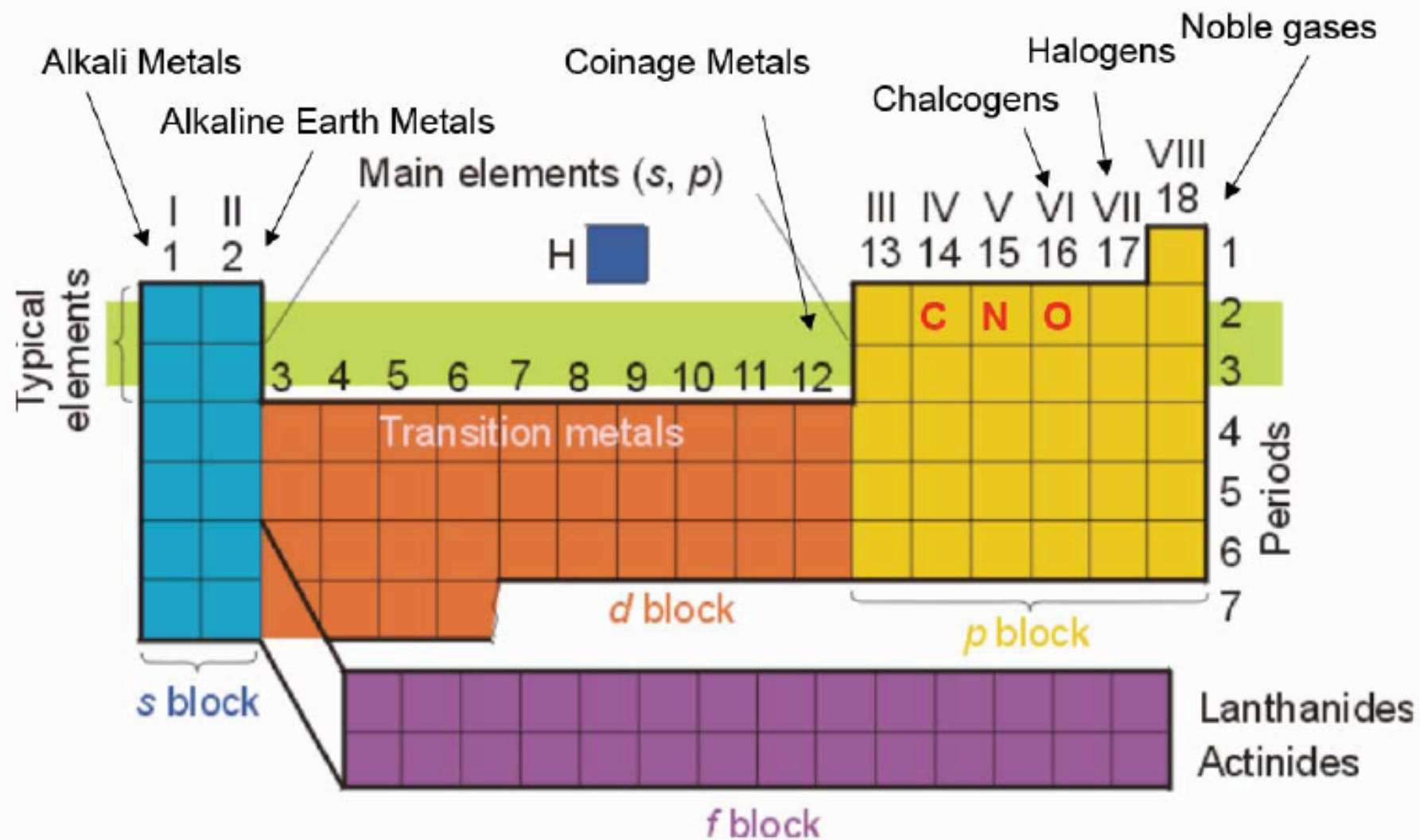
C, H, N, O

Inorganic Chemistry:

Non-living chemistry

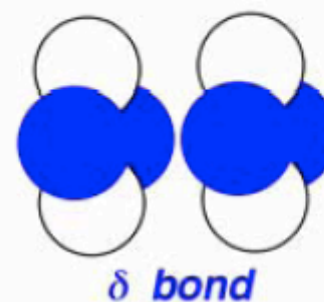
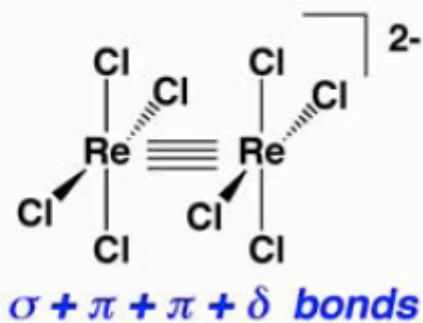
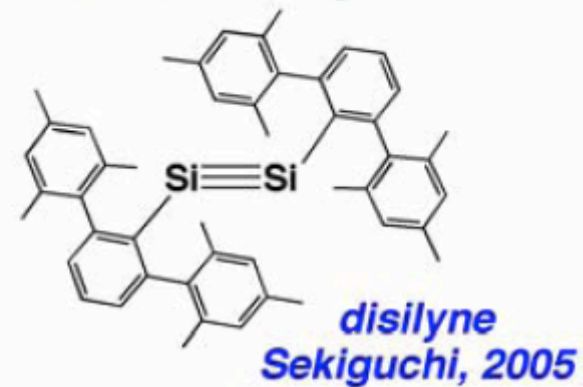
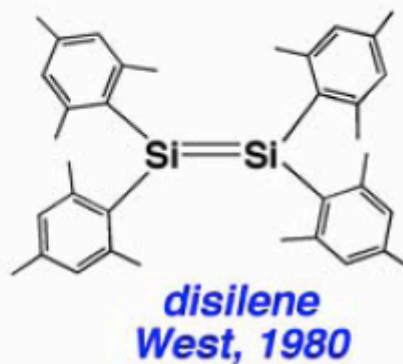
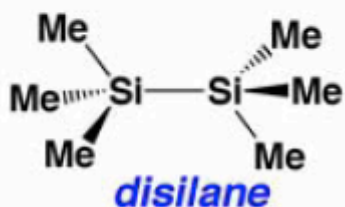
Chemistry of “everything else”

Chemistry of the entire periodic table

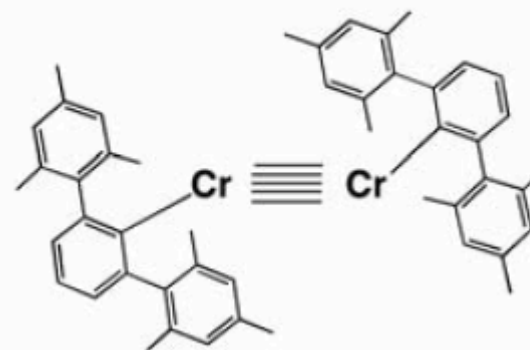


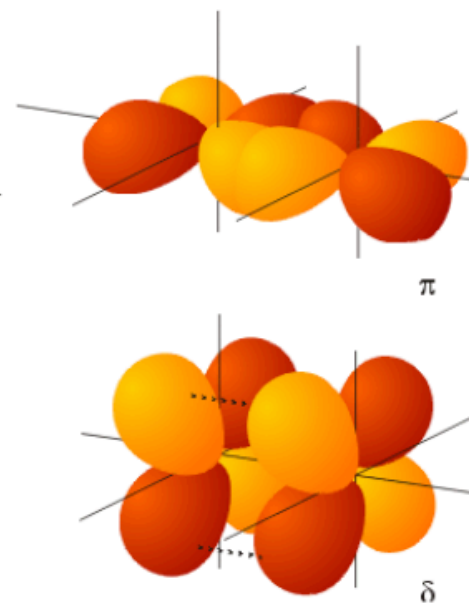
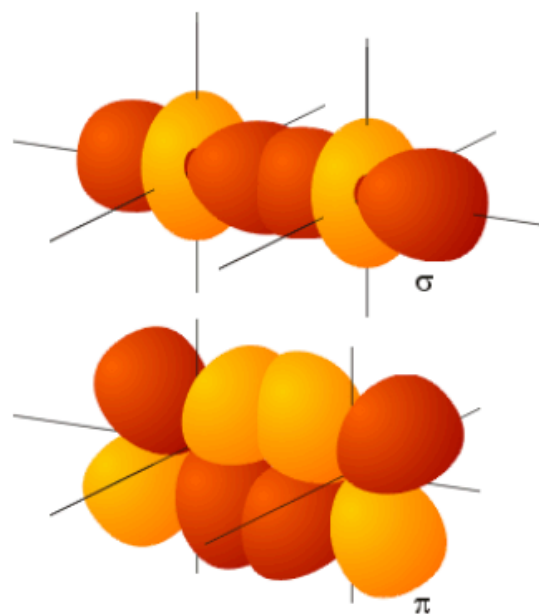
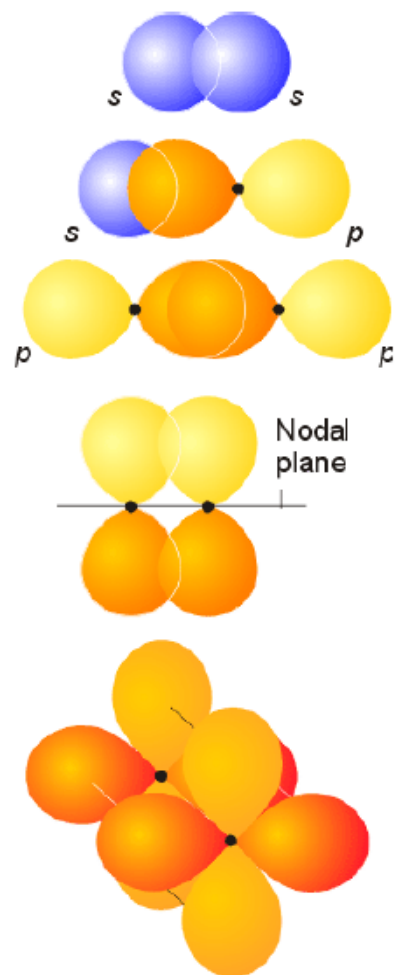
	Organic Compounds	Inorganic Compounds
Single Bond	✓	✓
Double Bond	✓	✓
Triple Bond	✓	✓
Quadruple bond	✗	✓
Coordination No.	Constant	Diverse
Geometry	Fixed	Diverse

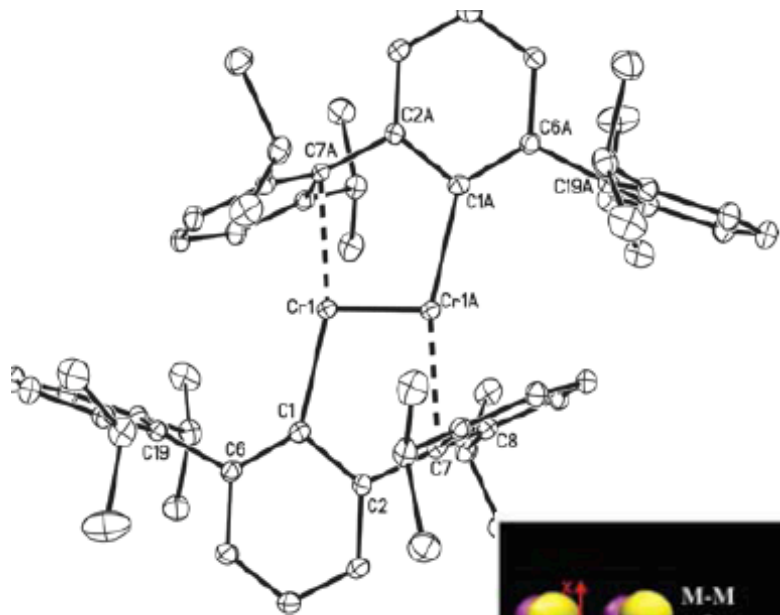
Multiple Bonds in Inorganic Chemistry



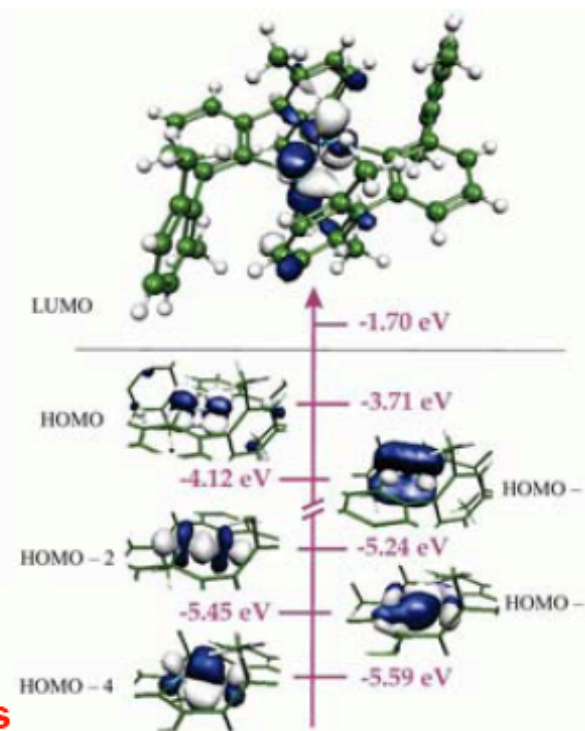
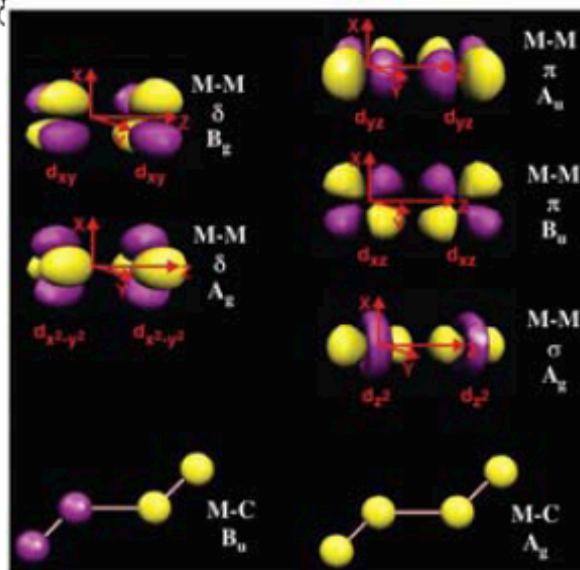
a pentuple bond
Power, 2005







Science 4 November 2005:
Vol. 310. no. 5749, pp. 844 - 847



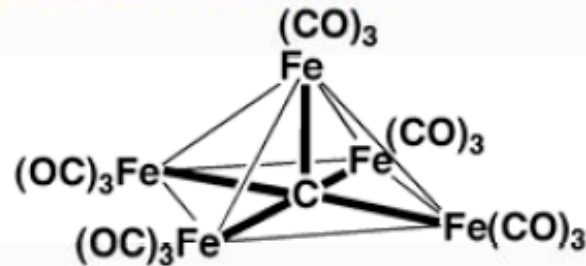
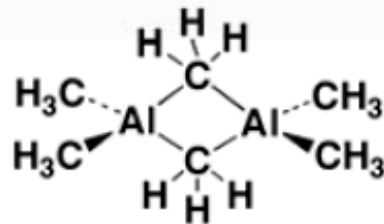
**A Stable Compound with
Fivefold Bonding Between Two Chromium(I) Centers**

Connectivity and Valence in Inorganic Chemistry

How many bonds can be formed to a single carbon atom?

organic chemistry: 2, 3 or 4 bonds

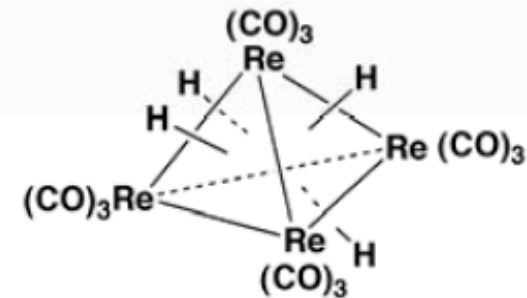
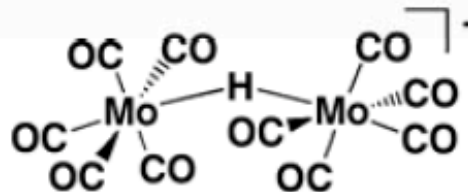
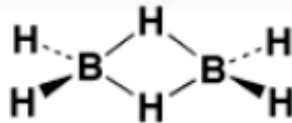
inorganic chemistry:



How many bonds can be formed to a single hydrogen atom?

organic chemistry: 1 bond

inorganic chemistry:



Common applications of inorganic chemistry

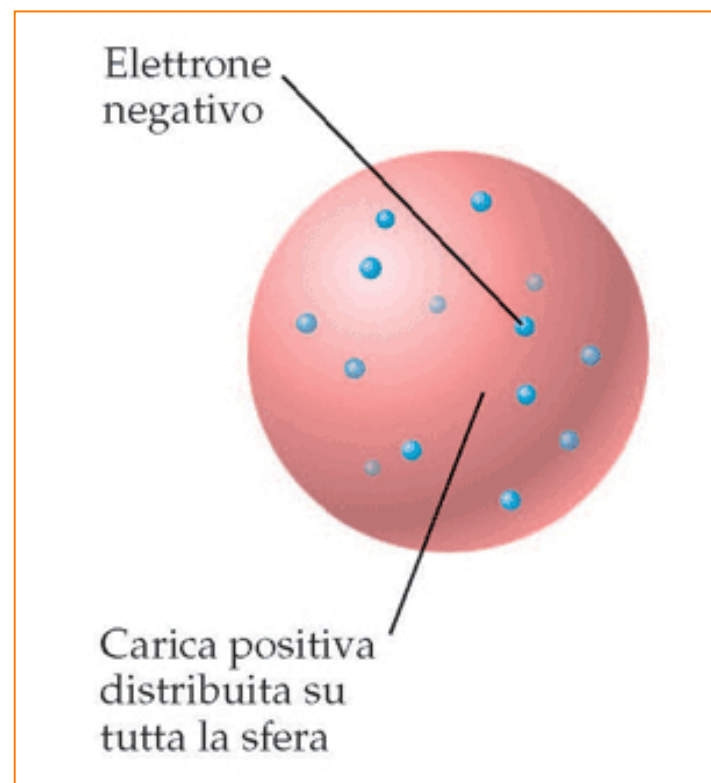
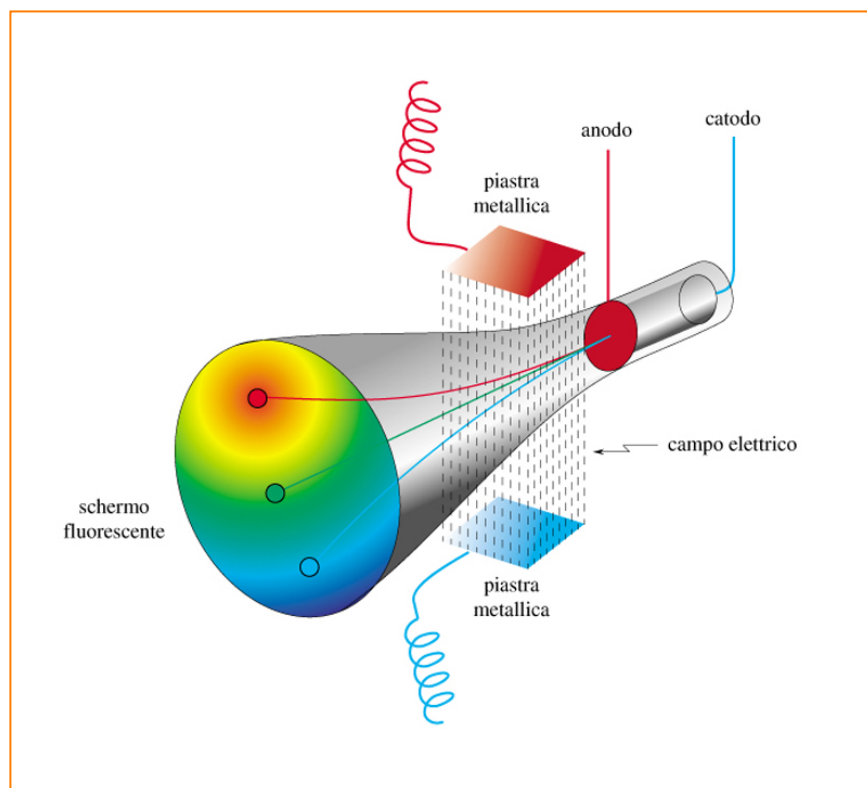
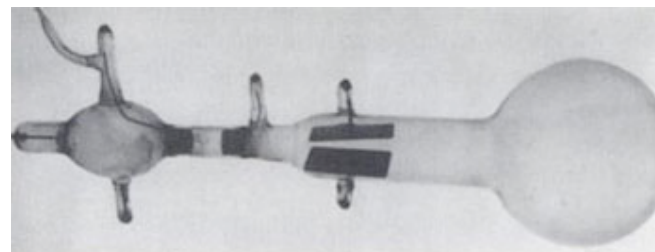


- **Catalysts:** aluminum oxides, zeolites, transition metals
- **Semiconductors:** Si, Ge, GaAs, InP
- **Polymers:** silicones, $(\text{SiR}_2)_n$, polyphosphazenes
- **Superconductors:** NbN, $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$, $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_z$
- **Magnetic Materials:** Fe, SmCo_5 , $\text{Nd}_2\text{Fe}_{14}\text{B}$
- **Lubricants:** graphite, MoS_2
- **Nanostructured materials:** nanoclusters, nanowires and nanotube
- **Fertilizers:** NH_4NO_3 , $(\text{NH}_4)_2\text{SO}_4$
- **Paints:** TiO_2 , PbCrO_4
- **Disinfectants/oxidants:** Cl_2 , Br_2 , I_2 , MnO_4^-
- **Water treatment:** $\text{Ca}(\text{OH})_2$, $\text{Al}_2(\text{SO}_4)_3$
- **Industrial processes:** H_2SO_4 , NaOH, CO_2
- **Organic synthesis:** reaction catalysts
- **Biology:** Vitamin B_{12} , hemoglobin, Fe-S protein

Struttura dell'atomo: il nucleo

Le tappe fondamentali delle scoperte sulla materia:

J.J. Thomson (1856-1940):



La struttura atomica

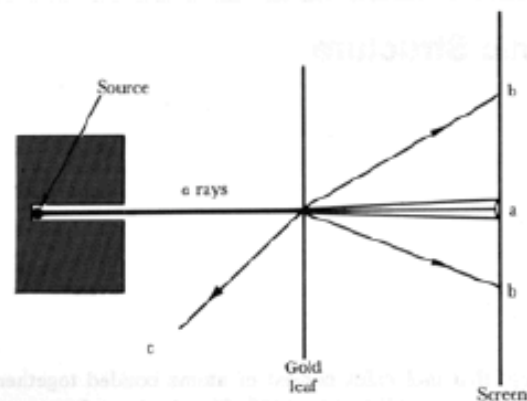
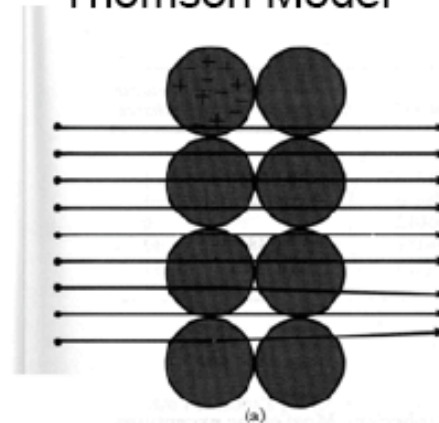


Figure 1-1 The experimental arrangement for Rutherford's measurement of the scattering of α particles by very thin gold foils. The source of the α particles was radioactive radium, which was encased in a lead block to protect the surroundings from radiation and to confine the α particles to a beam. The gold foil used was about 6×10^{-5} cm thick. Most of the α particles passed through the gold leaf with little or no deflection, at a. A few were deflected at wide angles, b, and occasionally a particle rebounded from the foil, c, and was detected by a screen or counter placed on the same side of the foil as the source.

