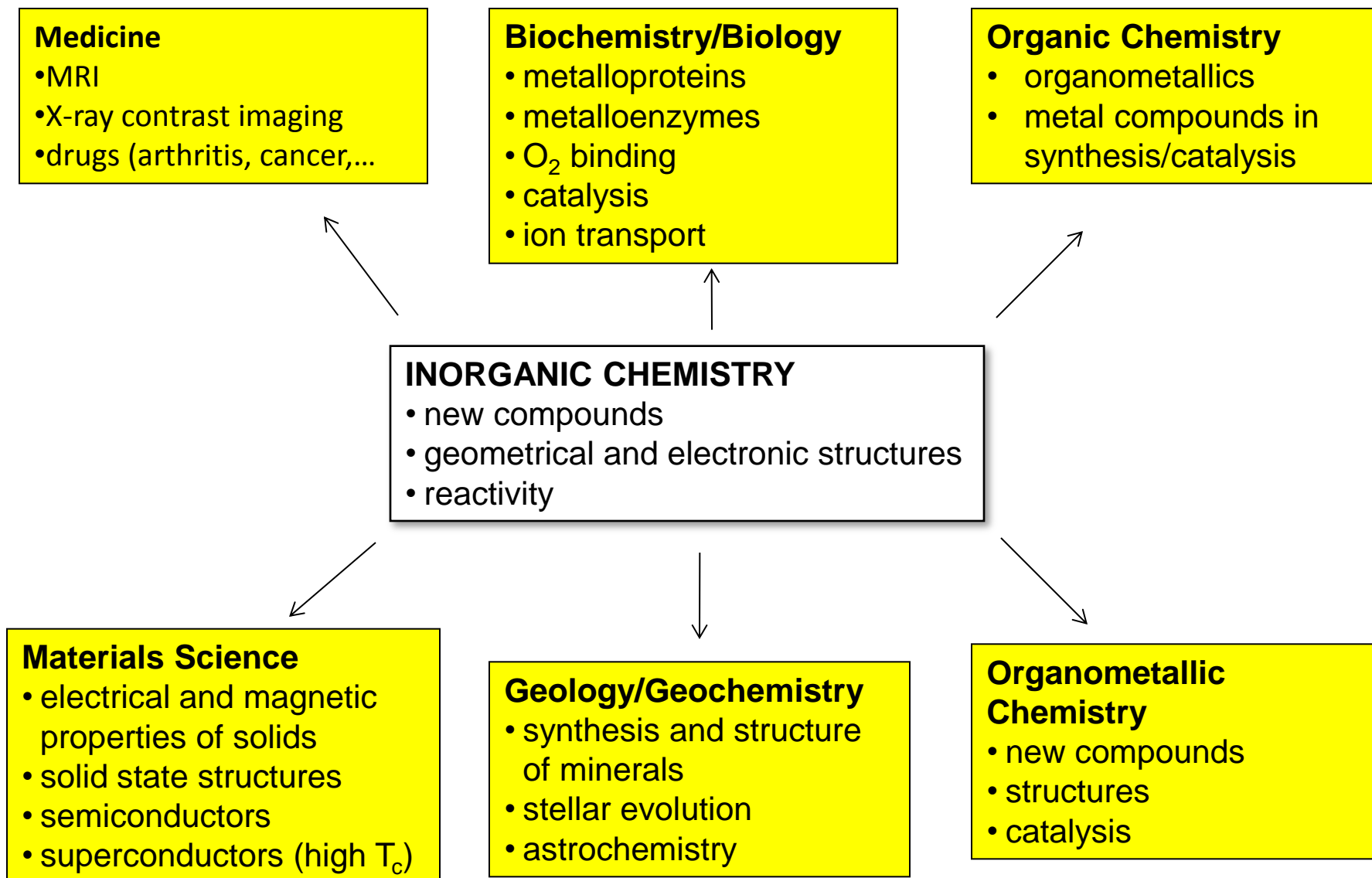


The Scope of Inorganic Chemistry



If some universal catastrophe were to engulf the world, and humankind
Could retain one scientific concept in order to rebuild civilization, what
would that one concept be?

Response for physicists (Richard Feynman in “Six Easy Pieces”):

The modern idea of atoms.

Response for chemists:

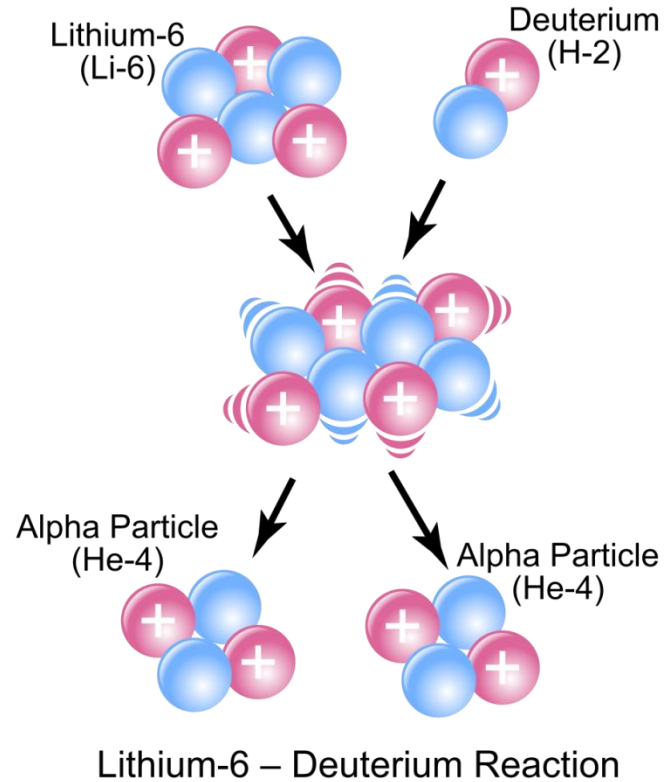
The periodic table

**The periodic table encapsulates the concept of elements,
organizes physical and chemical trends of substances,
and compares the structure of the different atoms—
All in a very small space.**

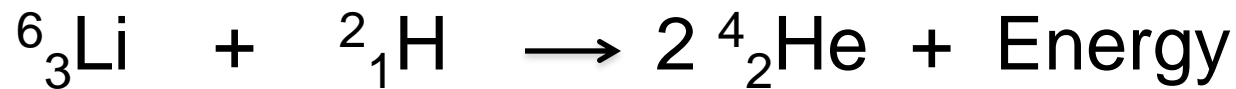
*Inorganic Chemists think they **own** the Periodic Table.*

So, How did it all start?