Thomson Model



Rutherford Model

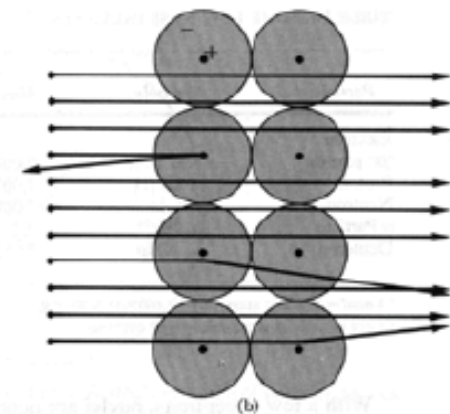
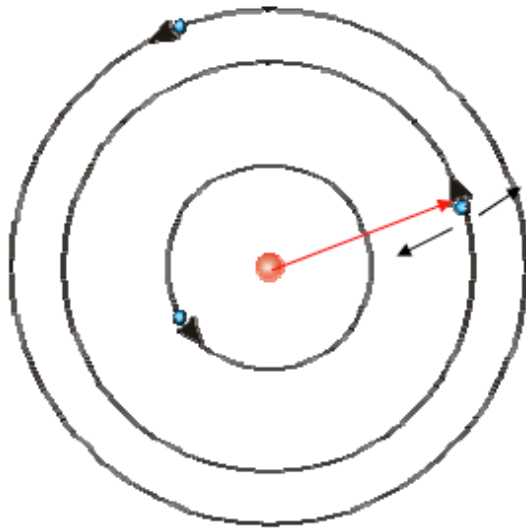


Figure 1-2 The expected outcome of the Rutherford scattering experiment, if one assumes (a) the Thomson model of the atom, and (b) the model deduced by Rutherford. In the Thomson model, mass is spread throughout the atom, and the negative electrons are embedded uniformly in the positive mass. There would be little deflection of the beam of positively charged α particles. In the Rutherford model all of the positive charge and virtually all of the mass is concentrated in a very small nucleus. Most α particles would pass through undeflected. But close approach to a nucleus would produce a strong swerve in the path of the α particle, and head-on collision would lead to its rebound in the direction from which it came.

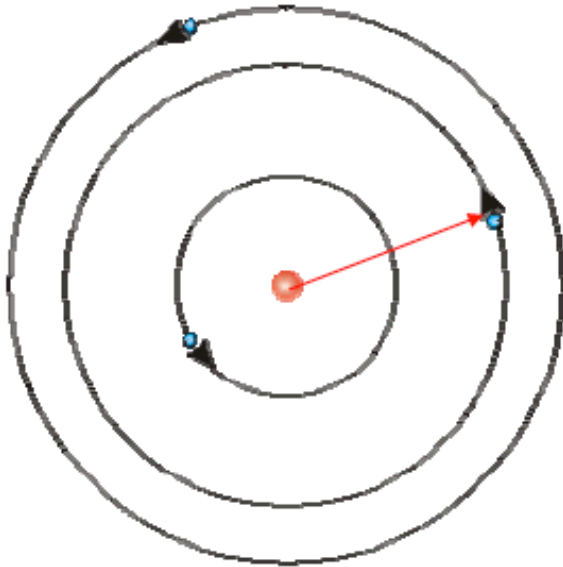
Il modello di Bohr

1913, Danish Physicist, Niels Bohr



Electrostatic F_e = Outward F_o

$$\frac{m_e v^2}{r} = \frac{e^2}{r^2}$$



$$\frac{m_e v^2}{r} = \frac{e^2}{r^2}$$

Total Energy:

$$\mathbf{E} = \mathbf{KE + PE}$$

$$\begin{aligned} E &= \frac{1}{2} m_e v^2 + \left(-\frac{e^2}{r} \right) \\ &= \frac{1}{2} \left(\frac{e^2}{r} \right) - \frac{e^2}{r} \\ &= -\frac{e^2}{2r} \end{aligned}$$



Energy Quantized (Planck Equation)

$$E = h\nu \longrightarrow \text{Frequency}$$



Angular Momentum of electron is quantized.

$$m_e v_e r = nh/2\pi$$



$$v = \frac{nh}{2\pi m_e r}$$

$$h = 6.62 \times 10^{-34} \text{ J.s}$$

 velocity



Velocity of the electron quantized

$$\frac{m_e v^2}{r} = \frac{e^2}{r^2}$$

$$v = \frac{nh}{2\pi m_e r}$$

$$\longrightarrow r_n = \frac{n^2 h^2}{4\pi^2 m_e e^2} = n^2 a_0$$

$r_1 = \text{Bohr radius} = a_0 = 0.529 \text{ \AA}$



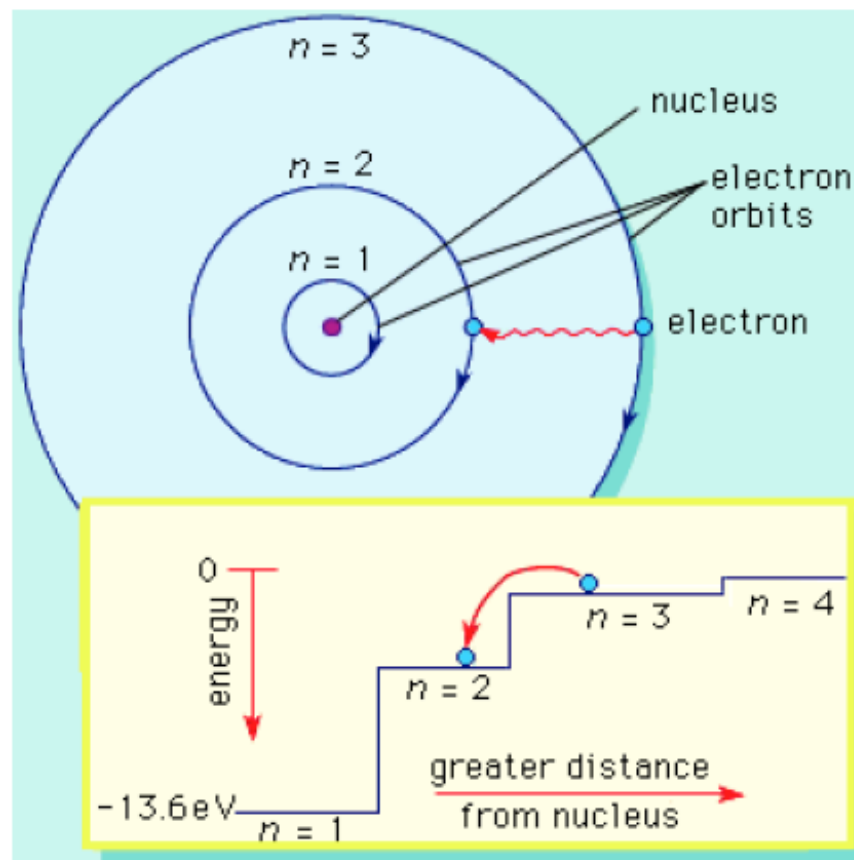
$$E = \frac{1}{2} m_e v^2 + \left(-\frac{e^2}{r}\right)$$

$$= \frac{1}{2} \left(\frac{e^2}{r}\right) - \frac{e^2}{r}$$

$$= -\frac{e^2}{2r}$$

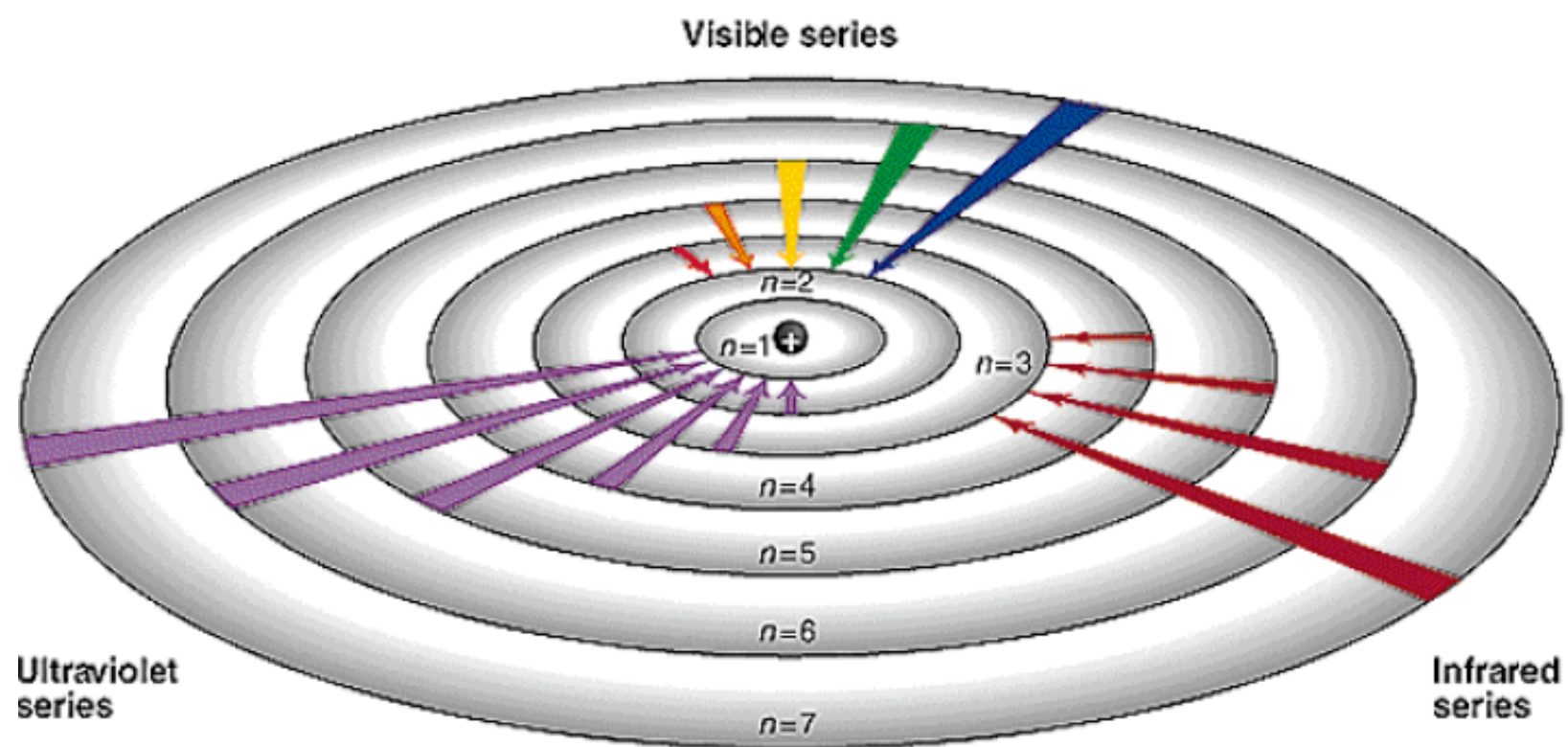
$$\longrightarrow E_n = -\frac{e^2}{2r_n} = -\frac{2\pi^2 m_e e^4}{n^2 h^2} = -\frac{k}{n^2}$$

$k = 13.606 \text{ eV}$

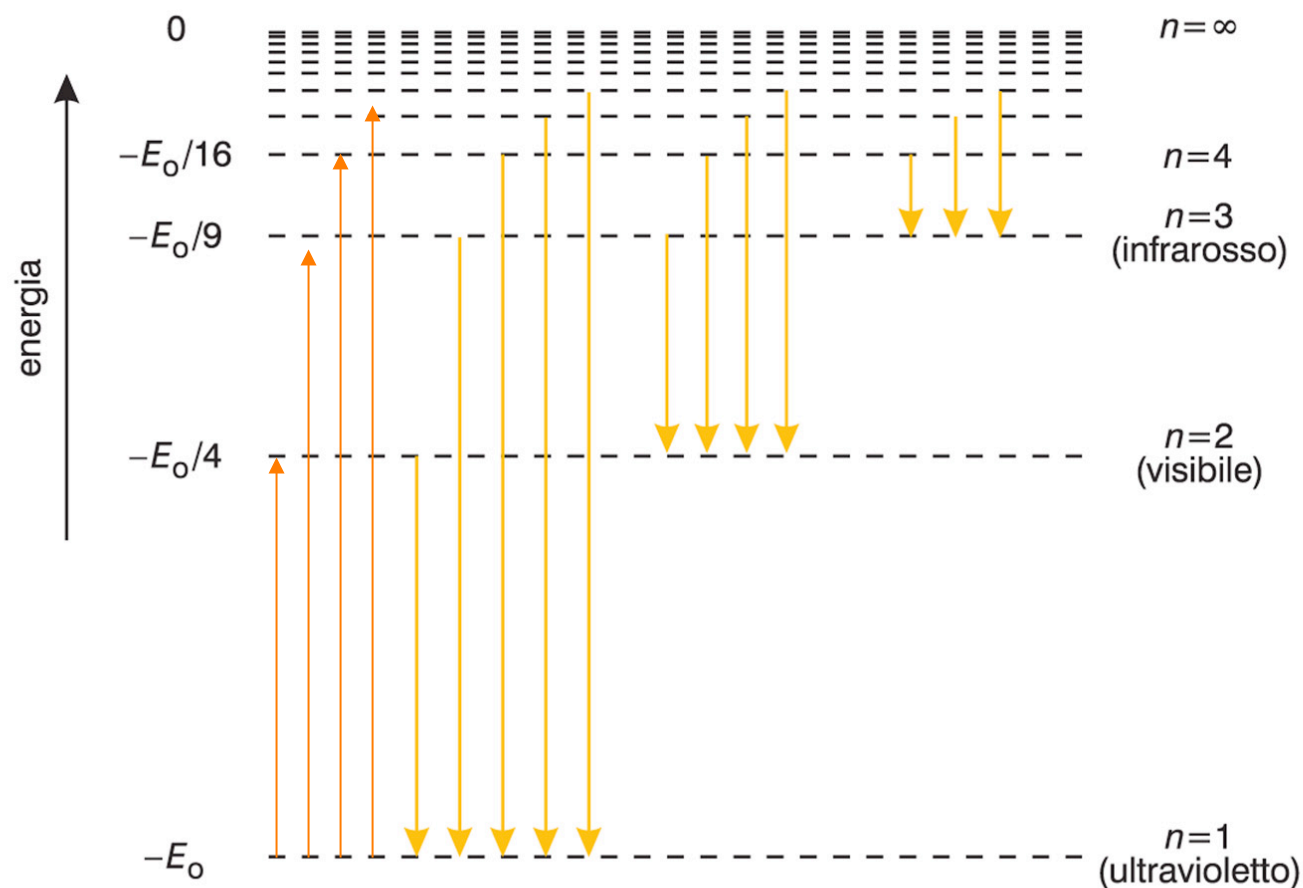


The electron travels in circular orbits around the nucleus. The orbits have quantized sizes and energies. Energy is emitted from the atom when the electron jumps from one orbit to another closer to the nucleus. Shown here is the first Balmer transition, in which an electron jumps from orbit $n = 3$ to orbit $n = 2$, producing a photon of red light with an energy of 1.89 eV and a wavelength of $656 \times 10^{-9} \text{m}$.

$$\Delta E = h\nu = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

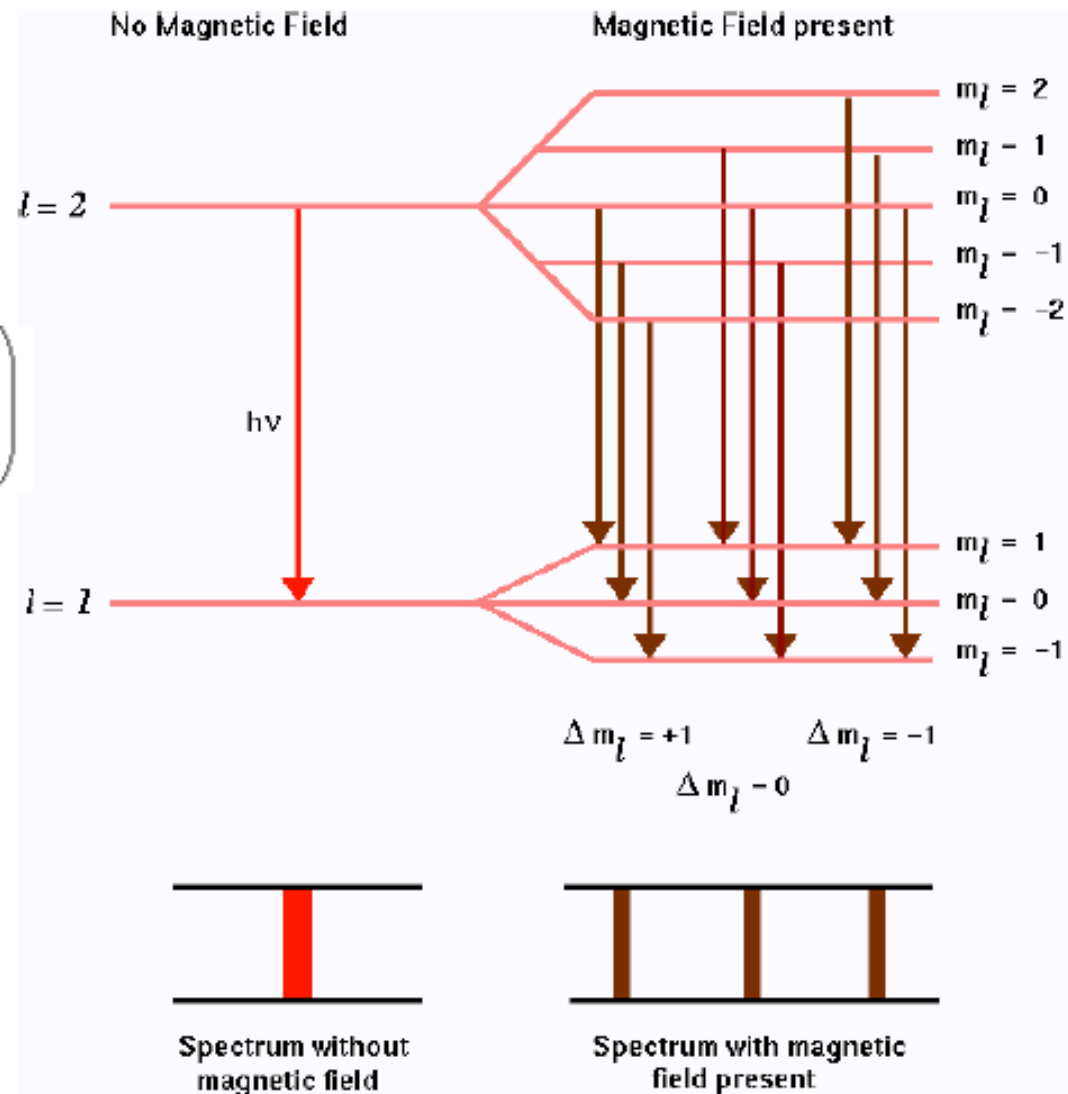


Transizioni tra i livelli energetici



Bohr Model can NOT explain Zeeman effect.

$$\Delta E = h\nu = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$



Spettri atomici

Spettrografi ad alta risoluzione misero in evidenza **multipletti** negli spettri atomi polielettronici.