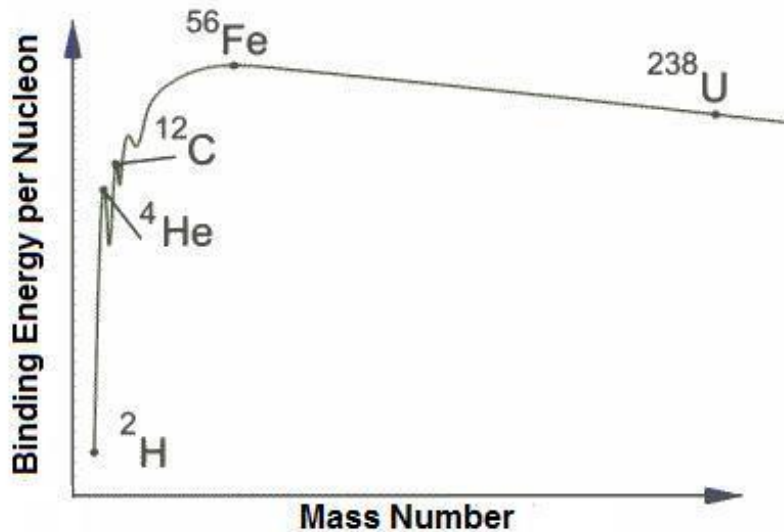
An example of nuclear FUSION and the creation of an unstable isotope of Be



${}^8_4\text{Be}$ with $t_{1/2}$ of
ca. 10^{-18} sec

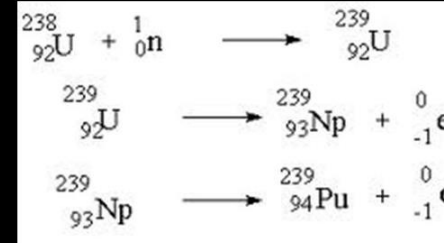


Stable vs. Unstable or Fissionable Nuclei

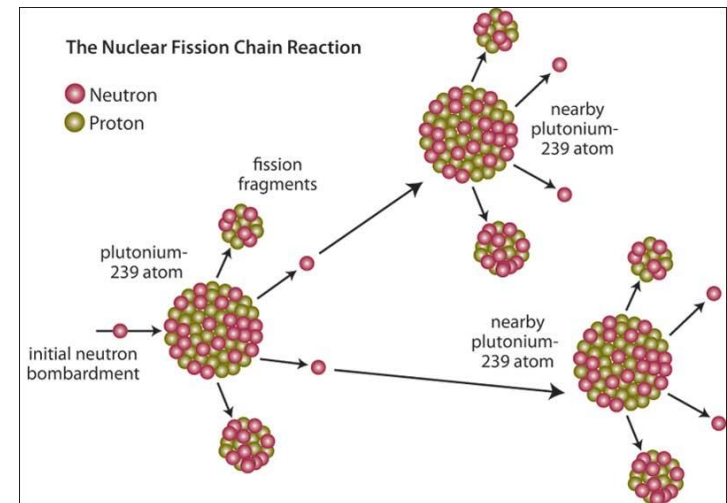


Project no. 1. Nuclear Reactions; Web Elements

Breeder Reactors



- Use U-238, a nonfissionable but much more plentiful isotope of uranium (99%).
- It undergoes transmutation into Pu-239 a fissionable isotope of plutonium



WebElements™ Periodic Table

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period																		
1	1 <u>H</u>																	2 <u>He</u>
2	3 <u>Li</u>	4 <u>Be</u>											5 <u>B</u>	6 <u>C</u>	7 <u>N</u>	8 <u>O</u>	9 <u>F</u>	10 <u>Ne</u>
3	11 <u>Na</u>	12 <u>Mg</u>											13 <u>Al</u>	14 <u>Si</u>	15 <u>P</u>	16 <u>S</u>	17 <u>Cl</u>	18 <u>Ar</u>
4	19 <u>K</u>	20 <u>Ca</u>	21 <u>Sc</u>	22 <u>Ti</u>	23 <u>V</u>	24 <u>Cr</u>	25 <u>Mn</u>	26 <u>Fe</u>	27 <u>Co</u>	28 <u>Ni</u>	29 <u>Cu</u>	30 <u>Zn</u>	31 <u>Ga</u>	32 <u>Ge</u>	33 <u>As</u>	34 <u>Se</u>	35 <u>Br</u>	36 <u>Kr</u>
5	37 <u>Rb</u>	38 <u>Sr</u>	39 <u>Y</u>	40 <u>Zr</u>	41 <u>Nb</u>	42 <u>Mo</u>	43 <u>Tc</u>	44 <u>Ru</u>	45 <u>Rh</u>	46 <u>Pd</u>	47 <u>Ag</u>	48 <u>Cd</u>	49 <u>In</u>	50 <u>Sn</u>	51 <u>Sb</u>	52 <u>Te</u>	53 <u>I</u>	54 <u>Xe</u>
6	55 <u>Cs</u>	56 <u>Ba</u>	* 71 <u>Lu</u>	* 72 <u>Hf</u>	* 73 <u>Ta</u>	* 74 <u>W</u>	* 75 <u>Re</u>	* 76 <u>Os</u>	* 77 <u>Ir</u>	* 78 <u>Pt</u>	* 79 <u>Au</u>	* 80 <u>Hg</u>	81 <u>Tl</u>	82 <u>Pb</u>	83 <u>Bi</u>	84 <u>Po</u>	85 <u>At</u>	86 <u>Rn</u>
7	87 <u>Fr</u>	88 <u>Ra</u>	* 103 <u>Lr</u>	* 104 <u>Rf</u>	* 105 <u>Db</u>	* 106 <u>Sg</u>	* 107 <u>Bh</u>	* 108 <u>Hs</u>	* 109 <u>Mt</u>	* 110 <u>Ds</u>	* 111 <u>Rg</u>	112 <u>Uu</u> b	113 <u>Uut</u>	114 <u>Uu</u> q	115 <u>Uu</u> p	116 <u>Uu</u> h	117 <u>Uus</u>	118 <u>Uuo</u>

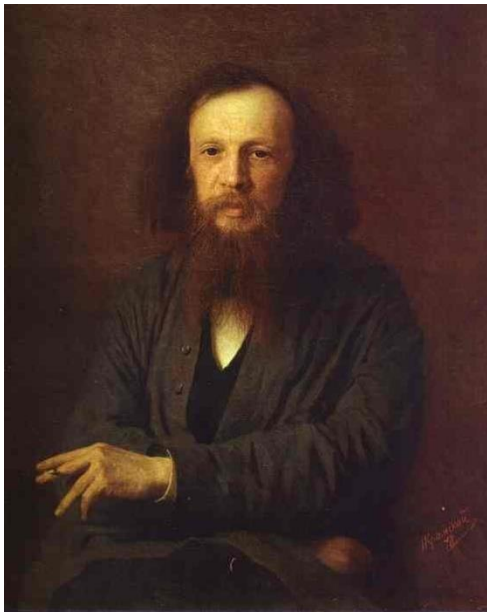
*Lanthanoids	* 71 <u>Lu</u>
**Actinoids	* 103 <u>Lr</u>

57 <u>La</u>	58 <u>Ce</u>	59 <u>Pr</u>	60 <u>Nd</u>	61 <u>Pm</u>	62 <u>Sm</u>	63 <u>Eu</u>	64 <u>Gd</u>	65 <u>Tb</u>	66 <u>Dy</u>	67 <u>Ho</u>	68 <u>Er</u>	69 <u>Tm</u>	70 <u>Yb</u>
89 <u>Ac</u>	90 <u>Th</u>	91 <u>Pa</u>	92 <u>U</u>	93 <u>Np</u>	94 <u>Pu</u>	95 <u>Am</u>	96 <u>Cm</u>	97 <u>Bk</u>	98 <u>Cf</u>	99 <u>Es</u>	100 <u>Fm</u>	101 <u>Md</u>	102 <u>No</u>

Mass Spectra computer:

<http://www.sisweb.com/mstools/isotope.htm>

<http://www.sisweb.com/mstools/isotope.htm>



Dimitri Mendeleev

1834-1907

A
Z E

			Ni = 59	Co = 59	Pd = 106,6
H = 1			Cu = 63,4		Ag = 108
	Be = 9,4	Mg = 24	Zn = 65,2		Cd = 112
	B = 11	Al = 27,4	? = 68		Ur = 116
	C = 12	Si = 28	? = 70		Sn = 118
	N = 14	P = 31	As = 75		Sb = 122
	O = 16	S = 32	Se = 79,4		Te = 128?
	F = 19	Cl = 35,5	Br = 80		J = 127
Li = 7	Na = 23	K = 39	Rb = 85,4		Cs = 133
		Ca = 40	Sr = 87,6		Ba = 137

Z = No. protons in nucleus, Atomic number

A = Mass number; no. of protons + neutrons in nucleus

Groups (American tradition)

IA IIA IIIB IVB VB VIB VIIB VIIIB IB IIB IIIA IVA VA VIA VIIA VIIIA

Groups (European tradition)

IA IIA IIIA IVA VA VIA VIIA VIII IB IIB IIIB IVB VB VIB VIIB 0

Groups (IUPAC)

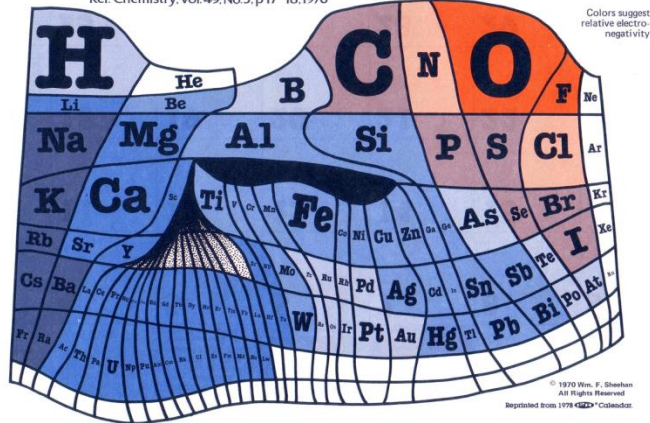
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

1																		2
3												5						10
Alkali Metals	Alkaline Earth Metals											13				Chalcogens	Halogens	Noble Gases
		21		22								30	31					
		39		40								48	49					
55	Alkaline Earth Metals	57	*	72								80	81					86
87		89	**	104								112						

*	58	Lanthanides																71
**	90	Actinides																103

The Elements According to Relative Abundance

A Periodic Chart by Prof. Wm. F. Sheehan, University of Santa Clara, CA 95053
 Ref. Chemistry, Vol. 49, No. 3, p. 17-18, 1976



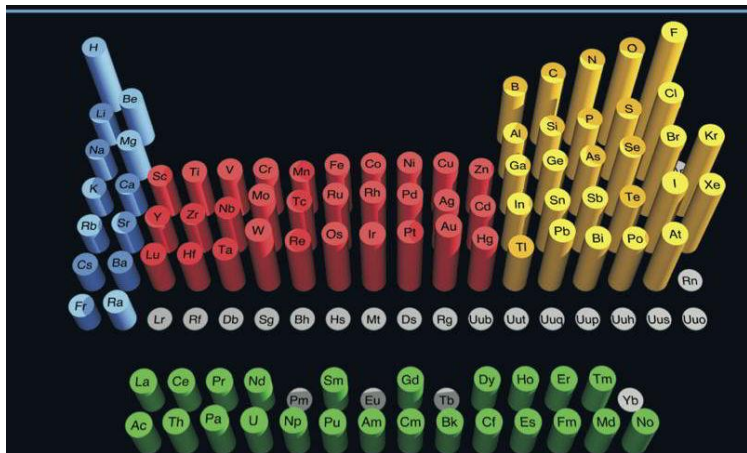
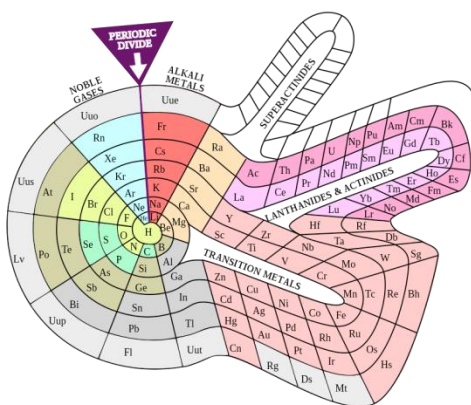
Colors suggest relative electronegativity.

© 1970 Wm. F. Sheehan
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 Reprinted from 1978 © Wm. F. Sheehan

Roughly, the size of an element's own niche ("I almost wrote square") is proportioned to its abundance on Earth's surface, and in addition, certain chemical similarities (e.g., Be and Al, or B and Si) are suggested by the positioning of neighbors.

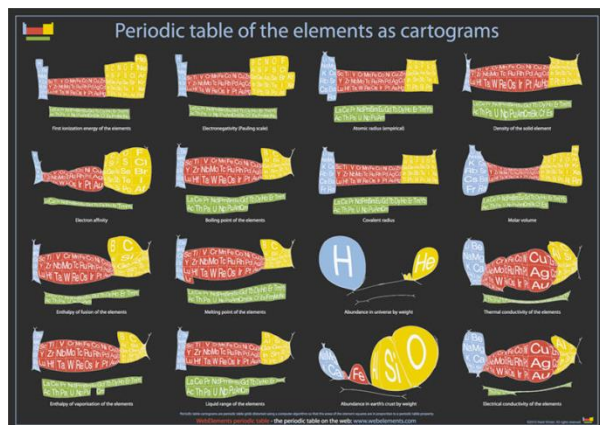
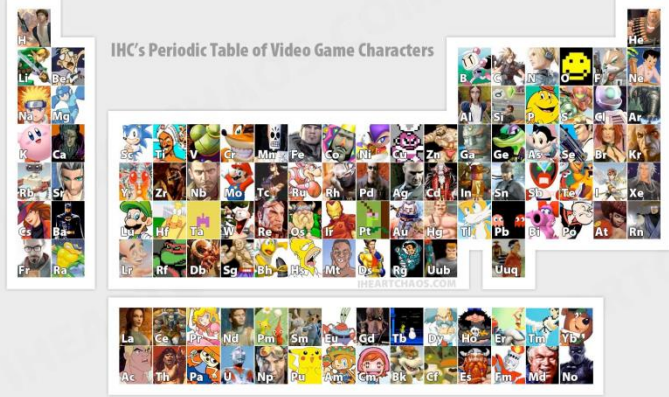
The chart emphasizes that in real life a chemist will probably meet O, Si, Al, ... and that he better do something about it. Periodic tables based upon elemental abundance would, of course, vary from planet to planet. . . W.F.S.