Sommerfeld: l'elettrone non descrive orbite circolari, ma ellittiche, in cui il nucleo dell'atomo rappresenta uno dei due fuochi.

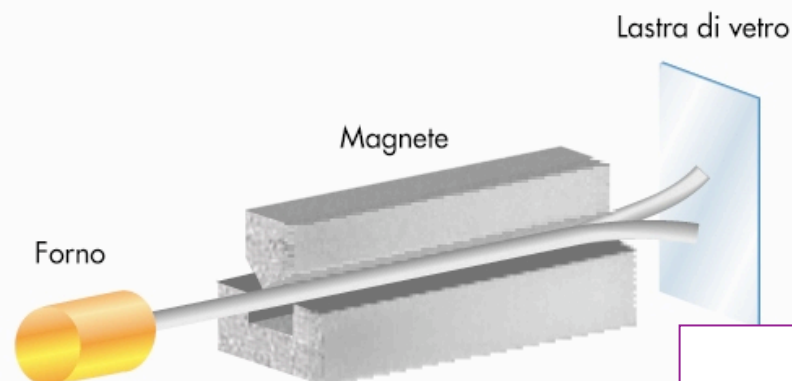
numero quantico angolare $0 < l < (n-1)$

Quando l'elettrone percorre la sua orbita genera un campo magnetico: studiando gli spettri degli atomi eccitati sottoposti ad un campo magnetico esterno, vennero osservati ulteriori sdoppiamenti (**effetto Zeeman**).

numero quantico magnetico $-l < m < +l$

Ad indicare che il piano dell'orbita può assumere solo determinate orientazioni rispetto alla direzione del campo esterno.

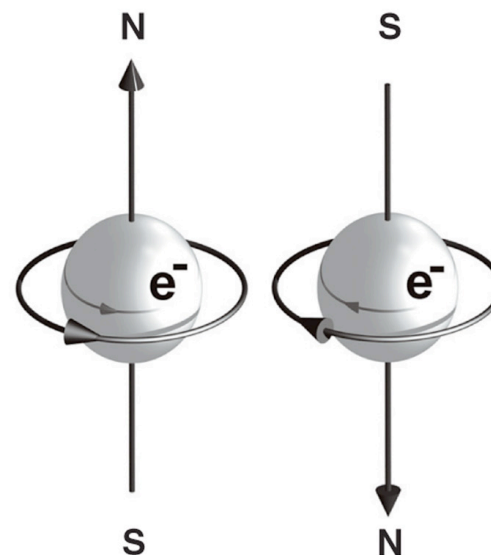
Spettri atomici



Fascio di atomi di argento in un campo non uniforme.
Fascio sdoppiato in modo simmetrico rispetto direzione originaria.

Elettrone ruota su sé stesso:
SPIN

numero quantico
magnetico di spin
 $m_s = \pm 1/2$

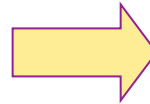


Allo spin elettronico «quantizzato»
sono associati numeri quantici di spin

$$m_s = +\frac{1}{2} \text{ e } m_s = -\frac{1}{2}$$

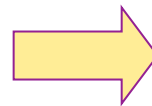
Modelli atomici

Inadeguatezza modello di Bohr:
miscela concetti fisica classica e
quantistica



Passaggio dal modello deterministico
di Bohr
a quello meccanico-ondulatorio di
Schrödinger

Abbiamo visto che la luce ha duplice
natura: ondulatoria e corpuscolare.
Quindi ad un'onda elettromagnetica è
associato un fotone con energia $E = h\nu$



Anche le particelle materiali,
piccole come l'elettrone, possono
avere un comportamento
dualistico.

1924, French physicist Louis de Broglie:

All matter possesses wave properties

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

$$h = 6.62 \times 10^{-34} \text{ J.s}$$



The uncertainty principle
1927, Werner Heisenberg

It is impossible to know simultaneously both the momentum and the position of a particle with certainty.



$$(\Delta p_x)(\Delta x) \geq \frac{h}{4\pi}$$

$$h = 6.62 \times 10^{-34} \text{ J} \cdot \text{s}$$

Modelli atomici

Principio di Indeterminazione di Heisenberg

Per descrivere il moto di un corpo è necessario conoscere i valori della sua posizione e della sua velocità:

questo non è possibile per l'elettrone in quanto non è possibile conoscerne contemporaneamente posizione e velocità.

$$\Delta x \cdot \Delta p \geq h / 4\pi$$

Dove Δx e Δp rappresentano gli errori commessi nella determinazione della posizione e della quantità di moto (mv): tanto maggiore è la precisione nella determinazione della posizione, tanto minore sarà quella della velocità e viceversa.

L'indeterminazione è tanto più trascurabile quanto maggiore è la massa.



Accuracy: one part per trillion

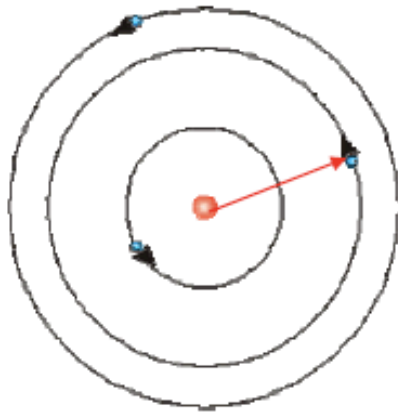
Baseball: 200g

Speed: 3000 cm/sec (67 miles/hour)

$$p = 6 \times 10^5 \text{ g} \cdot \text{cm} \cdot \text{sec}^{-1}$$

$$\Delta p = 6 \times 10^{-7} \text{ g} \cdot \text{cm} \cdot \text{sec}^{-1}$$

→ $\Delta x = 10^{-21} \text{ cm}$



Electron: 10^{-27} g

Same velocity

$$p = 3 \times 10^{-24} \text{ g} \cdot \text{cm} \cdot \text{sec}^{-1}$$

$$\Delta p = 3 \times 10^{-36} \text{ g} \cdot \text{cm} \cdot \text{sec}^{-1}$$

→ $\Delta x = 10^9 \text{ cm}$

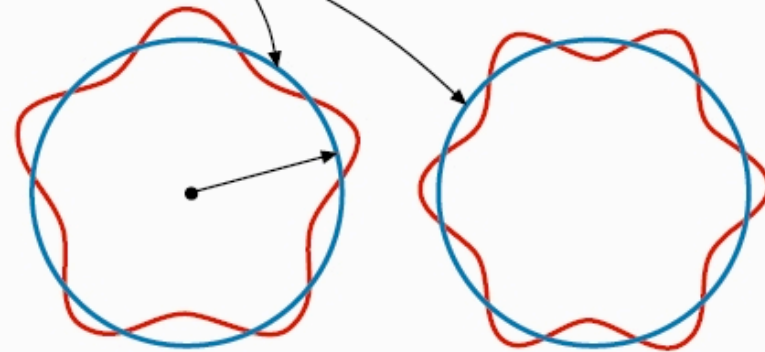


Modelli atomici

Equazione di Schrödinger

Si propose un modello ondulatorio: l'elettrone orbitante intorno al nucleo si comporta come un'onda stazionaria, quindi venne proposta un'equazione d'onda per rappresentarla.

Circonferenza = $2\pi r$



Tra le infinite soluzioni dell'equazione di Schrödinger, definite come funzioni d'onda, sono accettabili solo quelle che derivano da combinazioni di tre costanti, dette numeri quantici, che sono legate tra loro da relazioni ben definite: n , l , m .

Electron motion: wavefunction ψ

Describes spatial properties of electron.

Must be: single valued, continuous, normalized



Schrodinger wave equation (1926):

$$-\frac{h^2}{8\pi^2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi = E\psi$$

ψ : wavefunction / eigenfunction

x, y, z : coordinates

m : mass

h : Planck's

E : total energy

V : Potential energy



$$\longrightarrow \hat{H} \psi = E \psi$$

$\hat{H}$: Hamiltonian operator

Converting to polar coordinates:



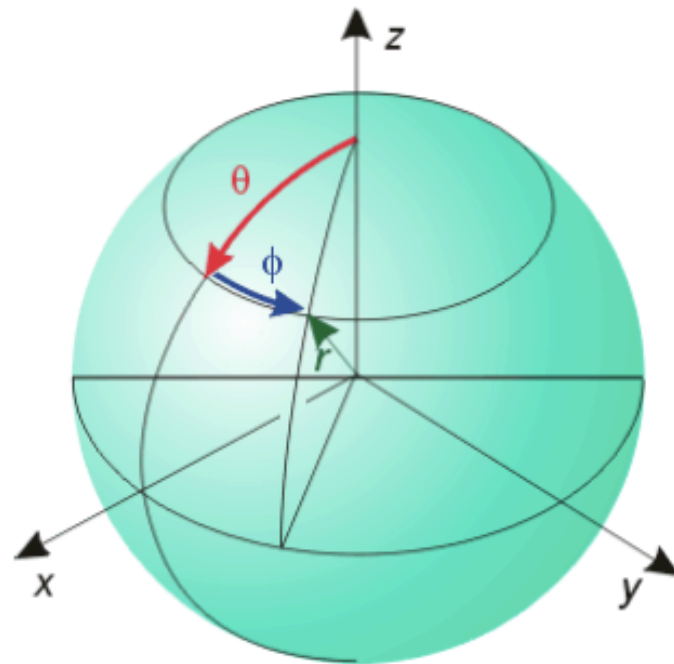
$$\psi_{n,l,m_l} = R_{n,l}(r) \cdot Y_{l,m_l}(\theta, \phi)$$

$$R_{n,l}(r)$$

Radial part

$$Y_{l,m_l}(\theta, \phi)$$

Angular part

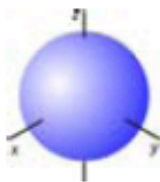


$n=1,2,3,4....$ = principle quantum number

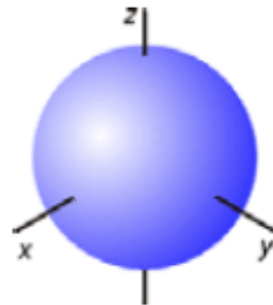
(1): determine the energy of the electron

(2): indicate approximately the effective volume of the orbital.

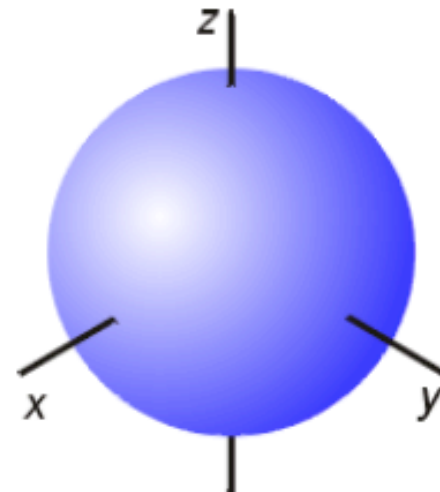
$$E_n = -\frac{e^2}{2r_n} = -\frac{2\pi^2 m_e e^4}{n^2 h^2} = -\frac{k}{n^2}$$



$n=1$

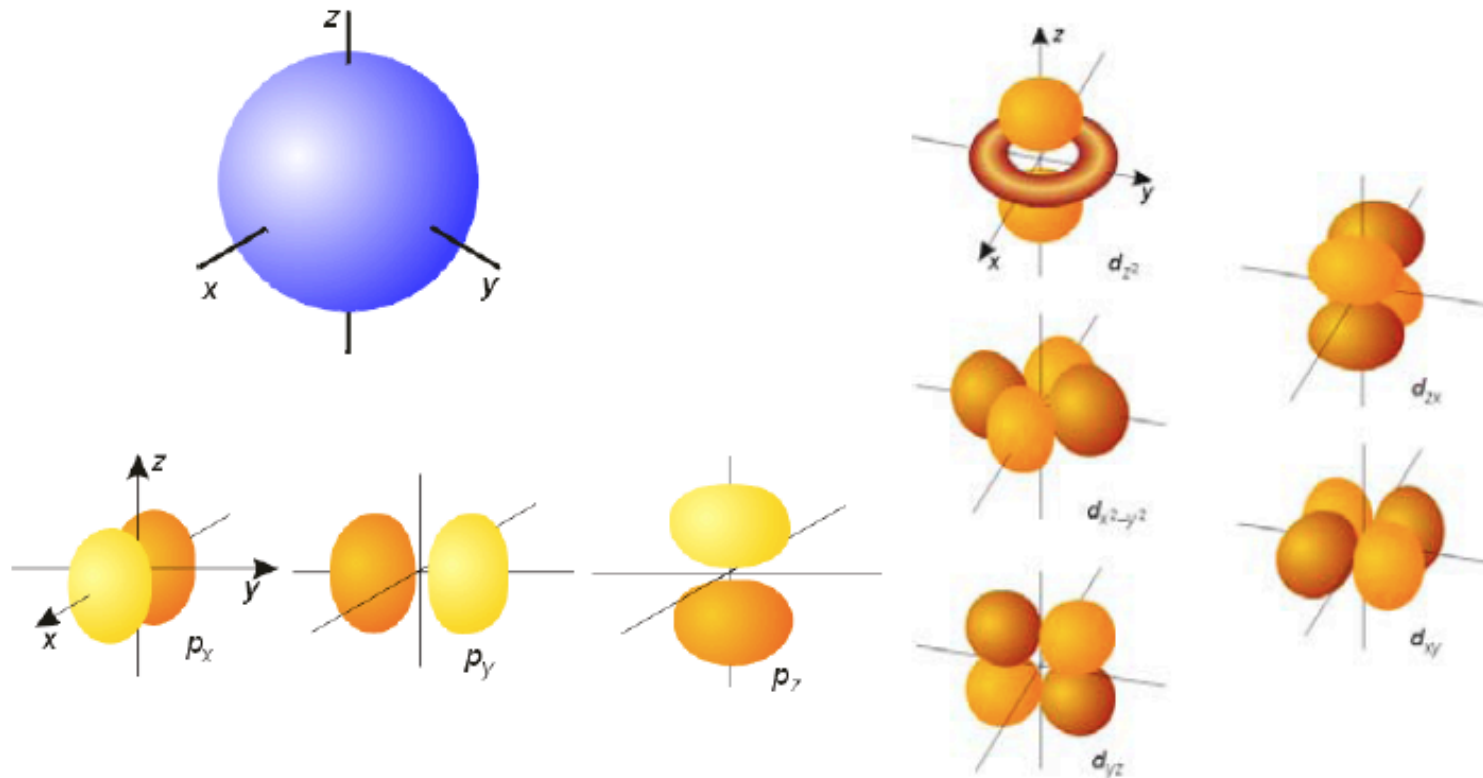


2



3

$l =$ angular momentum (or shape) quantum number
 0, 1, 2, 3, 4,
 s, p, d, f,
 Determine general shape of the orbital

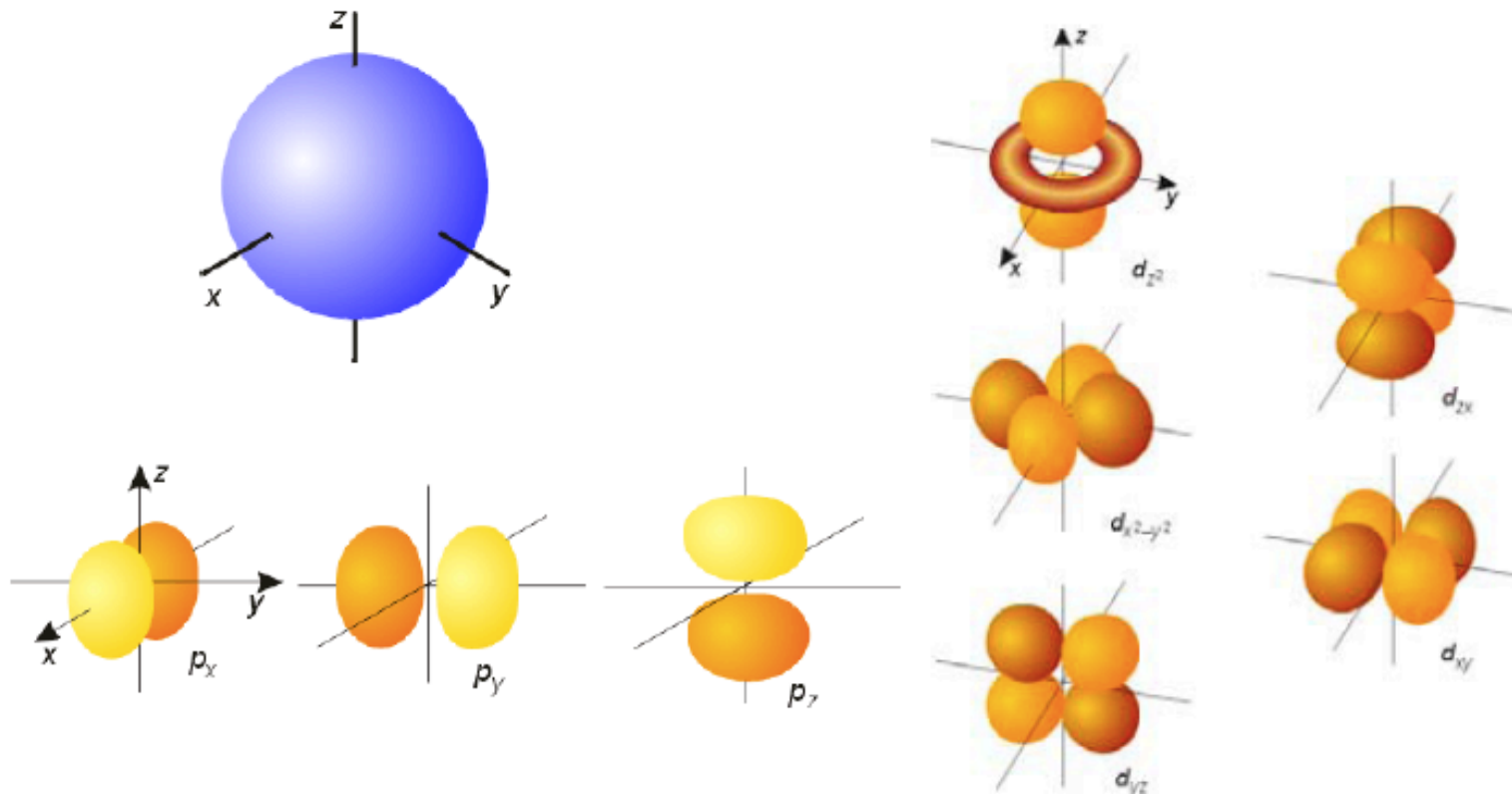


For each n , there are n possible angular momentum value

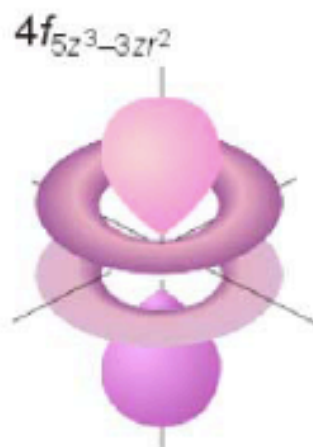
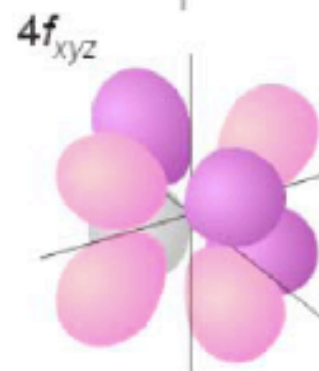
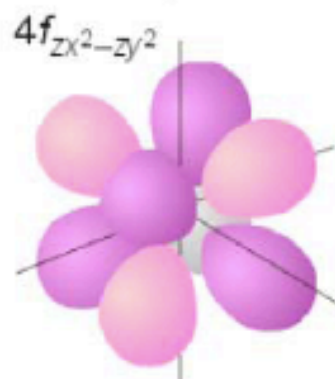
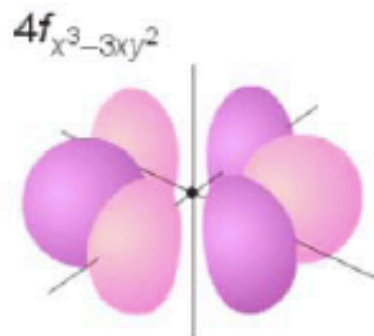
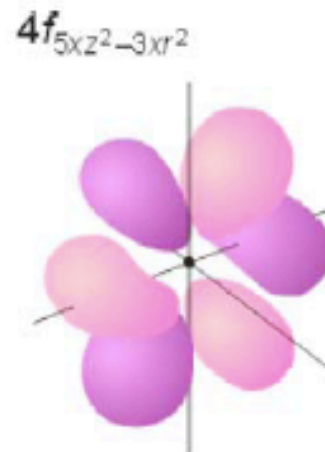
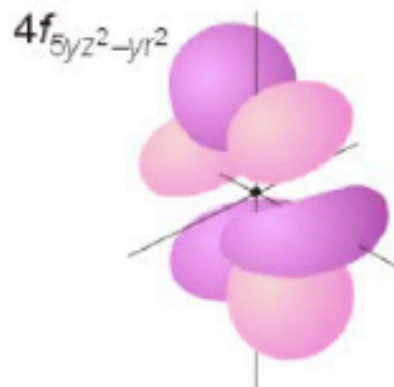
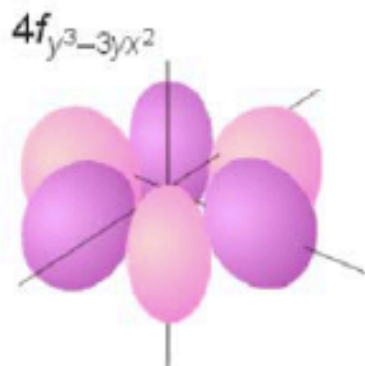
m_l = magnetic/orbital orientation quantum number

$0, \pm 1, \pm 2, \pm 3, \dots$

Determine orbital spatial orientation



For each l , there are $2l+1$ possible m_l value.