NOTE: TO ACCOMMODATE ALL ELEMENTS SOME DISTORTIONS WERE NECESSARY, FOR EXAMPLE SOME ELEMENTS



electronegativity: the power of an atom when in a molecule to attract electrons to itself. Electronegativity values are assigned to each element. The Pauling electronegativity scale is the most common.

IHC's Periodic Table of Video Game Characters



Color	Metal Flame Colors
Red	<p><i>Carmines</i>: Lithium compounds. Masked by barium or sodium.</p> <p><i>Scarlet or Crimson</i>: Strontium compounds. Masked by barium.</p> <p><i>Yellow-Red</i>: Calcium compounds. Masked by barium.</p>
Yellow	Sodium compounds, even in trace amounts. A yellow flame is not indicative of sodium unless it persists and is not intensified by addition of 1% NaCl to the dry compound.
White	<i>White-Green</i> : Zinc
Green	<p><i>Emerald</i>: Copper compounds, other than halides. Thallium.</p> <p><i>Blue-Green</i>: Phosphates, when moistened with H_2SO_4 or B_2O_3.</p> <p><i>Faint Green</i>: Antimony and NH_4 compounds.</p> <p><i>Yellow-Green</i>: Barium, molybdenum.</p>
Blue	<p><i>Azure</i>: Lead, selenium, bismuth, CuCl_2 and other copper compounds moistened with hydrochloric acid.</p> <p><i>Light Blue</i>: Arsenic and some of its compounds.</p> <p><i>Greenish Blue</i>: CuBr_2, antimony</p>
Violet	<p>Potassium compounds other than borates, phosphates, and silicates. Masked by sodium or lithium.</p> <p><i>Purple-Red</i>: Potassium, rubidium, and/or cesium in the presence of sodium when viewed through a blue glass.</p>

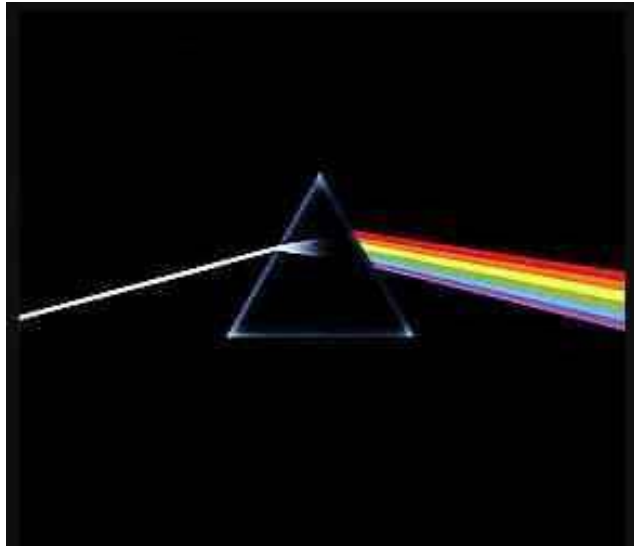
Atomic Emission (Spectroscopy)

- An emission spectrum requires first the addition of energy to a material.
- The addition of energy promotes electrons of that material from the ground state to the excited state.
- As the electrons “fall” from the excited state to the ground state, they emit the energy they absorbed in the form of electromagnetic radiation (heat, light, etc.)

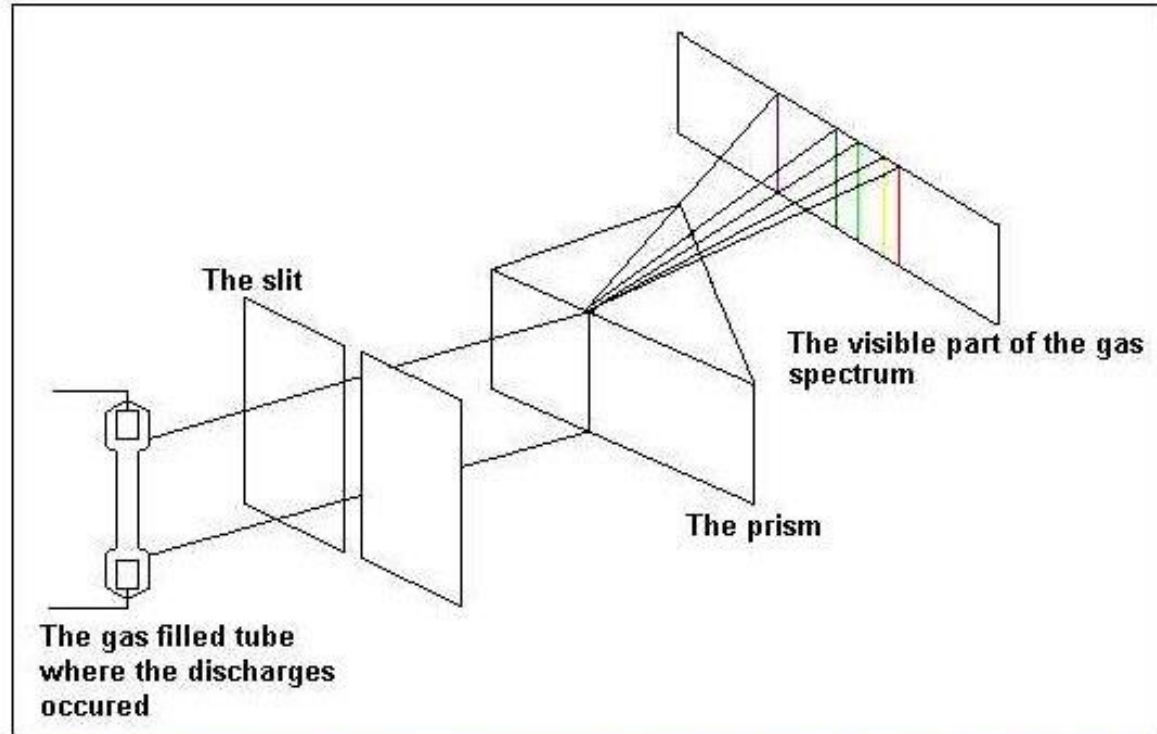
Comments

- Atomic emission is used in street lamps, fluorescent lights, and neon signs.
- Two common street lamps using this are the mercury lamp and the sodium lamp.
- “Neon” signs frequently implement the emission spectra of other gases such as argon and krypton.
- Very sophisticated instrumental techniques such as “flame photometry” and “atomic absorption” are based on the principles of atomic emission.

Continuous and Line Spectra



Dark Side of the Moon
Pink Floyd



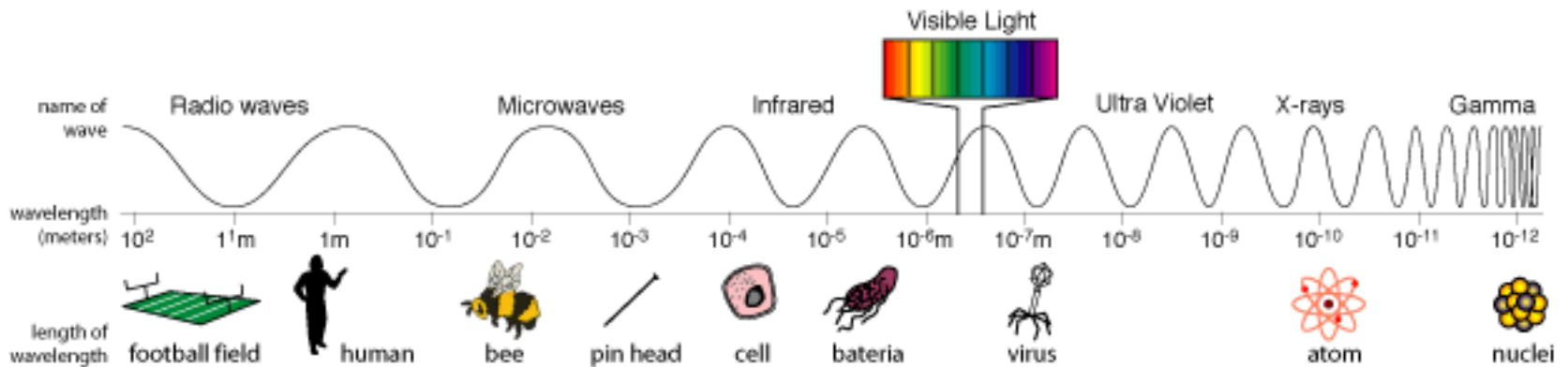
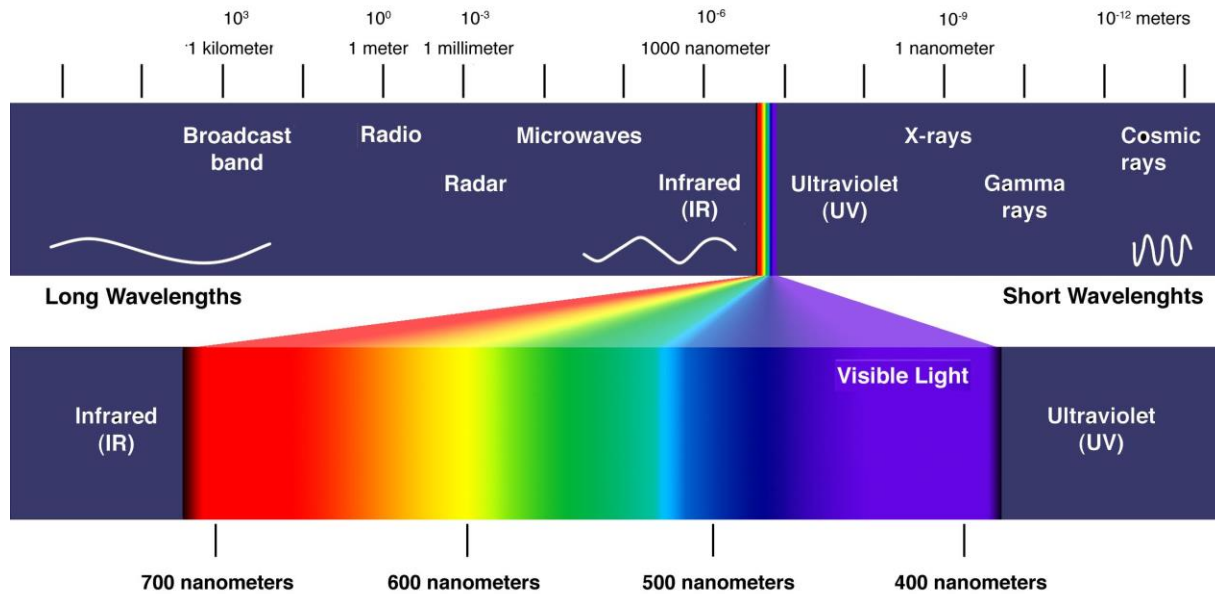
The discharges in the low pressure gas filled tube are the sources of the light which undergo refraction on the prism. We see the line spectrum of the gas.

Sodium Flame Spectrum

<http://webmineral.com/help/FlameTest.shtml>

Both neutral and singly ionized sodium contribute to the emission lines in this spectrum.

Electromagnetic Radiation Spectrum



In the news: January 20, 2016

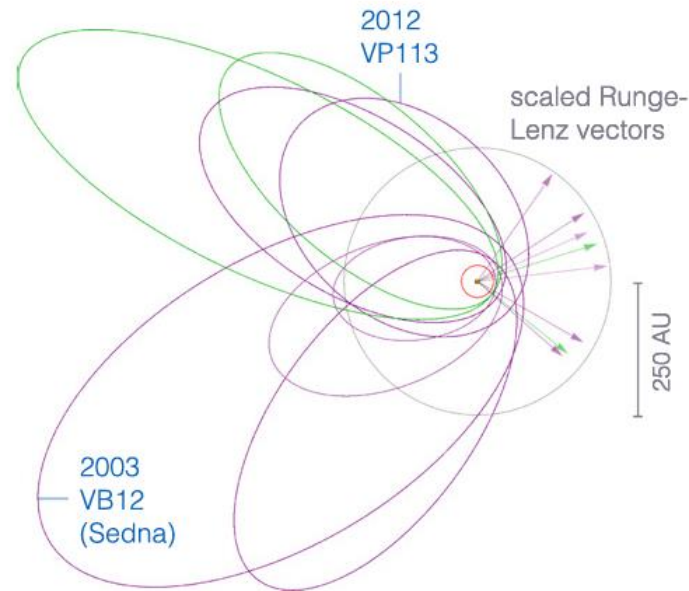
EVIDENCE FOR A DISTANT GIANT PLANET IN THE SOLAR SYSTEM

KONSTANTIN BATYGIN AND MICHAEL E. BROWN

Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA; kbatygin@gps.caltech.edu

Received 2015 November 13; accepted 2016 January 10; published 2016 January 20

BATYGIN & BROWN



Cumulatively, the presented results offer credence to the hypothesis that the observed structure of the distant Kuiper Belt can be explained by invoking perturbations from an unseen planetary mass companion to the solar system. Simultaneously, the suggestive nature of the results should be met with a healthy dose of skepticism, given the numerous assumptions made in the construction of our simple analytical model. In