$\ell = 3$

Solutions for Y

s orbital ($l=0, m=0$)

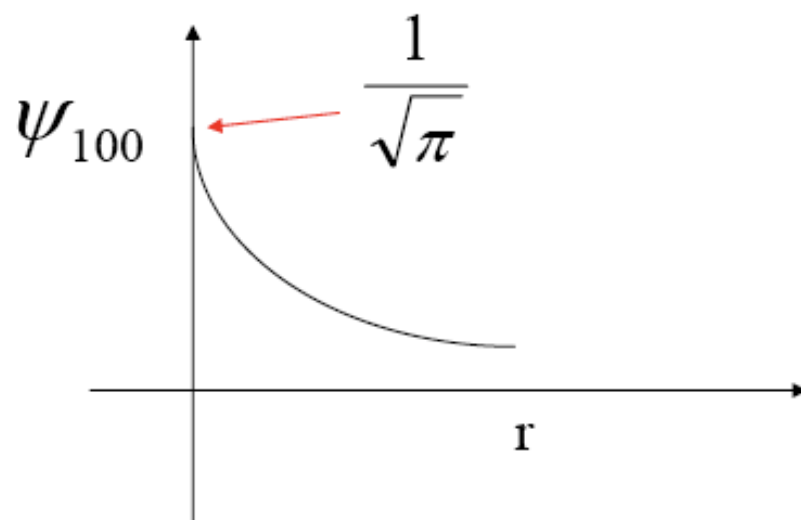


H 1s orbital:

$$\psi_{n,l,m_l} = R_{n,l}(r) \cdot Y_{l,m_l}(\theta, \phi)$$

$$\psi_{100} = (2e^{-r})\left(\frac{1}{2\sqrt{\pi}}\right)$$

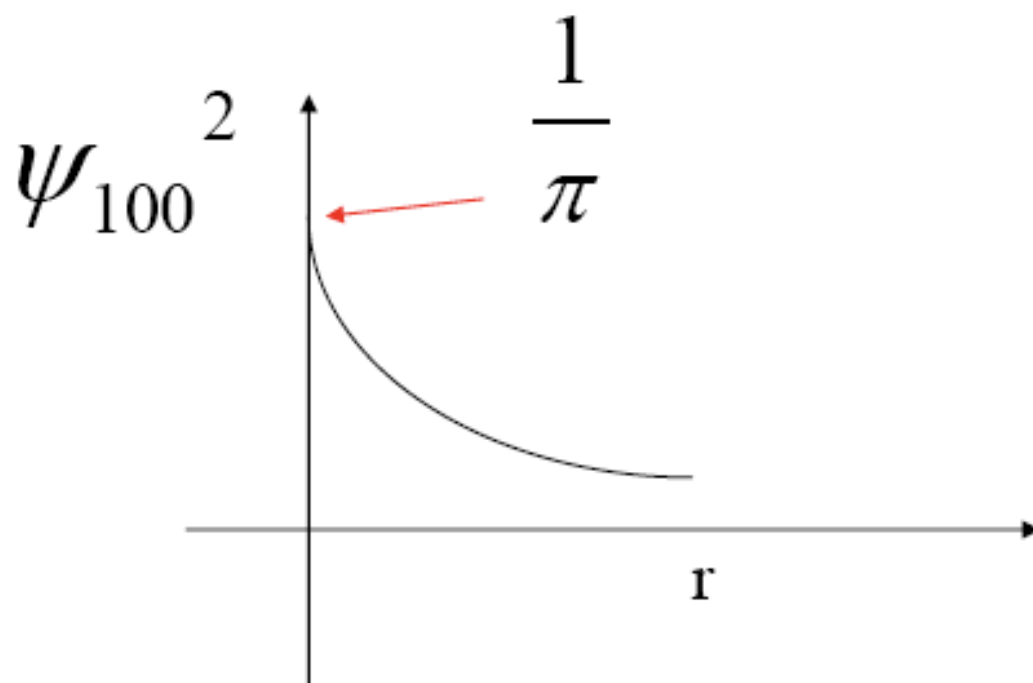
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Probability Density

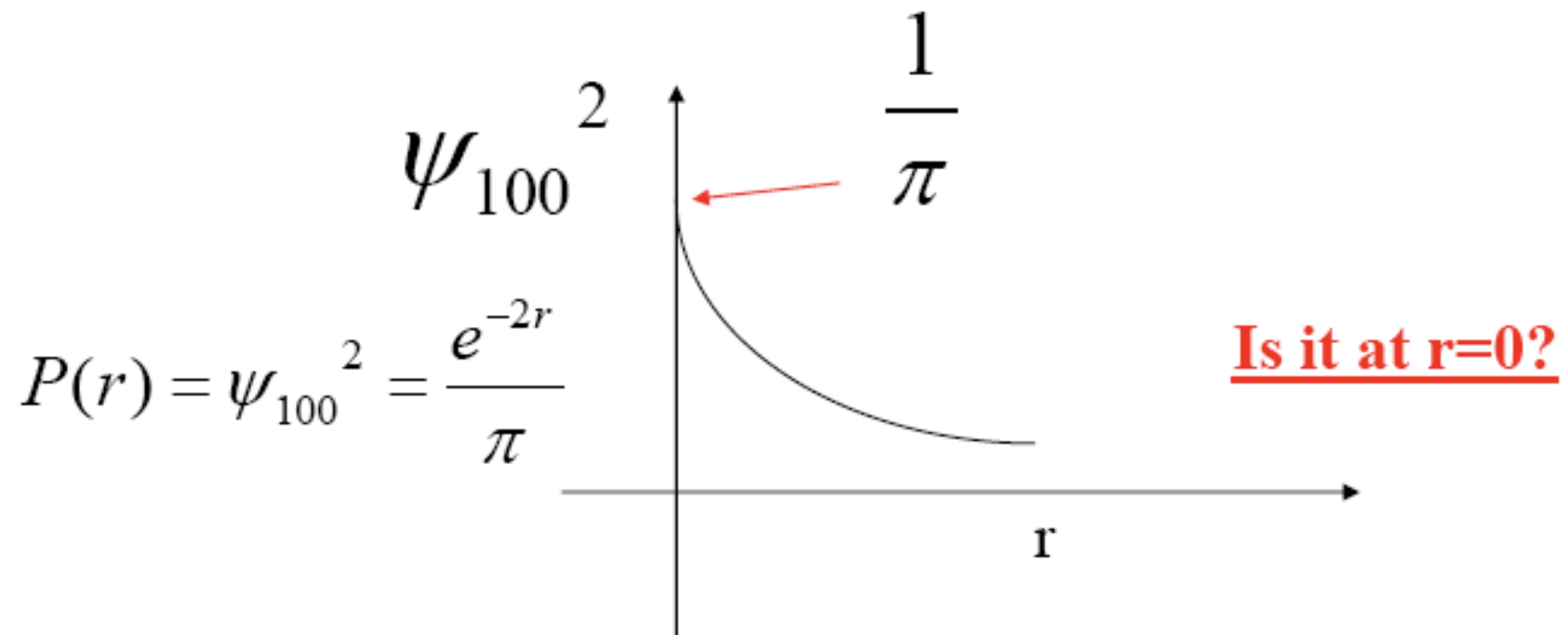
This probability function gives the probability of finding the electron at any point in space.

$$P(r) = \psi_{100}^2 = \frac{e^{-2r}}{\pi}$$



$$\int^{allspace} \psi^2 dV = 1$$

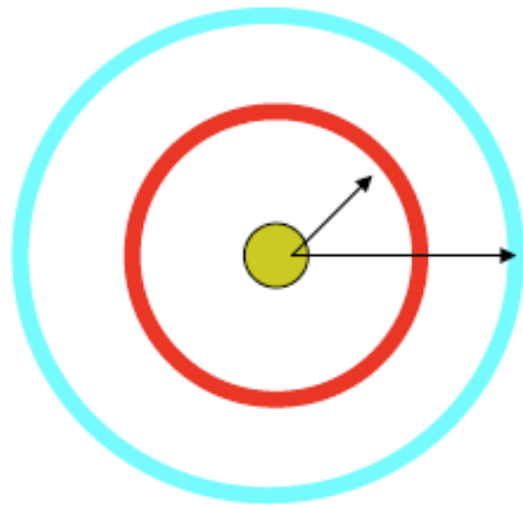
What radius is it most probable to find the electron?



Most probable radius: $r + dr$



Volume of the thin shell with thickness dr



$$4\pi r^2 dr$$

$$\text{Probability} = R^2(r) 4\pi r^2 dr$$

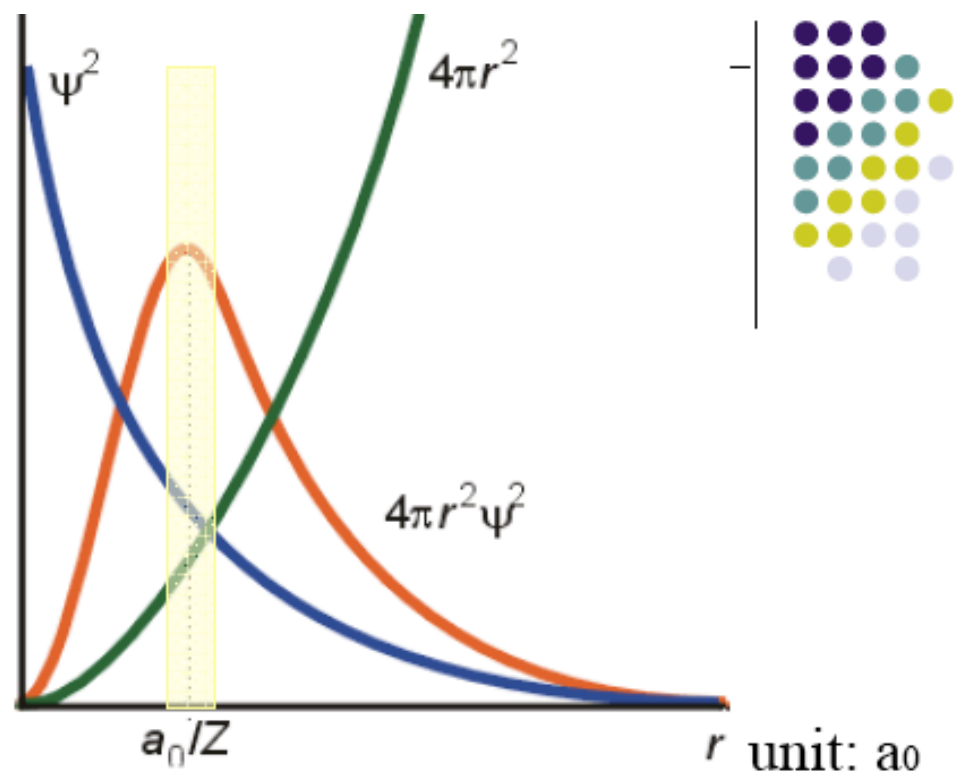
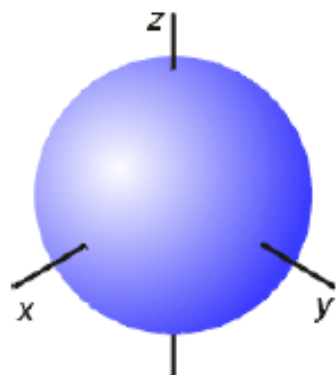
$$P / dr = R^2(r) 4\pi r^2$$

P/dr , **radial distribution function (RDF)**

compares the probability of finding electron at different r

Also called radial probability function

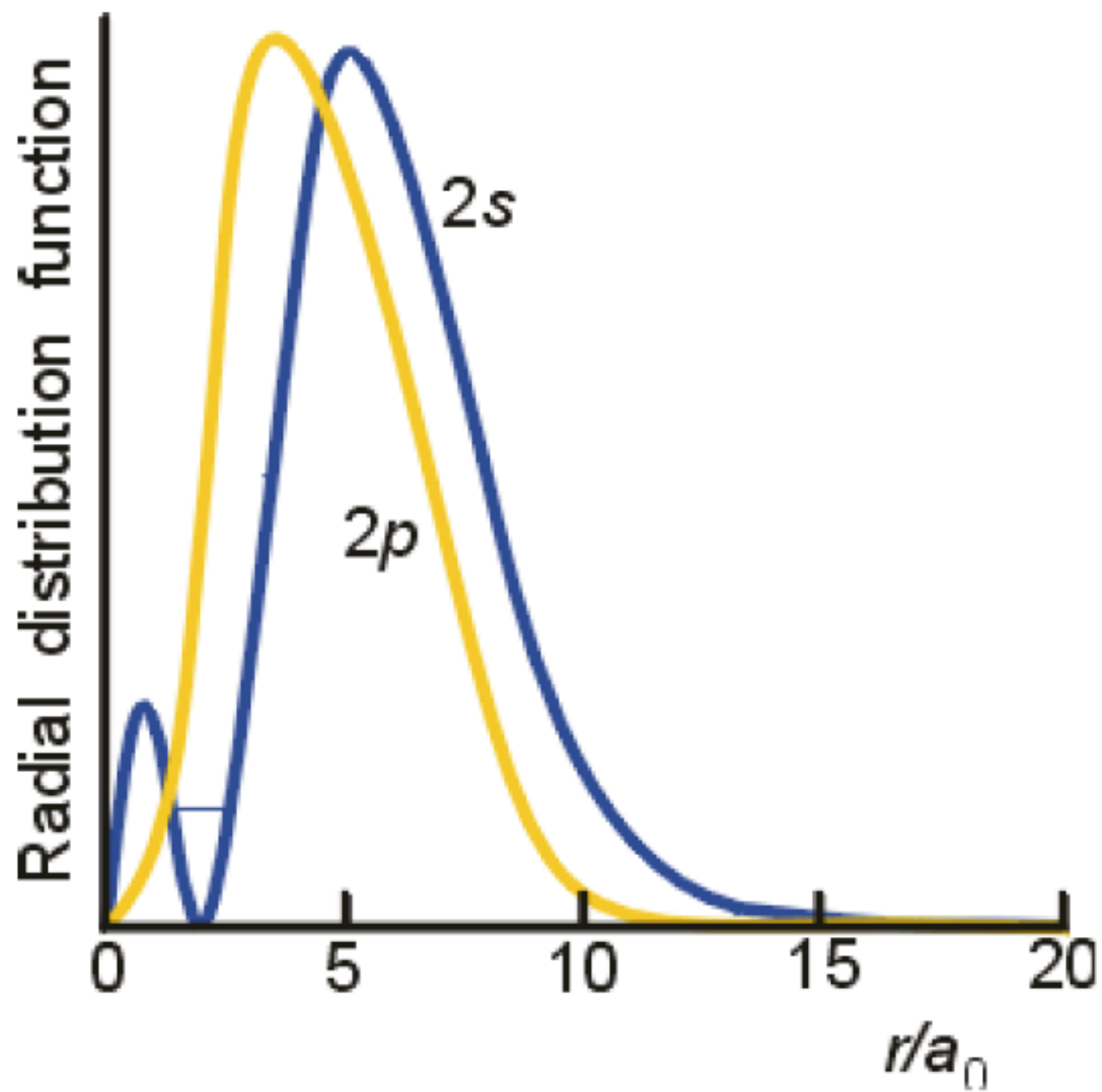
H 1s orbital:



$$RDF = 4\pi r^2 (2e^{-r})^2 = 16\pi r^2 e^{-2r}$$

Most probable radius:

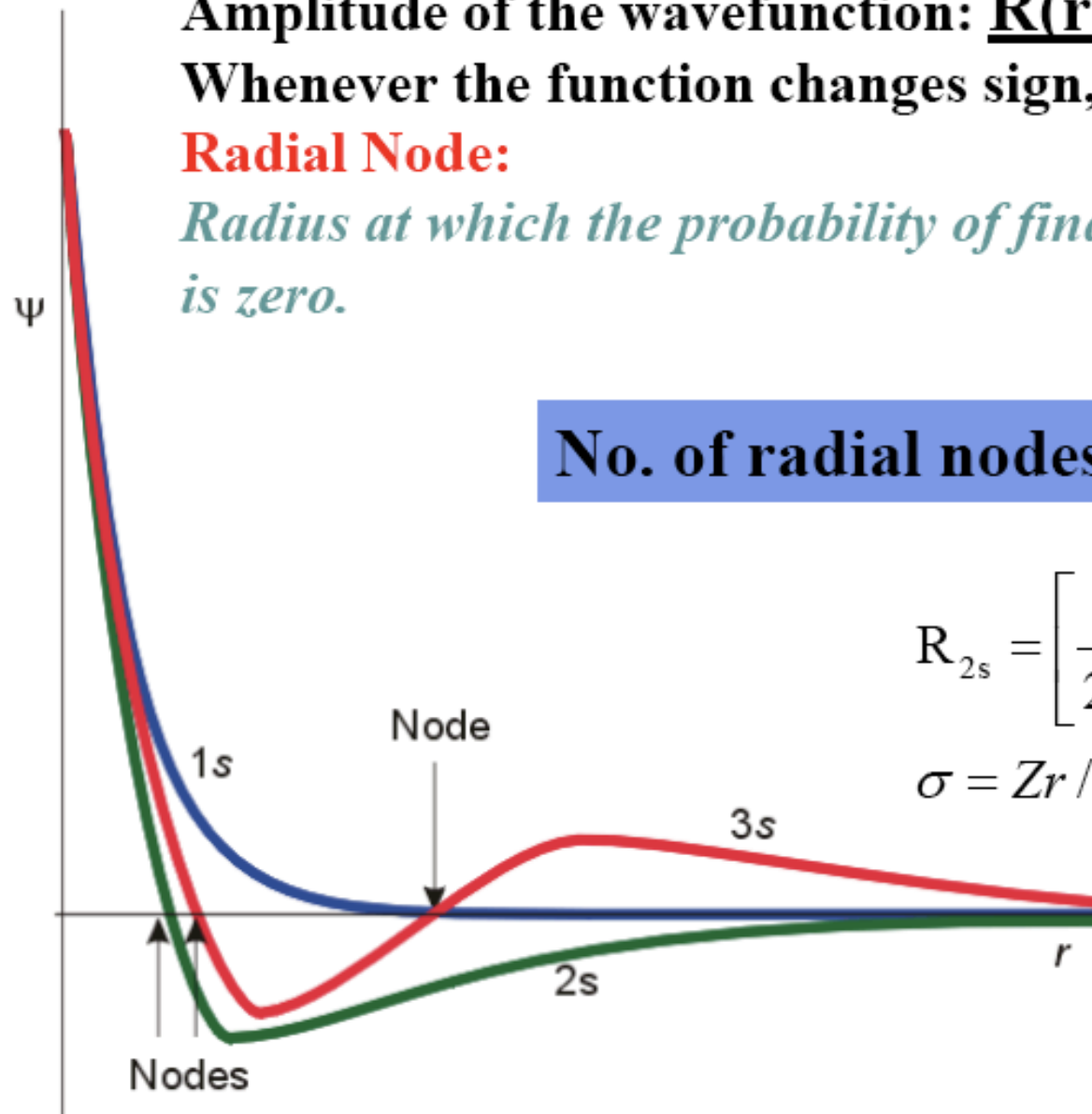
$$\frac{\partial(RDF)}{\partial r} = 0$$



Amplitude of the wavefunction: **R(r)**

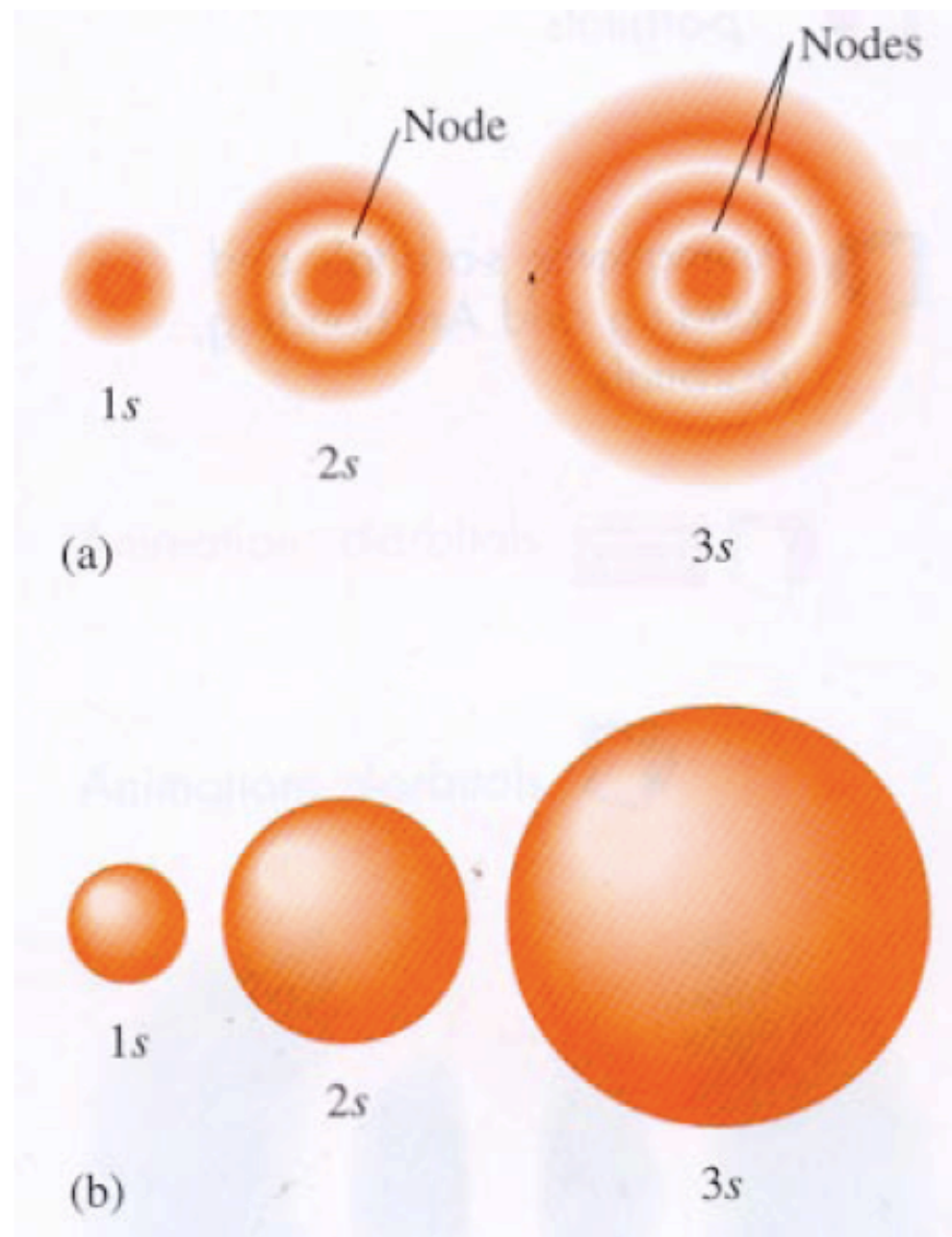
Whenever the function changes sign, there is a
Radial Node:

Radius at which the probability of finding the electron is zero.