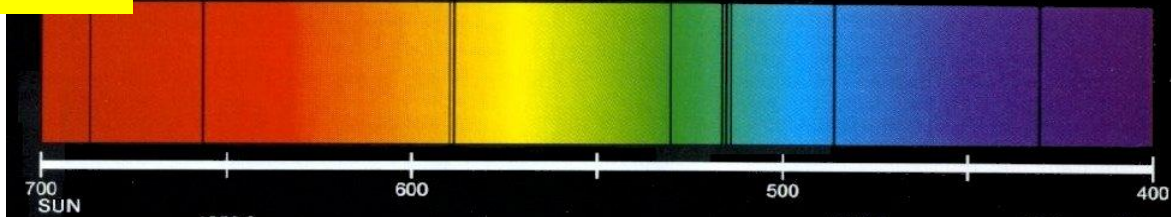
Lecture 2 362 January 22, 2016

*Paradigm Shift:
Development of Current
Atomic Theory*

Emission Spectra

C | 656,3 D₁ D₂ E b F G
 589,6 || 589 527 | 518,3 ||| 517,2 | 486,1 | 430,8

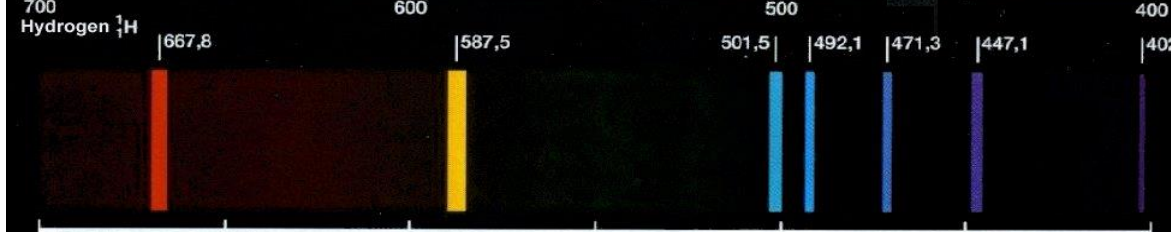
Sun



Hydrogen



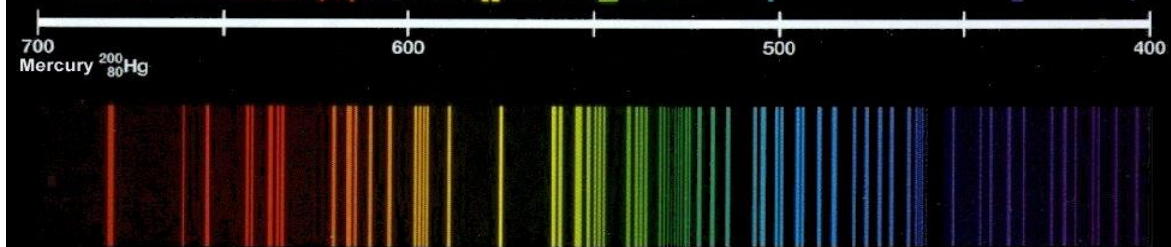
Helium



Mercury



Uranium



*Complexity increases
 With size of
 Element*

*What do these lines
 mean?????*

700 nm 600 nm 500 nm 400 nm

A Bit of History

TABLE 2.1 Discoveries in Atomic Structure

1896	A. H. Becquerel	Discovered radioactivity of uranium
1897	J. J. Thomson	Showed that electrons have a negative charge, with charge/mass = 1.76×10^{11} C/kg
1909	R. A. Millikan	Measured the electronic charge as 1.60×10^{-19} C; therefore, mass of electron = 9.11×10^{-31} kg
1911	E. Rutherford	Established the nuclear model of the atom: a very small, heavy nucleus surrounded by mostly empty space
1913	H. G. J. Moseley	Determined nuclear charges by X-ray emission, establishing atomic numbers as more fundamental than atomic masses



Z = No. protons in nucleus, Atomic number

A = Mass number; no. of protons + neutrons in nucleus



Marie Curie—1867-1934

So how to connect the physical properties of elements to the Periodic Table? Physicists! The current model of the atom belongs to Physicists!



DeBroglie



Planck



Schrodinger



Einstein



Heisenberg



Bohr

Pauli



Niels Bohr and wife Margrethe around 1930



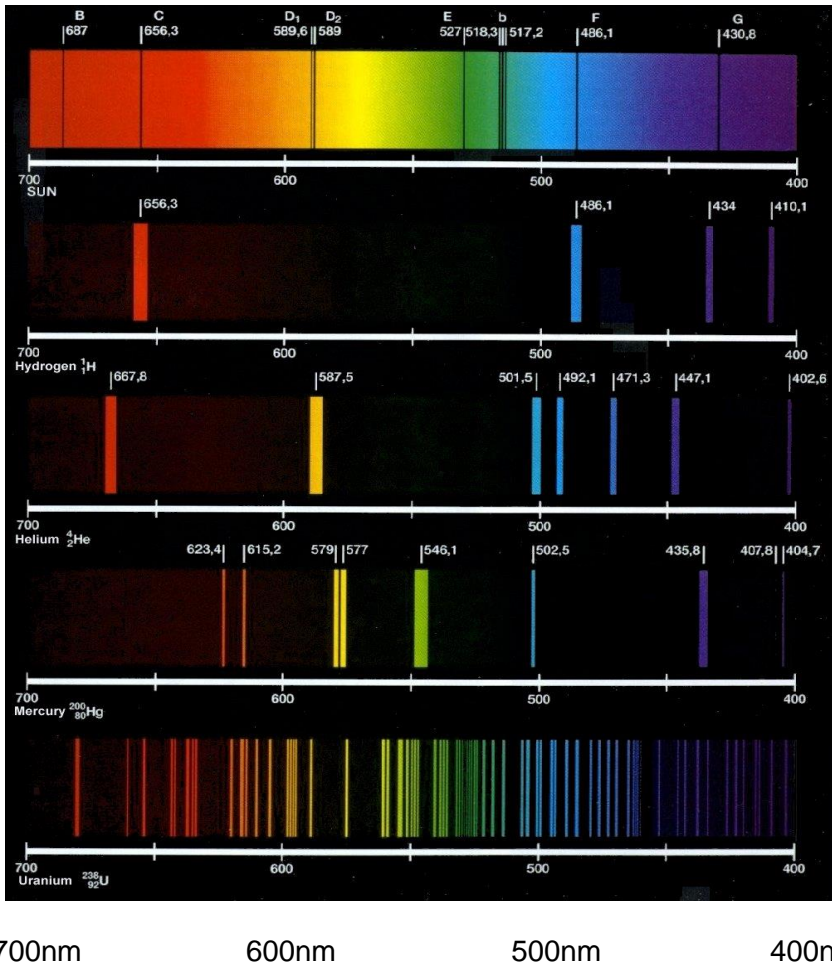
Taken from John L. Heilbron's "History: The Path to the quantum Atom",
Nature 498, 27-30, (06 June 2013)

Taken from John L. Heilbron's "History: The Path to the quantum Atom",
Nature 498, 27-30, (06 June 2013)

To develop his model, Bohr followed an analogy to the radiation theory of Max Planck (right). "... Bohr had developed a doctrine of multiple partial truths, each of which contained some bit of reality, and all of which together might exhaust it. "There exist so many different truths I can almost call it my religion that I think that everything that is of value is true."



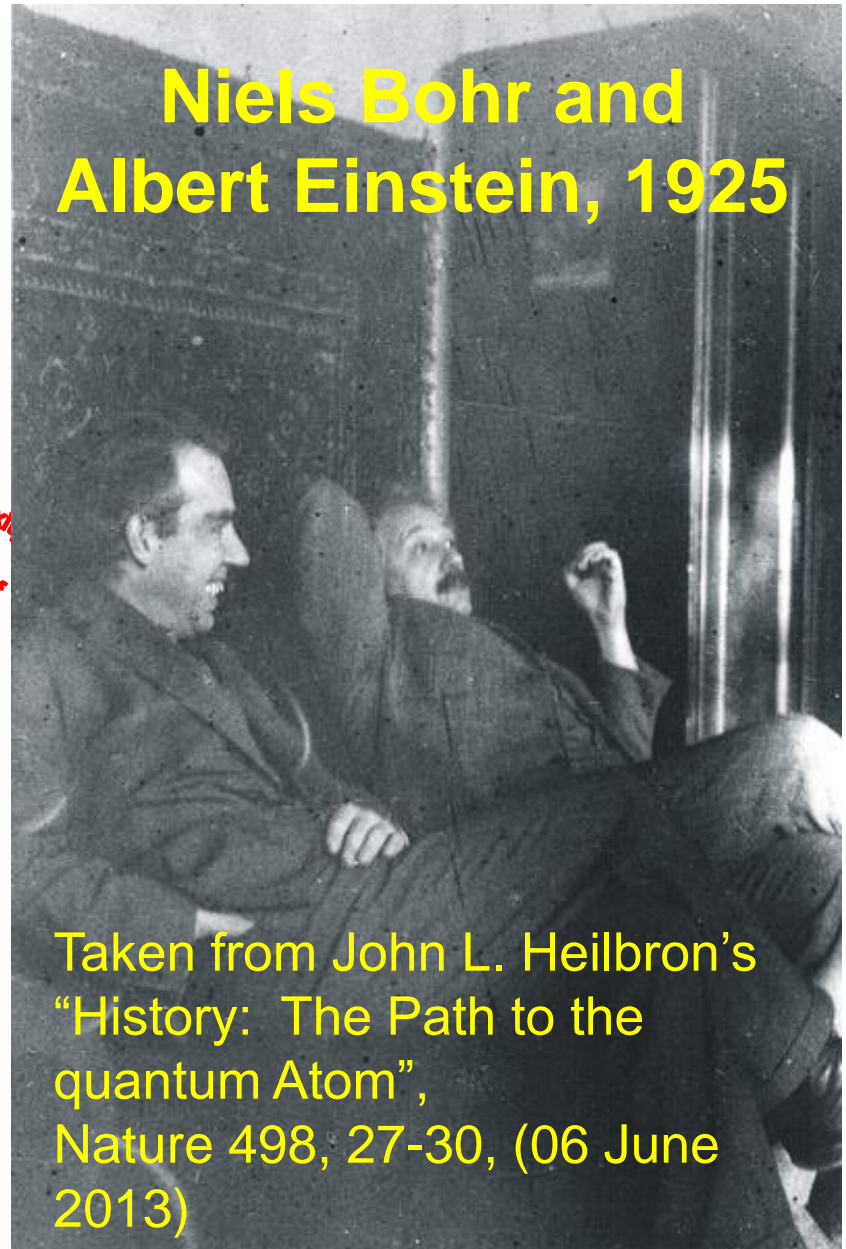
Lecture 2



Emission Spectra

Complexity increases with size of Element

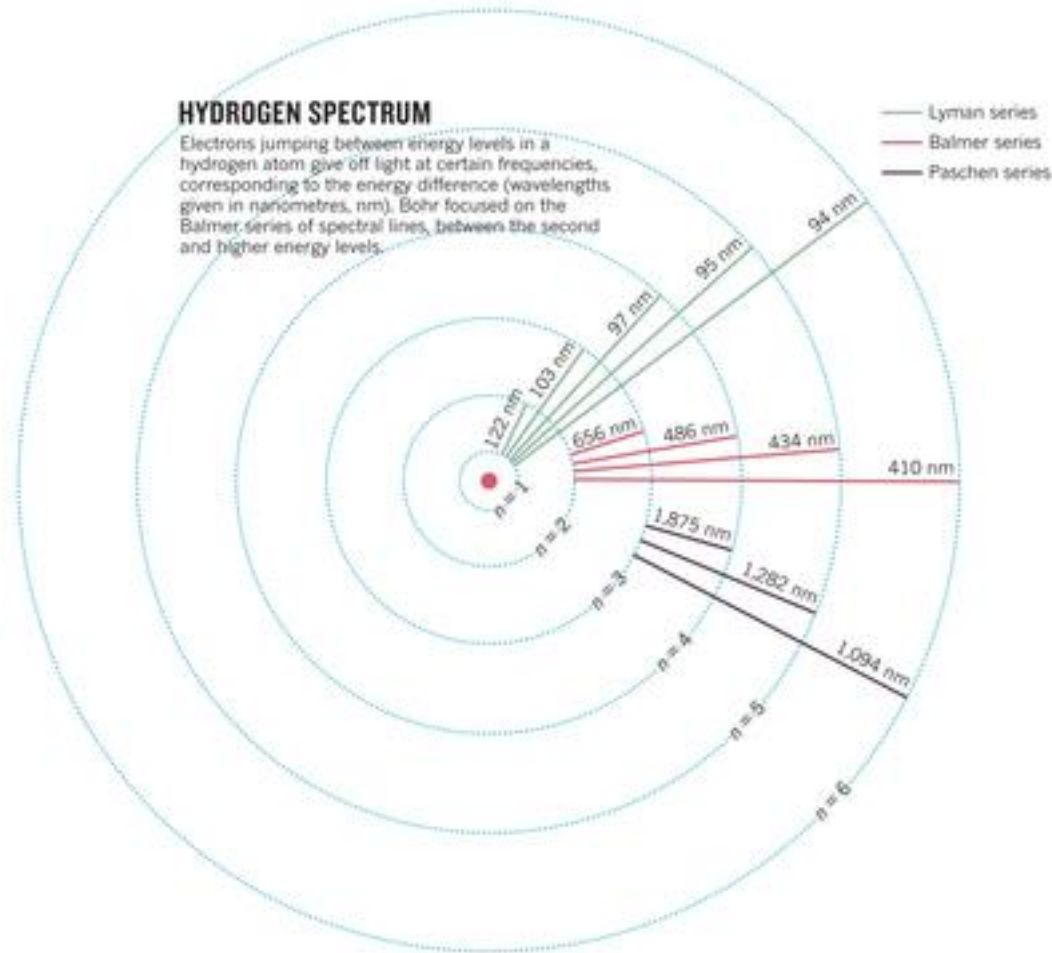
What do these lines mean?????