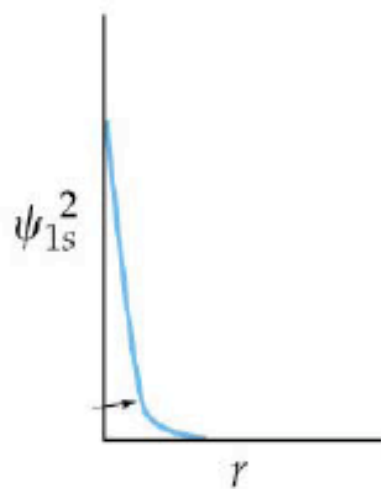


No. of radial nodes = $n - l - 1$

$$R_{2s} = \left[\frac{Z}{2a_0} \right]^{3/2} (2 - \sigma) e^{-\sigma/2}$$
$$\sigma = Zr / a_0$$

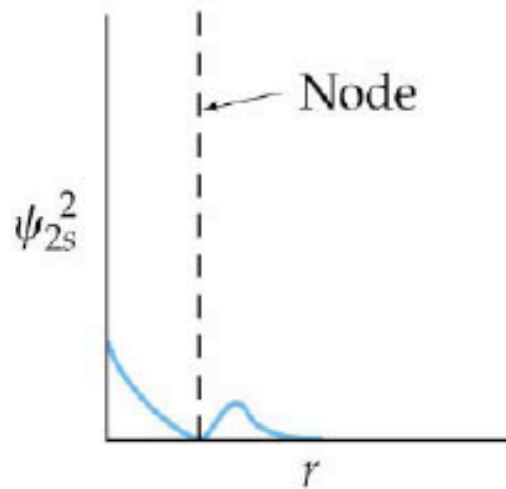


$1s$
 $n = 1, l = 0$



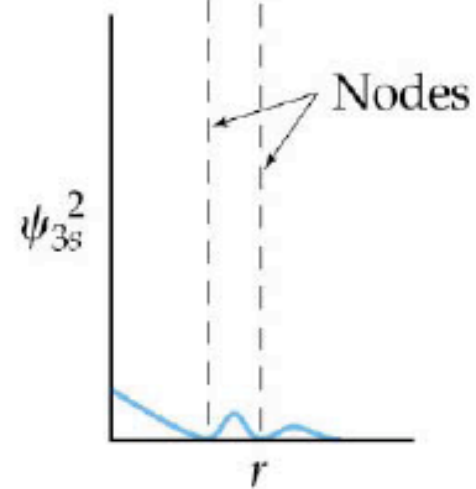
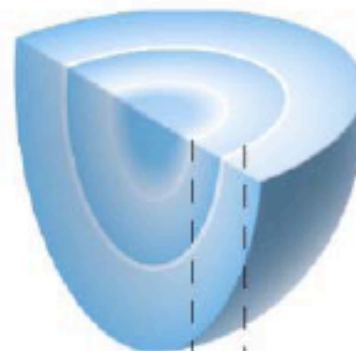
(a)

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

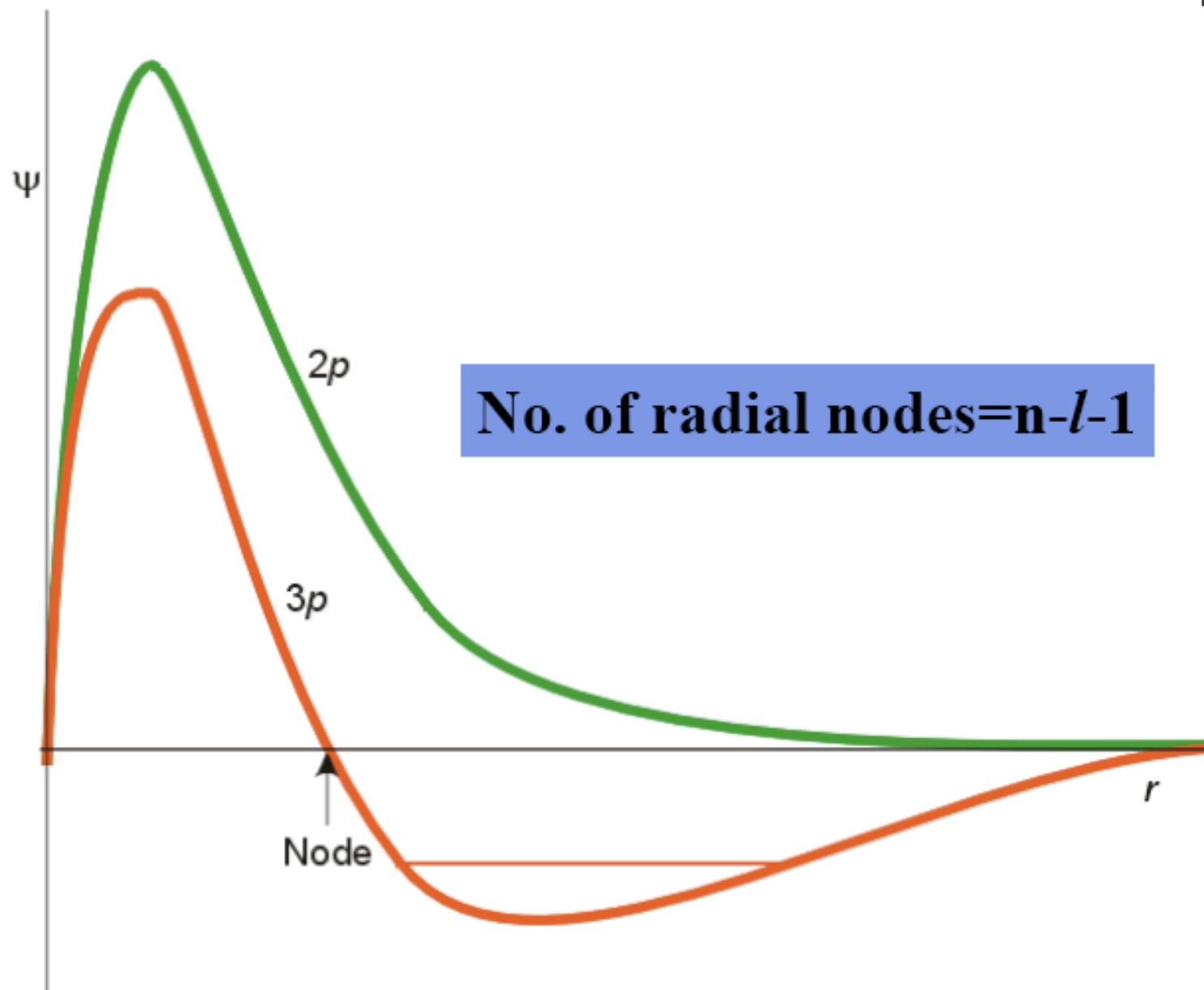


(b)

$3s$
 $n = 3, l = 0$



(c)



volume:

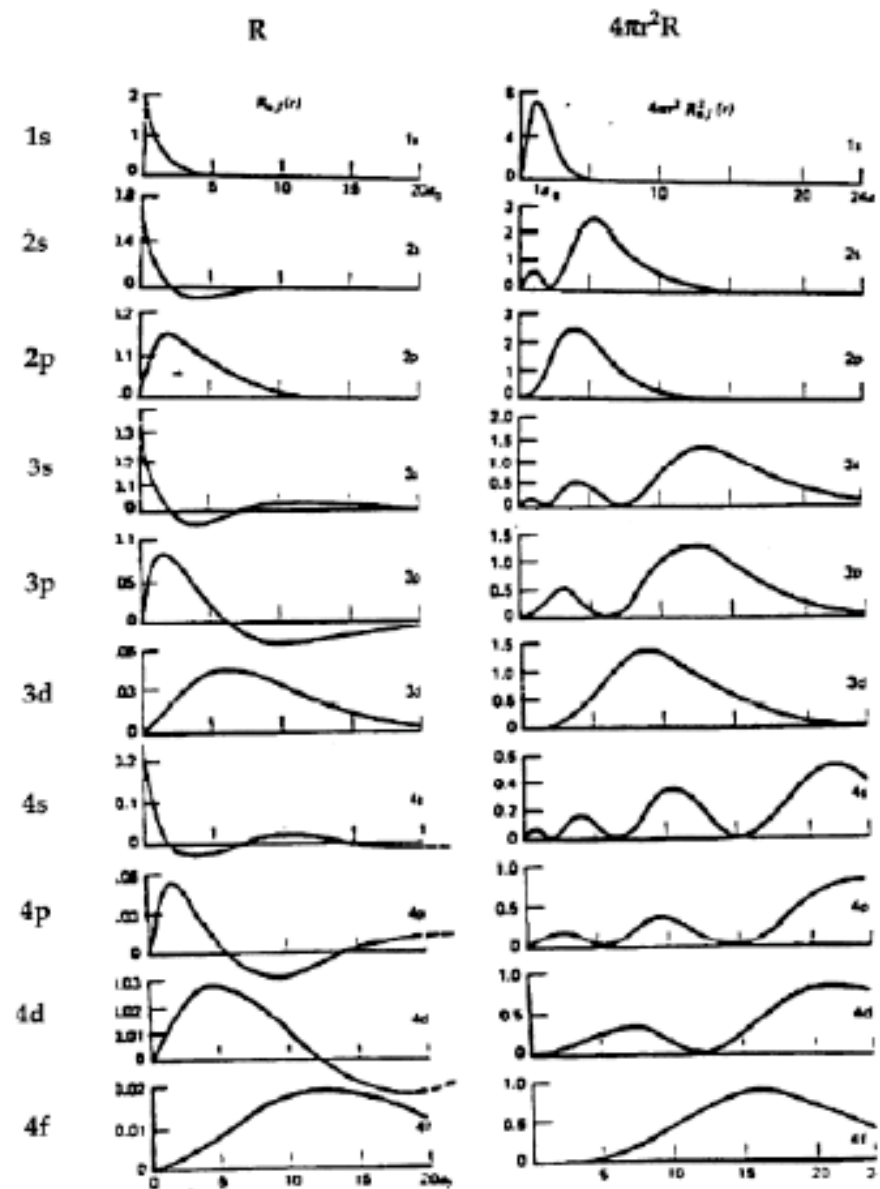
$$V = 4\pi r^3/3$$

incremental volume:

$$dV = 4\pi r^2 dr$$

weighted radial probability:

$$R^2 dV = 4\pi r^2 R^2 dr$$



Multielectron Atoms

Orbital energies for hydrogen atom:

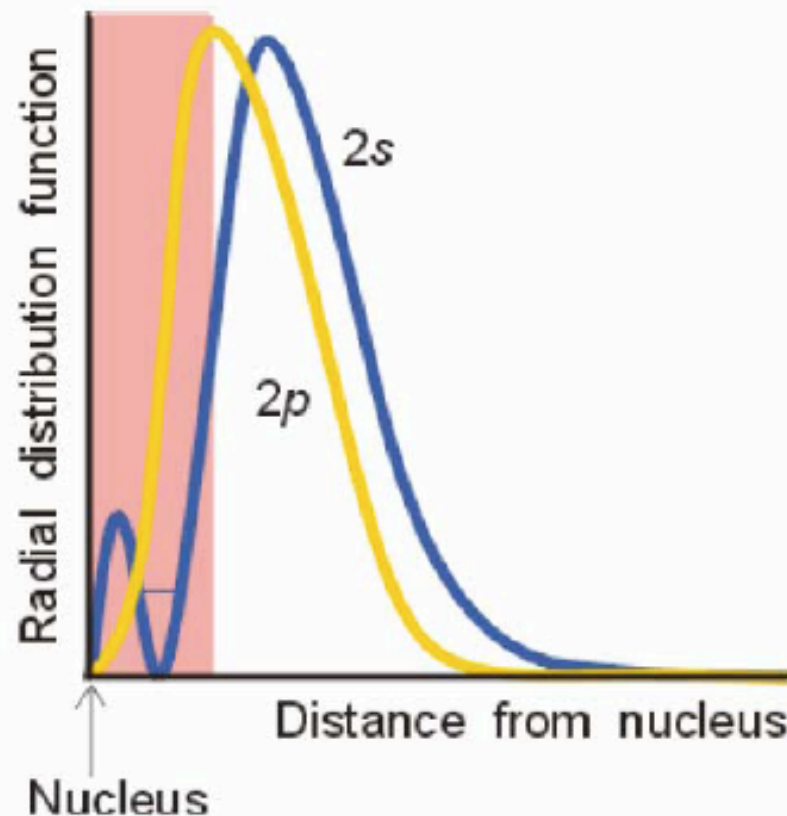
$1s < 2s = 2p < 3s = 3p = 3d$, etc....

Multielectron atom: three-body-problem; can't solve exactly

$1s < 2s < 2p < 3s < 3p$ etc....

1 electron approximation: borrow solutions to hydrogen atom; have to take into account shielding effects, electron-electron repulsion, spin correlation.

**Penetration
and
Shielding**

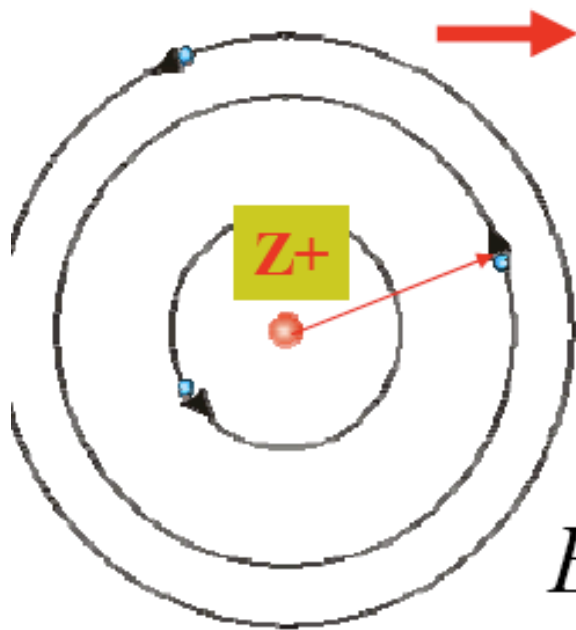


1 electron system: Hydrogen



How about many-electron system?

1 electron with nuclear charge Z



Increasing electrostatic interaction

Orbital contract

Orbital energy drops

$$V(r) = -\frac{Ze^2}{r}$$

$$E_n = -\frac{Z^2 \times 13.6 \text{ eV}}{n^2}$$

Example: For He^+ , $Z=2$, $E_1=-54.4 \text{ eV}$

For multi-electron atoms, Schrodinger equation can be set up, but can not be solved exactly.

Use approximation.



Build many-electron system:

1. Pauli exclusion principle:

No two electrons in an atom can have the same set of four quantum numbers (n, l, m_l, m_s)

m_s : spin quantum number
Quantized, $+1/2$ or $-1/2$



Each atomic orbital can contain at most two electrons.

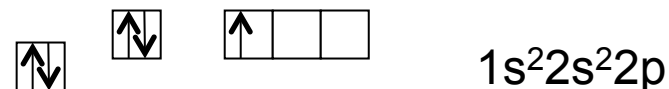
Principio di costruzione o Aufbau

E' possibile ricavare la configurazione elettronica degli atomi polielettronici partendo da quella dell'idrogeno ed aggiungendo un elettrone ed un protone fino ad arrivare all'atomo neutro dell'elemento con il numero atomico desiderato.

Regole:

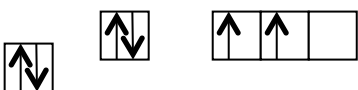
1. Si comincia dall'orbitale a più bassa energia.
2. **Principio di esclusione di Pauli:** "in un atomo non possono coesistere elettroni aventi tutti e quattro i numeri quantici uguali". Quindi essendo ogni orbitale caratterizzato da tre numeri quantici, su ognuno di essi possono trovarsi al massimo due elettroni aventi diverso valore di m_s (spin antiparallelo).

Boro, B, numero atomico = 5

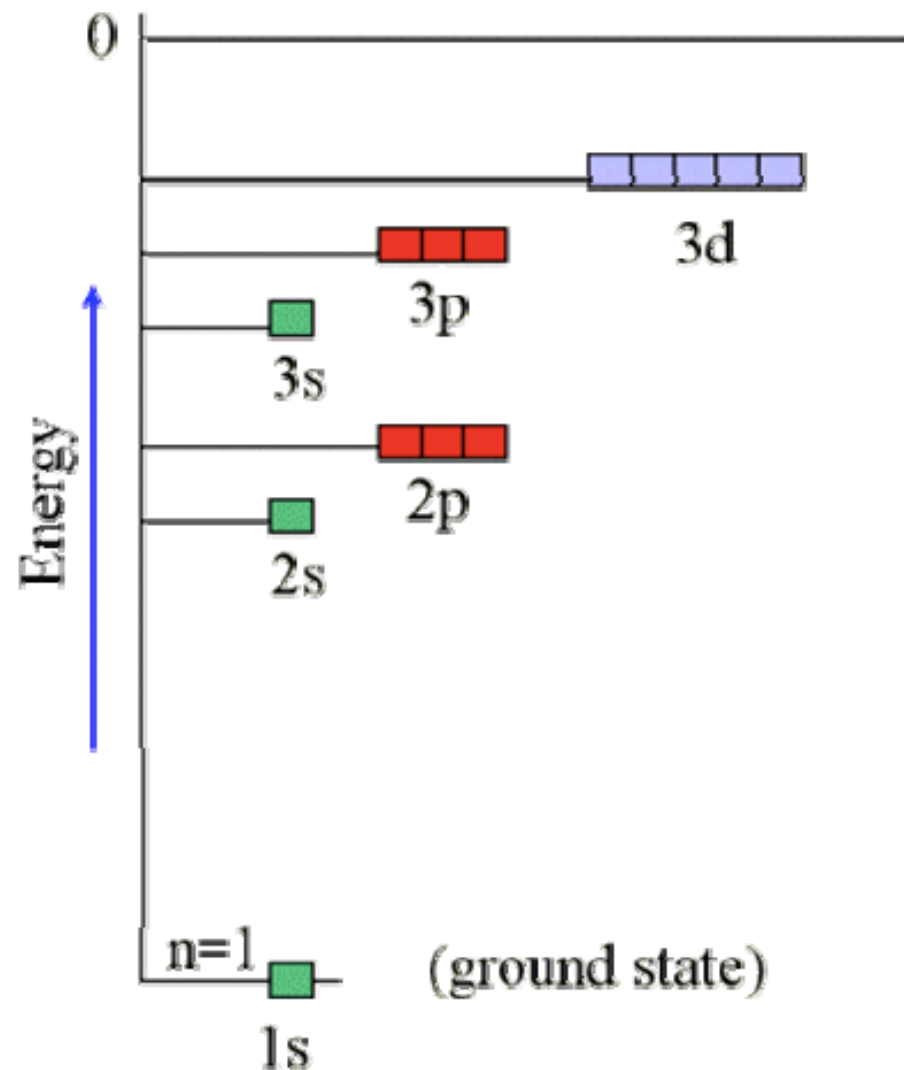


Carbonio, C, numero atomico = 6

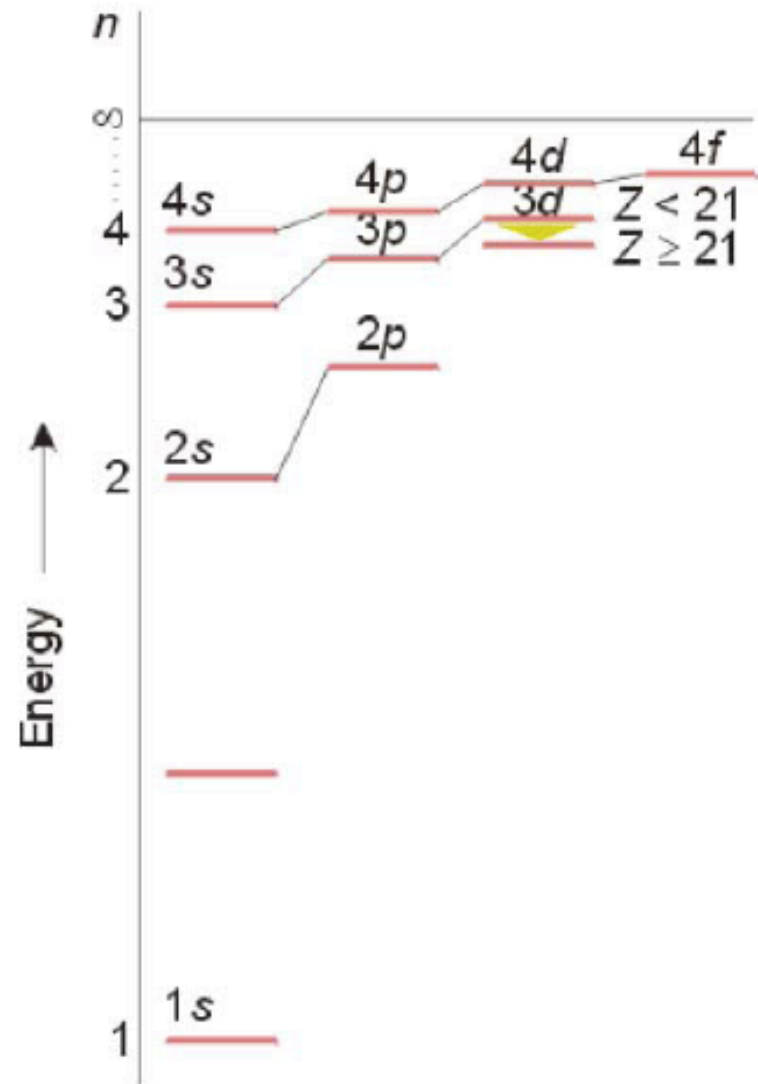
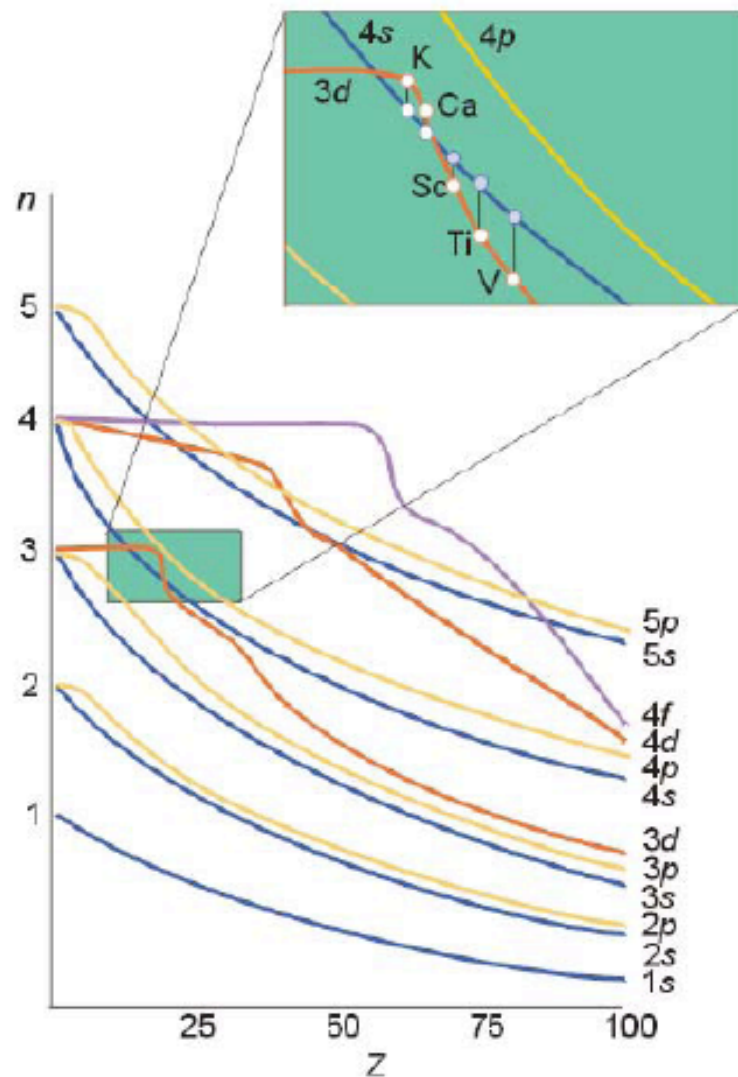
3. **Regola di Hund o della massima molteplicità:** la configurazione di minor energia di un atomo è quella che presenta il maggior numero di elettroni a spin paralleli.

Carbonio, C, numero atomico = 6  $1s^2 2s^2 2p^2$

Aufbau principle: electron fill the atomic orbitals from the lowest energy up.



Dependence of orbital energies on Z



Useful guideline for placement of valence electrons:

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f \sim 5d < 6p < 7s < 6d < 5f$

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d.....



Example:

He: 1,0,0, $\frac{1}{2}$ & 1,0,0, $-\frac{1}{2}$ $\rightarrow 1s^2$

Li: 1,0,0, $\frac{1}{2}$; 1,0,0, $-\frac{1}{2}$; 2,0,0, $\frac{1}{2}$ $\rightarrow 1s^2 2s^1$

Al: 13 electrons

$1s^2 2s^2 2p^6 3s^2 3p^1 = [Ne]3s^2 3p^1$

Core
electron

Valence
electron

Periodic Table and Periodicity

What is so special about it?

- Helps us to bring order into inorganic chemistry
- Concept of chemical periodicity
 - central to study of inorganic chemistry
- It systematizes and rationalizes
 - chemical facts
 - predict new ones
 - suggest fruitful areas for further research

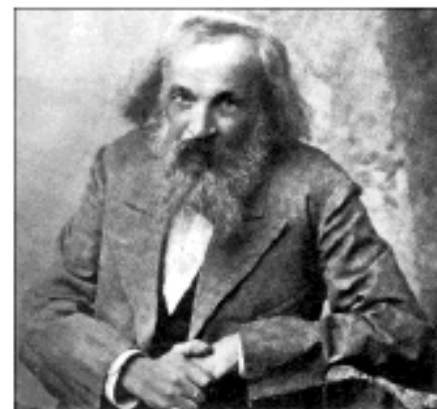
Periodic Law: The properties of chemical elements are not arbitrary, but depend upon the electronic structure of the atom and vary with the atomic number in a systematic way.

Therefore: periodic table may be useful for

- the interpretation of the periodic law in terms of the electronic structure of atoms
- the systematization of trends in physical & chemical properties, and to detect possible errors, anomalies, & inconsistencies
- the prediction of new elements & compounds and to suggest new areas of research

Dmitri Mendeleev

1869 : Proposed his periodic law that “the properties of the elements are a periodic function of their atomic weights”. He published several forms of periodic table, one containing 63 elements.



1834 - 1907

1871 : Mendeleev modified and improved his tables and predicted the discovery of 10 elements (now known as Sc, Ga, Ge, Tc, Re, Po, Fr, Ra, Ac and Pa). He described with amazing prescience the properties of four of these (Sc, Ga, Ge, Po). He did not predict the existence of noble gases and the number of lanthanide elements

History of the Periodic Table

- **1894-8:** Lord Rayleigh, W. Ramsay and **M. W. Travers** detected and isolated the noble gases (He, Ne, Ar, Kr, Xe).
- **1913:** N. Bohr explained the form of the periodic table on the basis of his theory of atomic structure and showed that there could be only 14 lanthanide elements.
- **1913 :** H. G. J. Moseley observed regularities in the characteristic X-ray spectra of the elements; he thereby discovered atomic numbers Z and provided justification for the ordinal sequence of the elements.
- **1940:** E. McMillan and P. Abelson synthesized the first transuranium element ^{93}Np . Others were synthesized by G. T. Seaborg during the next 15 years.

Glenn T. Seaborg

After co-discovering 10 new elements, in 1944 he moved 14 elements out of the main body of the periodic table to their current location below the Lanthanide series. These became known as the Actinide series.

1912 - 1999



Periodic Table of the Elements

1	2																	13	14	15	16	17	18
1A	New Original																	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	2																	5	6	7	8	9	10
1	2																	13	14	15	16	17	18
1	2																	5	6	7	8	9	10
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1	2																	5	6	7	8	9	10
1	2																						

Note: The subgroup numbers 1-16 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 112-118 are the IUPAC equivalents of those numbers.

IUPAC Nomenclature of elements with atomic number above 100

• Digit	Name	Abbreviation
•		
• 0	nil	n
• 1	un	u
• 2	bi	b
• 3	tri	t
• 4	quad	q
• 5	pent	p
• 6	hex	h
• 7	sept	s
• 8	oct	o
• 9	enn	e

E. g.,

114	Un-un-quad-ium	Uuq
118	Un-un-oct-ium	Uuo

Building Up the Periodic Table: The Basis

1. Various quantum numbers

2. Hund's Rule:

When more than one orbital has the same energy (e.g. p_x , p_y , p_z), electron occupy separate orbitals and do so with parallel spins.

3. Pauli (Exclusion) Principle

No more than two electrons shall occupy a single orbital and, if two do occupy a single orbital, then their spins must be paired.

or

"no two electrons can have the same four quantum numbers"

4. The order of orbitals for a given quantum number depends on

Shielding Effects (Z^)*

Penetration of orbitals

H	$1s^1$
He	$1s^2$
Li	$1s^2 2s^1$
.....	
F	$1s^2 2s^2 2p^5$
Ne	$1s^2 2s^2 2p^6$

Shielding

Energy of an electron in an atom is a function of Z^2/n^2 .

Nuclear charge (Z) increases more rapidly than principal quantum no. (n).

Therefore continuous increase expected in IE with increase in atomic number.

On the other hand

IE	H	1312	KJ mol ⁻¹
	Li	520	KJ mol ⁻¹

Why?

Reasons:

Average distance of 2s electron is greater than that of 1s.

The 2s electron is repelled by inner core $1s^2$ electrons, so that the former is much more easily removed – **shielding or screening** of the nucleus by inner electrons. Valence electron 'sees' only part of the total charge

Effective Nuclear charge

$$Z^* = Z - \sigma \quad (\sigma = \text{Screening Constant})$$

How to determine Z^* ?

If the electron resides in s or p orbital

1. Electrons in principal shell higher than the e- in question contribute 0 to σ
2. Each electron in the same principal shell contribute 0.35 to σ
3. Electrons in (n-1) shell each contribute 0.85 to σ
4. Electrons in deeper shell each contribute 1.00 to σ

Example: Calculate the Z^* for the 2p electron

Fluorine ($Z = 9$) $1s^2 2s^2 2p^5$

Screening constant for one of the outer electron (2p):

6 (six) (two 2s e- and four 2p e-) = $6 \times 0.35 = 2.10$

2 (two) 1s e- = $2 \times 0.85 = 1.70$

$$\sigma = 1.70 + 2.10 = 3.80$$

$$Z^* = 9 - 3.80 = 5.20$$

What is Z^* for 1s electron?

If the e- resides in a *d* or *f* orbital

1. All e-s in higher principal shell contribute 0
2. Each e- in same shell contribute 0.35
3. All inner shells in (n-1) and lower contribute 1.00

SLATER'S RULES

To calculate the shielding constant, σ , for an electron in an atom:

1. Write out the electronic configuration of the atom in the following order and groupings: (1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) ...
2. If the electron is in an (ns, np) group:
 - a) Electrons in groups to the right of the (ns, np) group contribute nothing to σ .
 - b) Each of the other electrons in the (ns, np) group contributes 0.35 to σ . (i.e., the shielding is 35% effective)
 - c) Each electron in the n-1 shell contributes 0.85 to σ .
 - d) Each electron in the n-2 shell or below contributes 1.00 to σ .

3. If the electron is in an (nd) or (nf) group:
- a) Electrons in groups to the right of the (nd) or (nf) group contribute nothing to σ .
 - b) Each of the other electrons in the (nd) or (nf) group contributes 0.35 to σ .
 - c) Each electron in groups to the left of the (nd) or (nf) group contributes 1.00 to σ .

Effective nuclear charge Z^* increases very slowly down a group for the “valence” i.e. outermost orbital e.g.

H	1.0	} Valence configuration same
Li	1.3	
Na	2.2	
K	2.2	
Rb	2.2	
Cs	2.2	

.....but increases rapidly along a period

Li	Be	B	C	N	O	F	Ne
1.3	1.95	2.6	3.3	3.9	4.6	5.2	5.9
$2s^1$	$2s^2$	$2p^1$	$2p^2$	$2p^3$	$2p^4$	$2p^5$	$2p^6$

Table 1.3 Effective nuclear charges, Z_{eff}

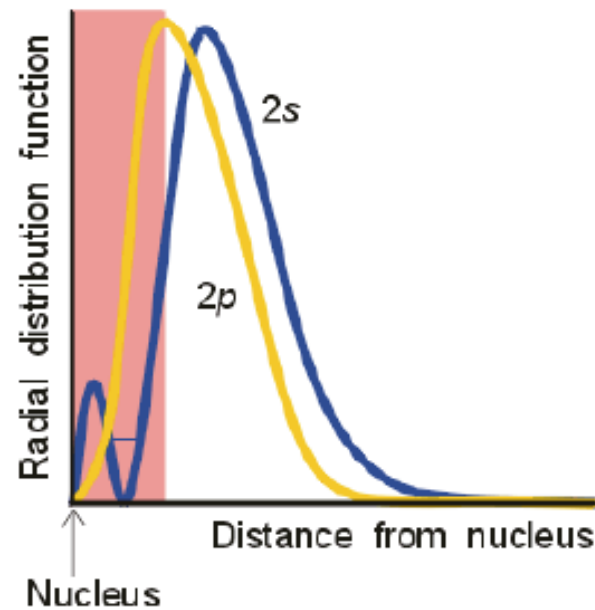
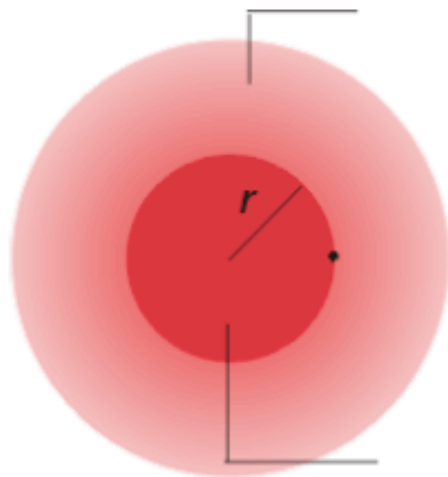
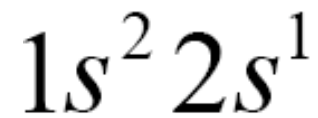
	H								He
<i>Z</i>	1								2
1s	1.00								1.69
	Li	Be	B	C	N	O	F		Ne
<i>Z</i>	3	4	5	6	7	8	9		10
1s	2.69	3.68	4.68	5.67	6.66	7.66	8.65		9.64
2s	1.28	1.91	2.58	3.22	3.85	4.49	5.13		5.76
2p			2.42	3.14	3.83	4.45	5.10		5.76
	Na	Mg	Al	Si	P	S	Cl		Ar
<i>Z</i>	11	12	13	14	15	16	17		18
1s	10.63	11.61	12.59	13.57	14.56	15.54	16.52		17.51
2s	6.57	7.39	8.21	9.02	9.82	10.63	11.43		12.23
2p	6.80	7.83	8.96	9.94	10.96	11.98	12.99		14.01
3s	2.51	3.31	4.12	4.90	5.64	6.37	7.07		7.76
3p			4.07	4.29	4.89	5.48	6.12		6.76

Table 1-3*Shriver & Atkins Inorganic Chemistry, Fourth Edition*

© 2006 by D. F. Shriver, P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller, and F. A. Armstrong

Penetration of Atomic Orbitals

- Energy levels for hydrogen show no distinction between energies of different types of orbitals (s, p, d, f) in a given quantum level.
- Li nucleus : 3 protons; it has +3 nuclear charge
If Li has only one electron (Li^{2+}), this electron would reside 1s orbital; strong attraction to nucleus. Therefore, size of this 1s orbital is smaller than it is for hydrogen (+1 nuclear charge)
- Li with 2e-; Some repulsion between electrons, but size of 1s still smaller than it has for hydrogen
- Uncharged Li has 3 electrons. Two electrons in 1s; 3rd electron in 2nd quantum shell which is larger than the 1s shell.
- Therefore, expect 3rd e- to be attracted by +3 nuclear charge and repelled by two 1s electrons and hence 'see' an effective nuclear charge of 1.3.
- If 3rd electron could penetrate close to nucleus, effective nuclear charge would be > 1.3



2s orbital penetrates the inner 1s electron shell better than 2p.

2s electron feel a greater effective nuclear charge $\rightarrow$ lower E for 2s

$$Z_{eff}(2s^1) > Z_{eff}(2p^1) \longrightarrow E(2s) < E(2p)$$

Ground State: $1s^2 2s^1$



For $Z > 1$:

$E(ns) < E(np) < E(nd) < E(nf)$ for given n

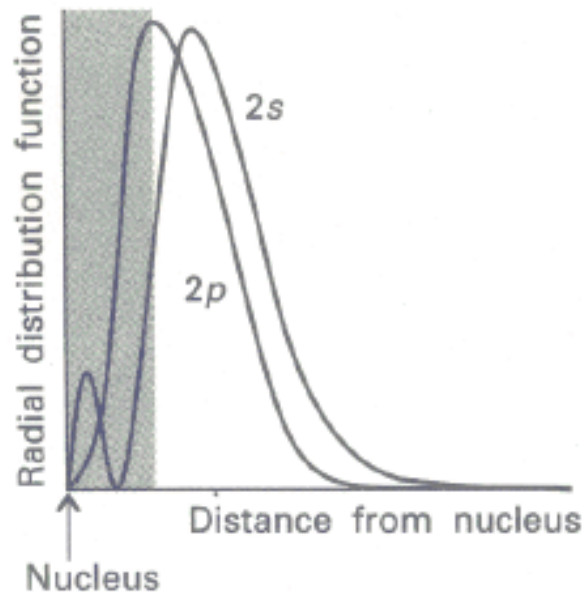
Z_{eff} : $\longrightarrow$ low

Penetrating ability: $\longrightarrow$ poor

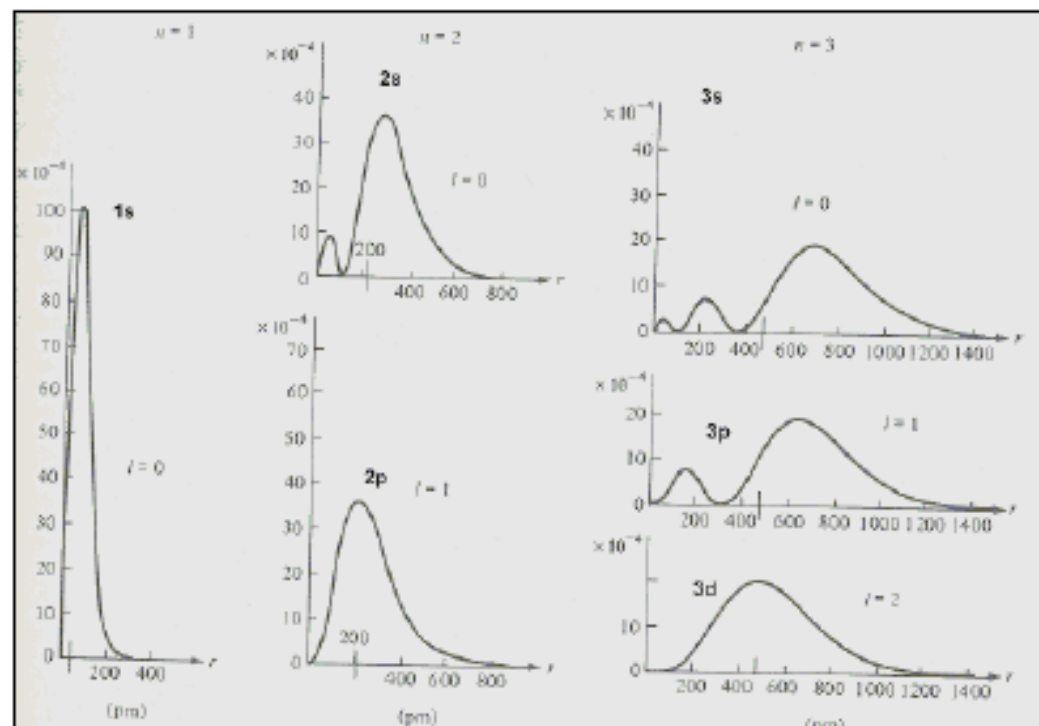
$$Z_{\text{eff}} = Z - \sigma$$

Shielding constant

Penetration of orbitals



1.18 The penetration of a 2s electron through the inner core is greater than that of a 2p electron because the latter vanishes at the nucleus. Therefore, the 2s electrons are less shielded than the 2p electrons.



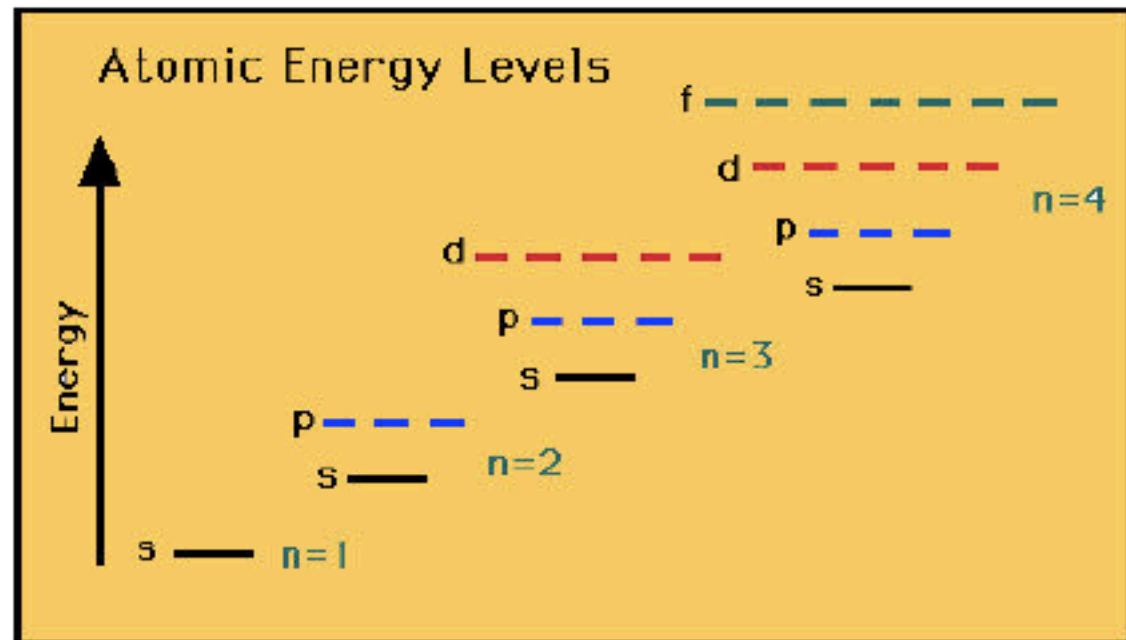
The penetration potential of an orbital varies as:

$$ns > np > nd > nf$$

The energy of the orbitals for a given n varies as:

$$ns < np < nd < nf$$

Considerations of principles such as penetration and shielding have enabled atomic orbitals to be arranged in rough order of increasing energy (order of filling of orbitals).



How do you fill electrons ?

H $1s^1$
 He $1s^2$
 Li $1s^2 2s^1$

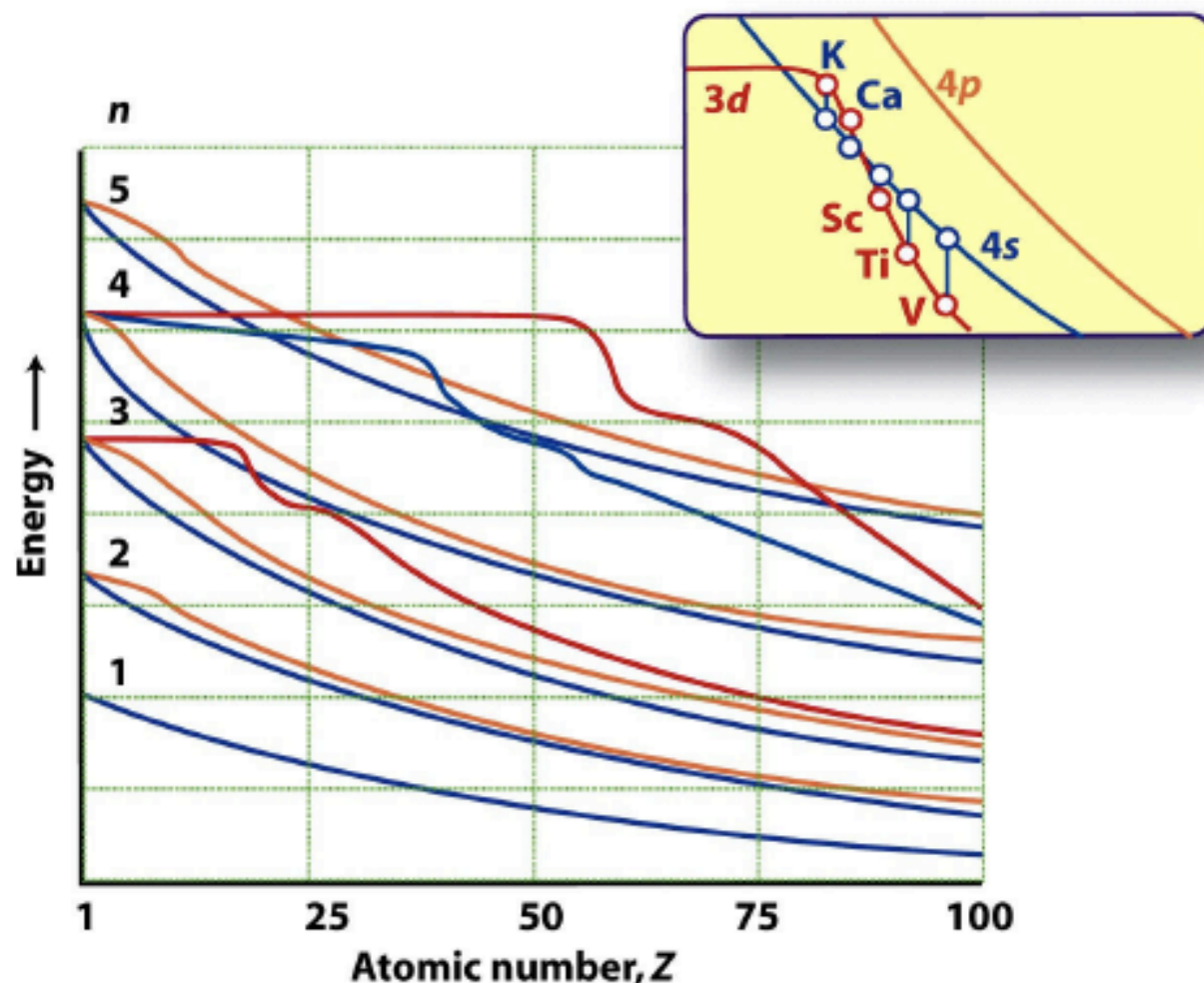
 F $1s^2 2s^2 2p^5$
 Ne $1s^2 2s^2 2p^6$

 Na $[\text{Ne}] 3s^1$
 Al $[\text{Ne}] 3s^2 3p^1$

 Ar $[\text{Ne}] 3s^2 3p^6$

 Now what next
 ?
 19 K $[\text{Ar}] 4s^1$
 20 Ca $[\text{Ar}] 4s^2$

 then? Sc



Sc (at. No. 21) $[\text{Ar}] 3d^3 4s^0$ or $[\text{Ar}] 3d^2 4s^1$ - Is this correct?
 NO; Why?

- For most of the d-block, both spectroscopic determination of the ground states and computation show that it is advantageous to occupy higher energy 4s orbitals, even if 3d is lower (Why?)
- Two electrons present in the same *d-orbital* repel each other more strongly than do two electron in a *s-orbital*. Therefore, occupation of orbitals of higher energy can result in a reduction in the repulsion between electrons that would occur if the lower-energy 3d orbitals were occupied.
- It is essential to consider all contributions to the energy of a configuration, and just not one-electron orbital energies
- Spectroscopic data show that GS configurations of d-block elements are of the form $3d^n 4s^2$, with 4s orbitals full occupied.

Sc (at. No. 21) is $[\text{Ar}]3d^1 4s^2$

**This order is followed in most cases
- but not always!**

Two atomic configurations do not follow the
nuclear sequence of filling of orbitals

$Z = 24$ Cr [Ar] $3d^5 4s^1$; not [Ar] $3d^4 4s^2$

$Z = 29$ Cu [Ar] $3d^{10} 4s^1$; not [Ar] $3d^9 4s^2$

As atomic number increases, energy of 3d orbitals decrease relative to both 4s and 4p; at $z = 29$, energy of 3d becomes much lower than 4s, hence order of filling
 $3d < 4s < 4p$

Filling of Orbitals (Aufbau)

- Transition series: filling order: 4s, 3d
- removal order (cation formation): 4s, 3d (not 3d, 4s)

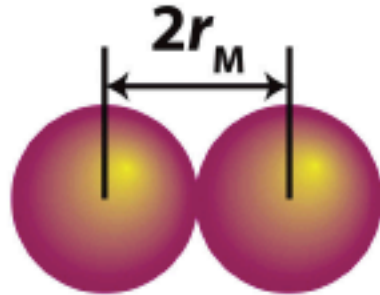
e.g. Ti [Ar] 4s² 3d²

- Ti²⁺ [Ar] 3d² (not [Ar] 4s²) Why?
- When 2 electrons are removed, regardless of where they come from, all atomic orbitals contract (Z^* increases because of net ionic charge and reduced shielding)
- Contraction has a small effect on 4s orbital which owes its low energy to its deep penetration
- Contraction in d orbital causes a considerable decrease in energy – this decrease is evidently enough to lower the energy of 3d **well** below 4s

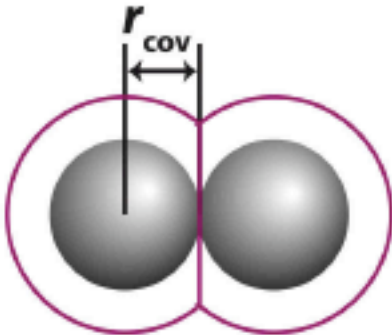
Periodic properties

- *Atomic size (radius),*
- *Ionic size (radius),*
- *Atomic volume*
- *Ionization energy,*
- *Electron affinity*
- *Electronegativity.*

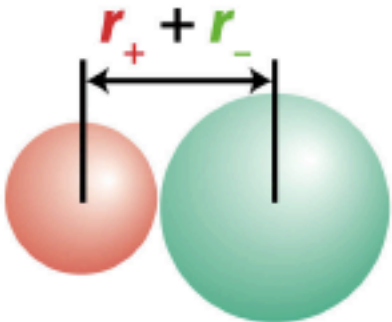
Atomic Radius



The **METALLIC RADIUS** is half of the experimentally determined distance between the nuclei of nearest neighbors in the solid



The **COVALENT RADIUS** of a non-metallic element is half of the experimentally determined distance between the nuclei of nearest neighbors in the solid



The **IONIC RADIUS** of an element is related to the distance between the nuclei of neighboring cations and anions

Ionic radius of O^{2-} is $1.40 \text{ \AA}$;

What is the ionic radius for Mg^{2+} ?

Measure the Mg-O distance in MgO and subtract $1.40 \text{ \AA}$

Atomic Radius

In a period, left to right

1. n (number of shells) remain constant.
2. Z increases (by one unit)
3. Z^* increases (by 0.65 unit)
4. Electrons are pulled close to the nucleus by the increased Z^*

So atomic radius decreases with increase in atomic number (in a period left to right)

In a group, top to bottom

1. n increases
2. Z increases
3. No dramatic increase in Z^* - almost remains constant

So atomic radius increases moving down the group

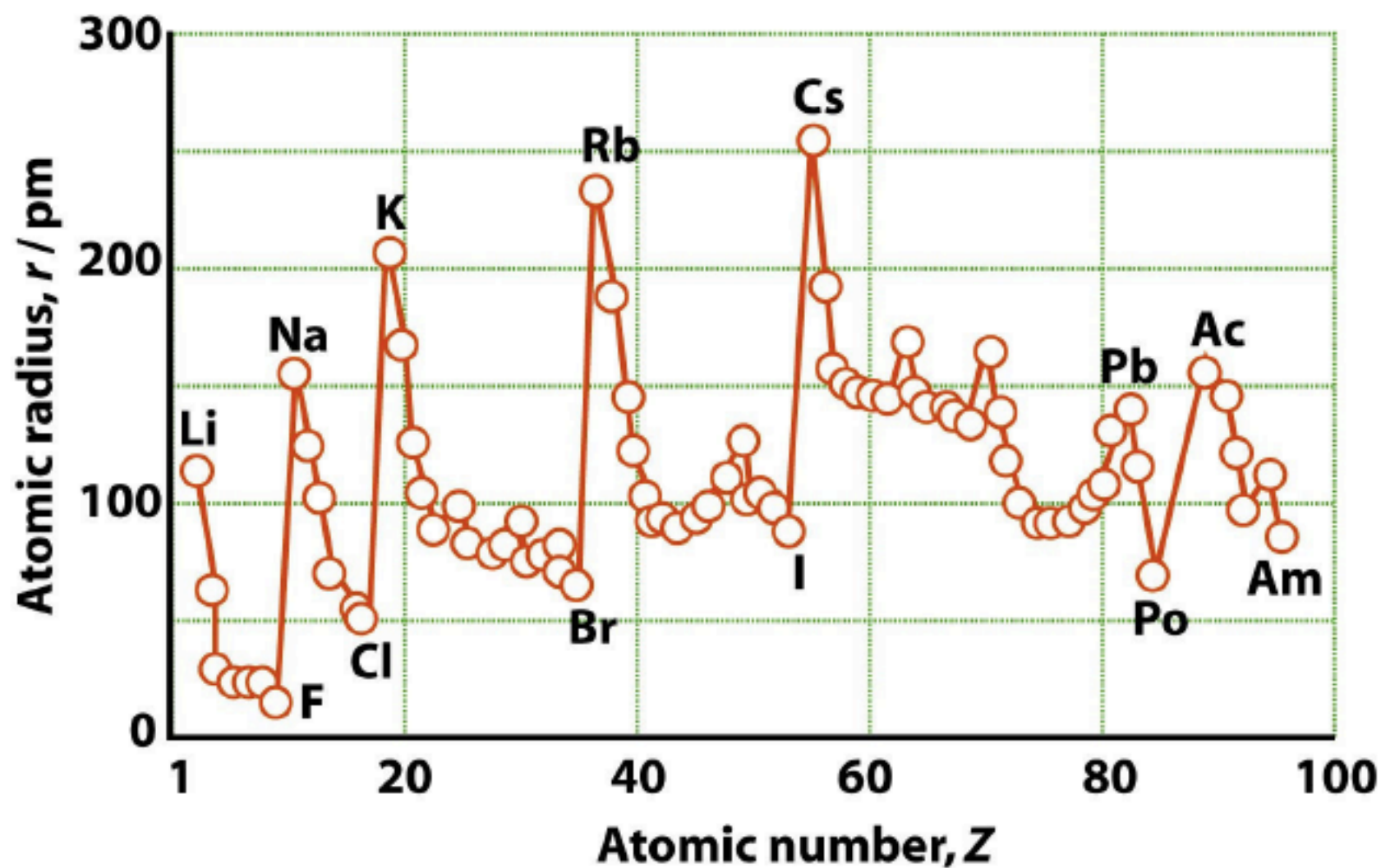


Figure 1-24

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Atomic Radii

DECREASING ATOMIC RADIUS

I	II	III	IV	V	VI	VII	VIII
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr
Rb	Sr	In	Sn	Sb	Te	I	Xe
Cs	Ba	Tl	Pb	Bi	Po	At	Rn

INCREASING ATOMIC RADIUS

Metallic Radius

Metallic radii in the third row d-block are similar to the second row d-block, but not larger as one would expect given their larger number of electrons

Lanthanide Contraction

f-orbitals have poor shielding properties;
low penetrating power.

Table 1.4 Atomic radii, r/pm^*

Li	Be												B	C	N	O	F
157	112												88	77	74	66	64
Na	Mg												Al	Si	P	S	Cl
191	160												143	118	110	104	99
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	
235	197	164	147	135	129	137	126	125	125	128	137	153	122	121	117	114	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	
250	215	182	160	147	140	135	134	134	137	144	152	167	158	141	137	133	
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi			
272	224	172	159	147	141	137	135	136	139	144	155	171	175	182			

*The values refer to coordination number 12 (see Section 3.2).

Decreases with increase in atomic number in a period left to right
Increases moving along a group top to bottom

Table 1.5 Ionic radii, r/pm^*

Li⁺ 59(4) 76(6)	Be²⁺ 27(4)	B³⁺ 11(4)			N³⁻ 146	O²⁻ 135(2) 138(4) 140(6) 142(8)	F⁻ 128(2) 131(4) 133(6)
Na⁺ 99(4) 102(6) 118(8)	Mg²⁺ 49(4) 72(6) 89(8)	Al³⁺ 39(4) 53(6)			P³⁻ 212	S²⁻ 184(6)	Cl⁻ 181(6)
K⁺ 138(6) 151(8) 159(10) 160(12)	Ca²⁺ 100(6) 112(8) 123(10) 134(12)	Ga³⁺ 62(6)			As³⁻ 222	Se²⁻ 198(6)	Br⁻ 196(6)
Rb⁺ 152(6) 160(8) 173(12)	Sr²⁺ 118(6) 125(8) 144(12)	In³⁺ 79(6) 92(8)	Sn²⁺ 83(6) 93(8)	Sn⁴⁺ 69(6)		Te²⁻ 221(6)	I⁻ 220(6)
Cs⁺ 167(6) 174(8) 188(12)	Ba²⁺ 149(6) 156(8) 175(12)	Tl³⁺ 88(6) Tl⁺ 164(6)					

* Numbers in parentheses are the coordination number of the ion. For more values, see *Resource section 1*.

All anions are larger than their parent atoms;

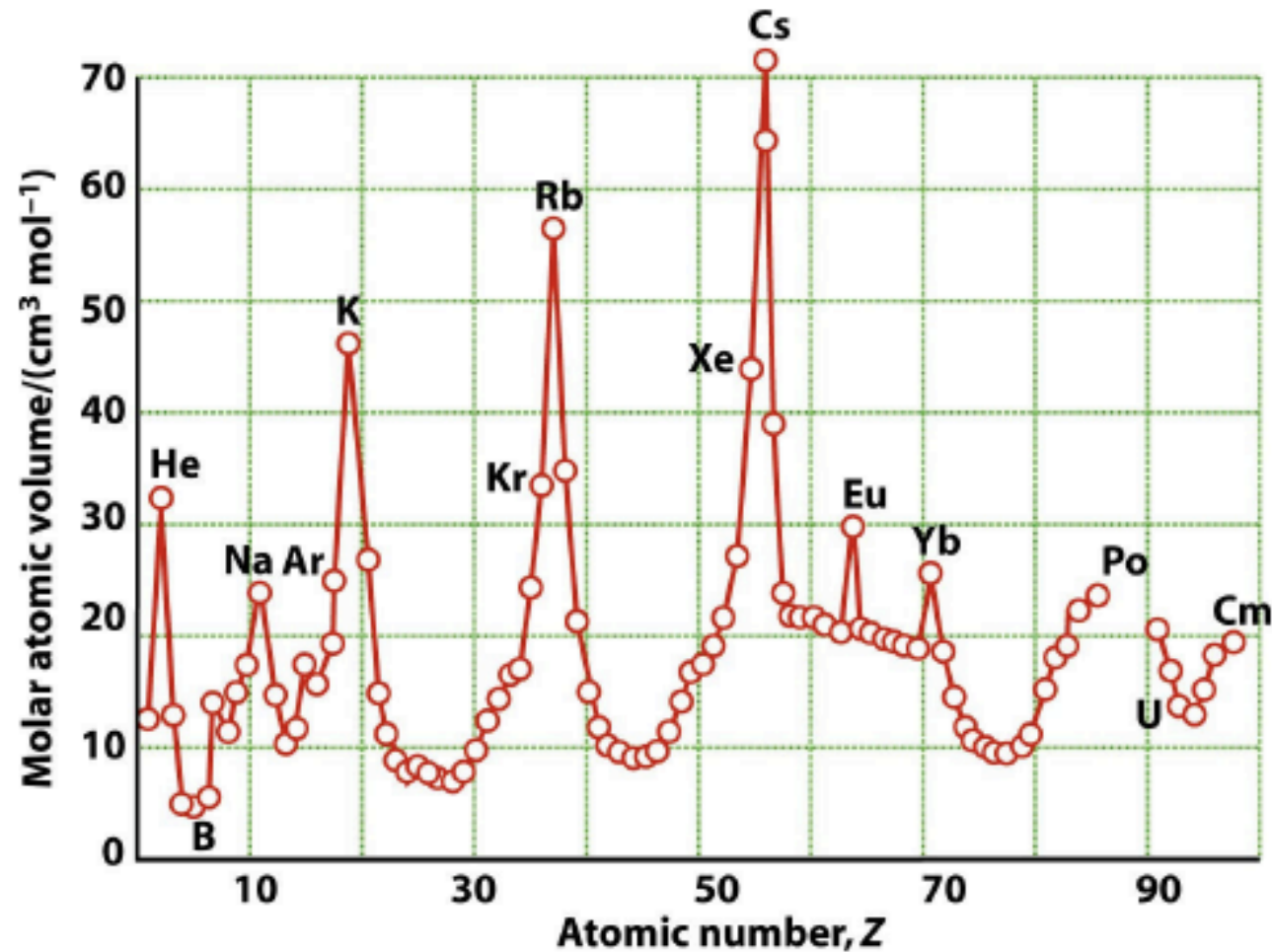
The cations are smaller

Table 1-5

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Molar Atomic Volume $\rightarrow$ Volume per mole of atoms of the element



Density, melting point, etc. depend on atomic volume;
related to compactness or the lack of it

Ionisation Energy (IE)

The minimum energy needed to remove an electron from a gas phase atom

Depends on

- (a) Size of the atom - IE decreases as the size of the atom increases
- (b) Nuclear Charge - IE increases with increase in nuclear charge
- (c) The type of electron - Shielding effect

1 st IE	H	1312	KJ mol ⁻¹
	Li	520	KJ mol ⁻¹

Reasons

1. Average distance of 2s electron is greater than that of 1s
2. Penetration effect
3. Electronic configuration

On moving down a group

1. nuclear charge increases
2. Z^* due to screening is almost constant
3. number of shells increases, hence atomic size increases.
4. there is a increase in the number of inner electrons which shield the valence electrons from the nucleus

Thus IE decreases down the group

On moving across a period

1. the atomic size decreases
2. nuclear charge increases

Thus IE increases along a period

Exception: B, O ionization energy lower than Be, N: empty or half filled orbitals contribute to the stability.

Similarly: Al, S

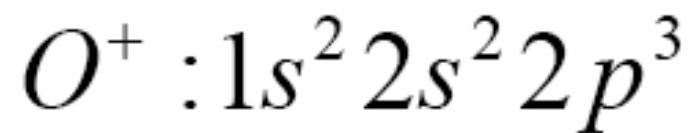
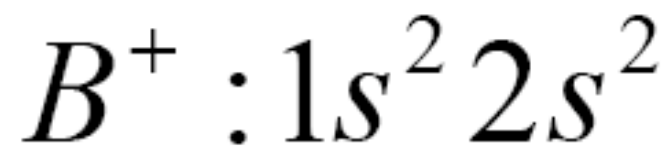
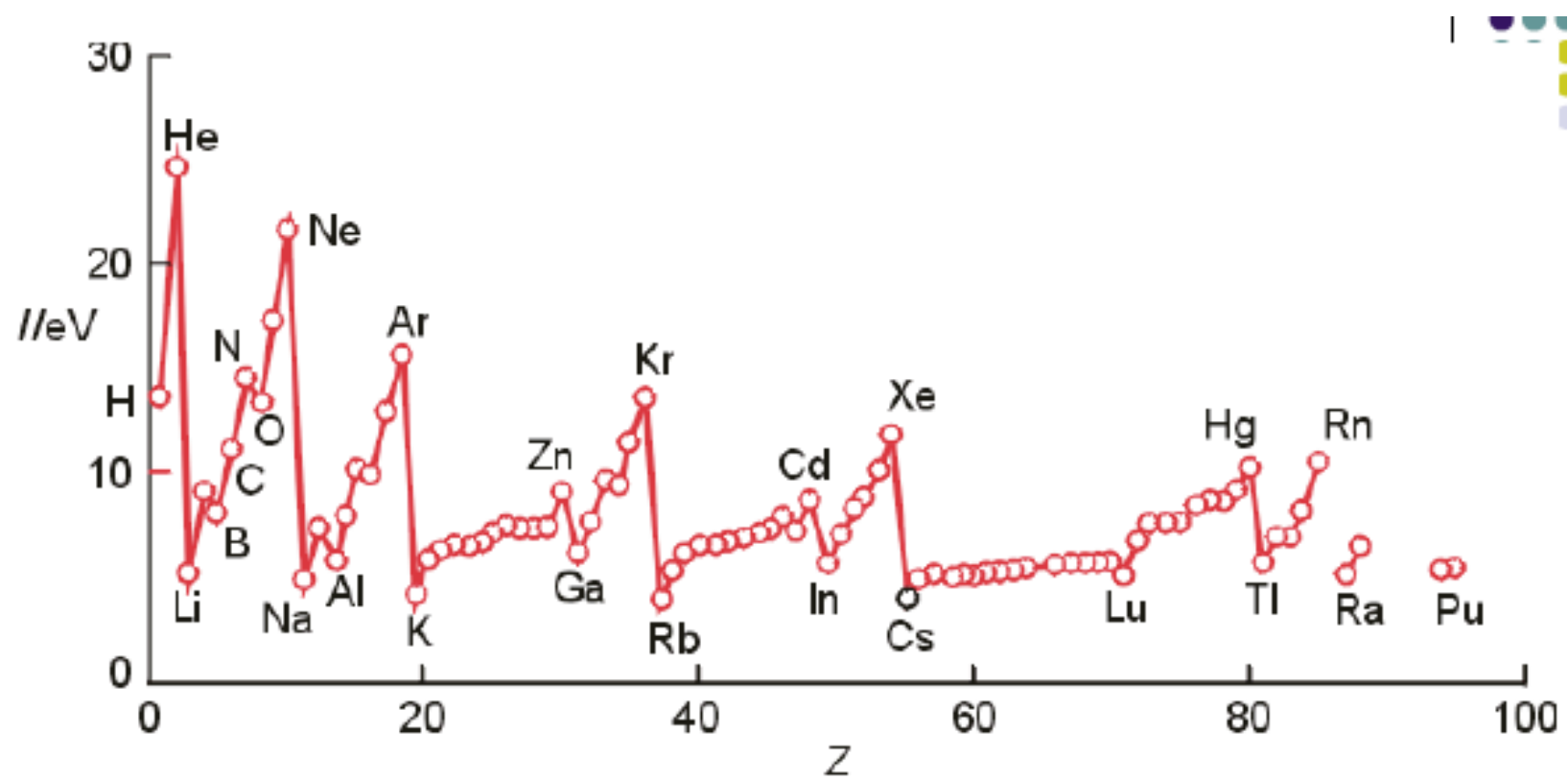


Table 1.6 First and second (and some higher) ionization energies of the elements, $I/(kJ\ mol^{-1})$

H							He
1312							2373
							5259
Li	Be	B	C	N	O	F	Ne
513	899	801	1086	1402	1314	1681	2080
7297	1757	2426	2352	2855	3386	3375	3952
11809	14844	3660	4619	4577	5300	6050	6122
		25018					
Na	Mg	Al	Si	P	S	Cl	Ar
495	737	577	786	1011	1000	1251	1520
4562	1476	1816	1577	1903	2251	2296	2665
6911	7732	2744	3231	2911	3361	3826	3928
		11574					
K	Ca	Ga	Ge	As	Se	Br	Kr
419	589	579	762	947	941	1139	1351
3051	1145	1979	1537	1798	2044	2103	3314
4410	4910	2963	3302	2734	2974	3500	3565
Rb	Sr	In	Sn	Sb	Te	I	Xe
403	549	558	708	834	869	1008	1170
2632	1064	1821	1412	1794	1795	1846	2045
3900	4210	2704	2943	2443	2698	3197	3097
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
375	502	590	716	704	812	926	1036
2420	965	1971	1450	1610	1800	1600	
3400	3619	2878	3080	2466	2700	2900	

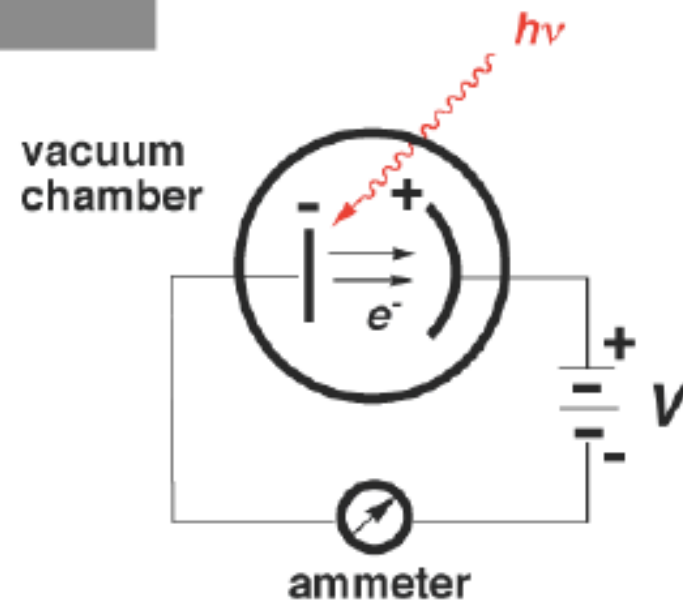
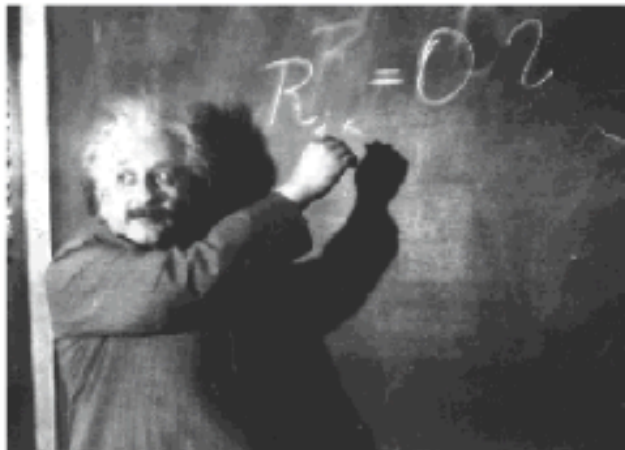
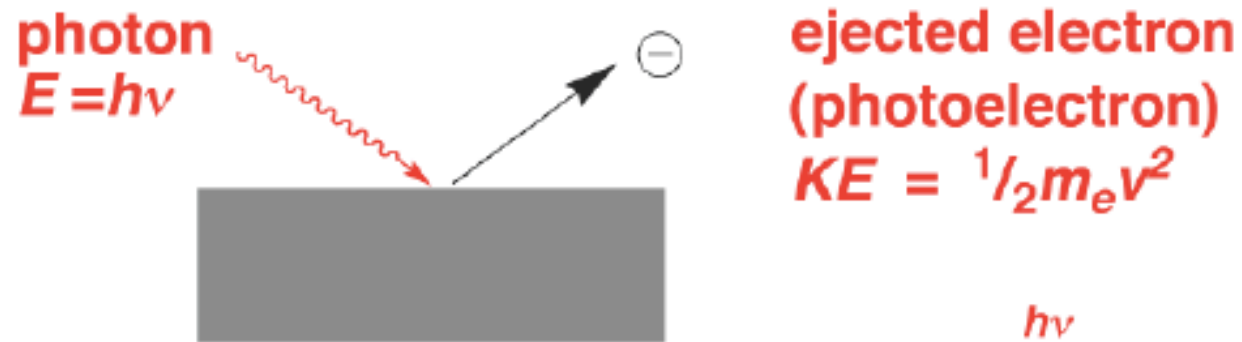
Table 1-6

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Measurement of Ionization Energies: Einstein and the Photoelectric Effect

Einstein's photoelectric law: $h\nu = IE + \frac{1}{2}m_e v^2$



Electron affinity (EA)

- the amount of energy associated with the gain of electrons

The greater the energy released in the process of taking up the extra electron, greater is the EA

The EA of an atom measures the tightness with which it binds an additional electron to itself.

On moving across a period,

- the atomic size decreases and hence the force of attraction exerted by the nucleus on the electrons increases. Consequently, the atom has a greater tendency to attract additional electron i.e., its electron affinity increases
- EA values of metals are low while those of non-metals are high
- Halogens have high electron affinities. This is due to their strong tendency to gain an additional electron to change into the stable ns^2np^6 configuration

On moving down a group,

- the atomic size increases and therefore, the effective nuclear attraction decreases and thus electron affinity decreases

Table 1.7 Electron affinities of the main-group elements, $E_a/(\text{kJ mol}^{-1})^*$

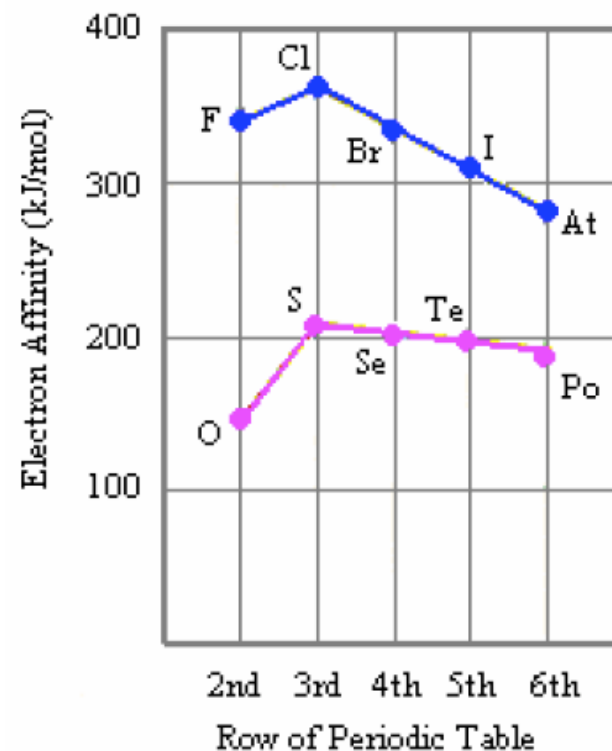
H							He
72							−48
Li	Be	B	C	N	O	F	Ne
60	≤ 0	27	122	−8	141 −780	328	−116
Na	Mg	Al	Si	P	S	Cl	Ar
53	≤ 0	43	134	72	200 −492	349	−96
K	Ca	Ga	Ge	As	Se	Br	Kr
48	2	29	116	78	195	325	−96
Rb	Sr	In	Sn	Sb	Te	I	Xe
47	5	29	116	103	190	295	−77

* The first values refer to the formation of the ion X^- from the neutral atom; the second value to the formation of X^{2-} from X^- .

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- ↗ maximum for halogens
- ↗ usually positive, difficult to measure, but can be negative.
- ↗ **EA(F) lower than EA(Cl):**
smaller diameter, strong e-e repulsion



Electronegativity

measure of the tendency of an element to attract electrons to itself

On moving down the group,

- Z increases but Z^* almost remains constant
- number of shells (n) increases
- atomic radius increases
- force of attraction between added electron and nucleus decreases

Therefore EN decreases moving down the group

On moving across a period left to right

- Z and Z^* increases
- number of shells remains constant
- atomic radius decreases
- force of attraction between added electron and nucleus increases

Hence EN increases along a period

Trend 1. EN decrease down a group

Trend 2: EN increase across a period



H 2.20																	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 2.00	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.60	Mo 2.16	Tc 1.90	Ru 2.20	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	
Cs 0.79	Ba 0.89	La 1.10	Hf 1.30	Ta 1.50	W 2.36	Re 1.90	Os 2.20	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 2.04	Pb 2.33	Bi 2.02	Po 2.00	At 2.20	

Electronegativity (EN)



The power of an atom in a molecule to attract electrons to itself

Mulliken definition: $EN = 1/2(IE_1 + EA)$

Pauling definition:

$$EN_A - EN_B = 0.208 \sqrt{DE_{AB} - \sqrt{DE_{A^2} DE_{B^2}}}$$

$$EN(F) = 3.98$$

DE = bond dissociation energy in kcal/mol

EN(A) - EN(B) small $\rightarrow$ A-B bonding mostly covalent

EN(A) - EN(B) large $\rightarrow$ A-B bonding has ionic component

Electronegativity: Allred and Rochow

To gauge the ability of an atom in a molecule to attract an electron, Allred and Rochow used the electrostatic force of attraction between an atom and an electron placed at the covalent radius of the atom:

$$\text{force} = e^2 Z_{\text{eff}} / r^2$$

where r is the covalent radius, e is the charge on an electron and Z_{eff} is the effective charge of the electron due to the nucleus and its surrounding electrons. The force correlates well with the Pauling electronegativity scale and the Allred-Rochow electronegativity values are calculated with the formula:

$$c = 0.744 + 0.359 Z_{\text{eff}} / r^2$$

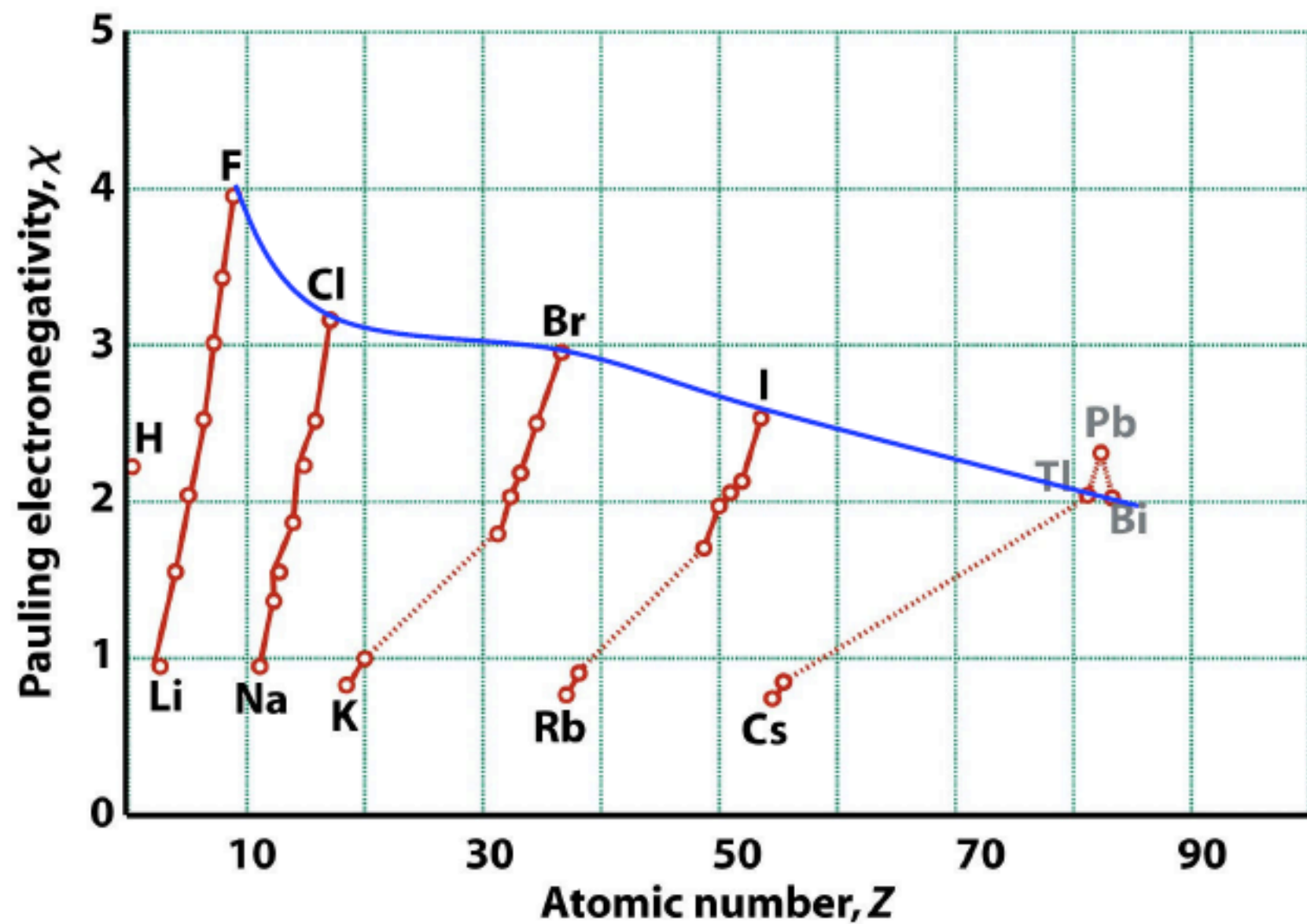


Figure 1-27

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Table 1.8 Pauling χ_P , Mulliken, χ_M , and Allred–Rochow, χ_{AR} , electronegativities

H								He
2.20								5.5
3.06								
2.20								
Li	Be	B	C	N	O	F		Ne
0.98	1.57	2.04	2.55	3.04	3.44	3.98		
1.28	1.99	1.83	2.67	3.08	3.22	4.43		4.60
0.97	1.47	2.01	2.50	3.07	3.50	4.10		5.10
Na	Mg	Al	Si	P	S	Cl		Ar
0.93	1.31	1.61	1.90	2.19	2.58	3.16		
1.21	1.63	1.37	2.03	2.39	2.65	3.54		3.36
1.01	1.23	1.47	1.74	2.06	2.44	2.83		3.30
K	Ca	Ga	Ge	As	Se	Br		Kr
0.82	1.00	1.81	2.01	2.18	2.55	2.96		3.0
1.03	1.30	1.34	1.95	2.26	2.51	3.24		2.98
0.91	1.04	1.82	2.02	2.20	2.48	2.74		3.10
Rb	Sr	In	Sn	Sb	Te	I		Xe
0.82	0.95	1.78	1.96	2.05	2.10	2.66		2.6
0.99	1.21	1.30	1.83	2.06	2.34	2.88		2.59
0.89	0.99	1.49	1.72	1.82	2.01	2.21		2.40