Niels Bohr and Albert Einstein, 1925

Taken from John L. Heilbron's "History: The Path to the quantum Atom", Nature 498, 27-30, (06 June 2013)

The Bohr Atom: electrons in concentric rings



Taken from John L. Heilbron's "History: The Path to the quantum Atom",
Nature 498, 27-30, (06 June 2013)

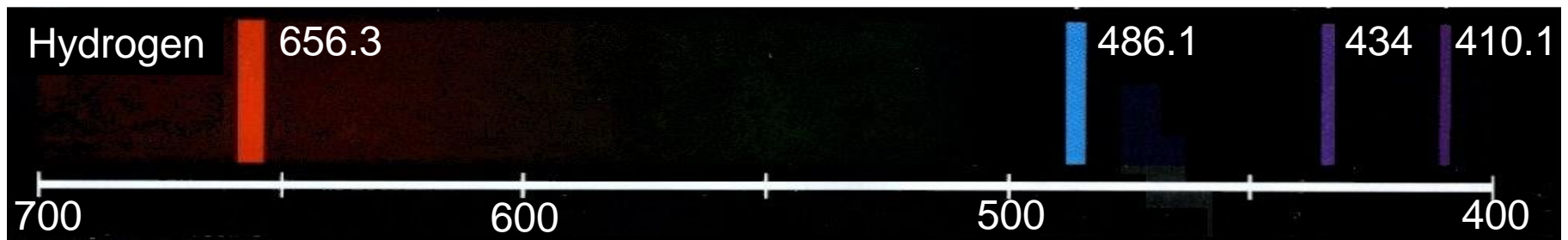
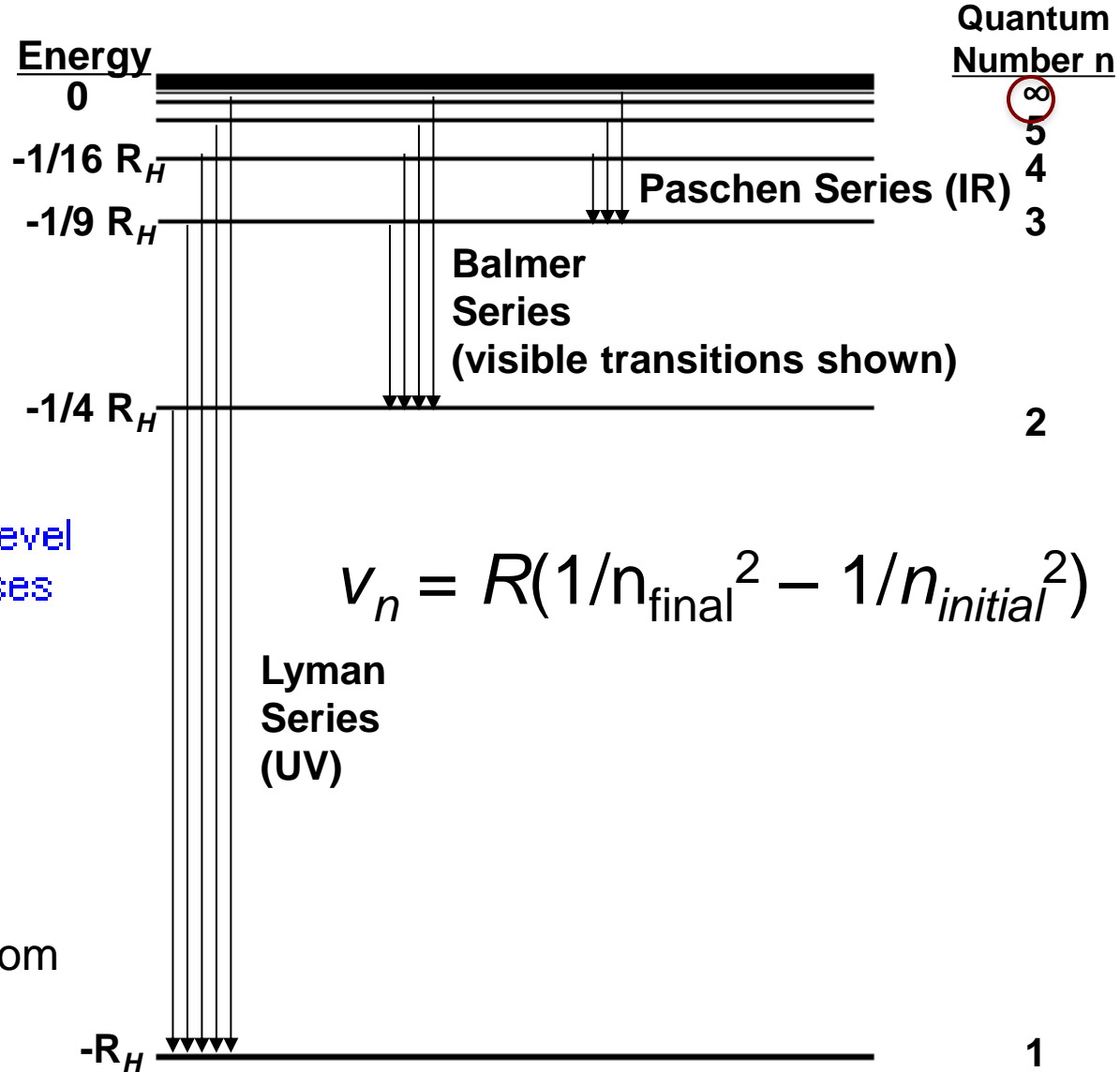
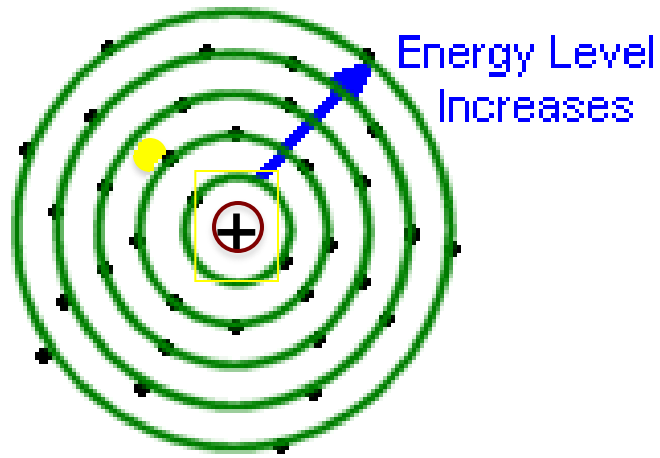
The Balmer formula expresses the frequencies of some lines in the spectrum of hydrogen in simple algebra:

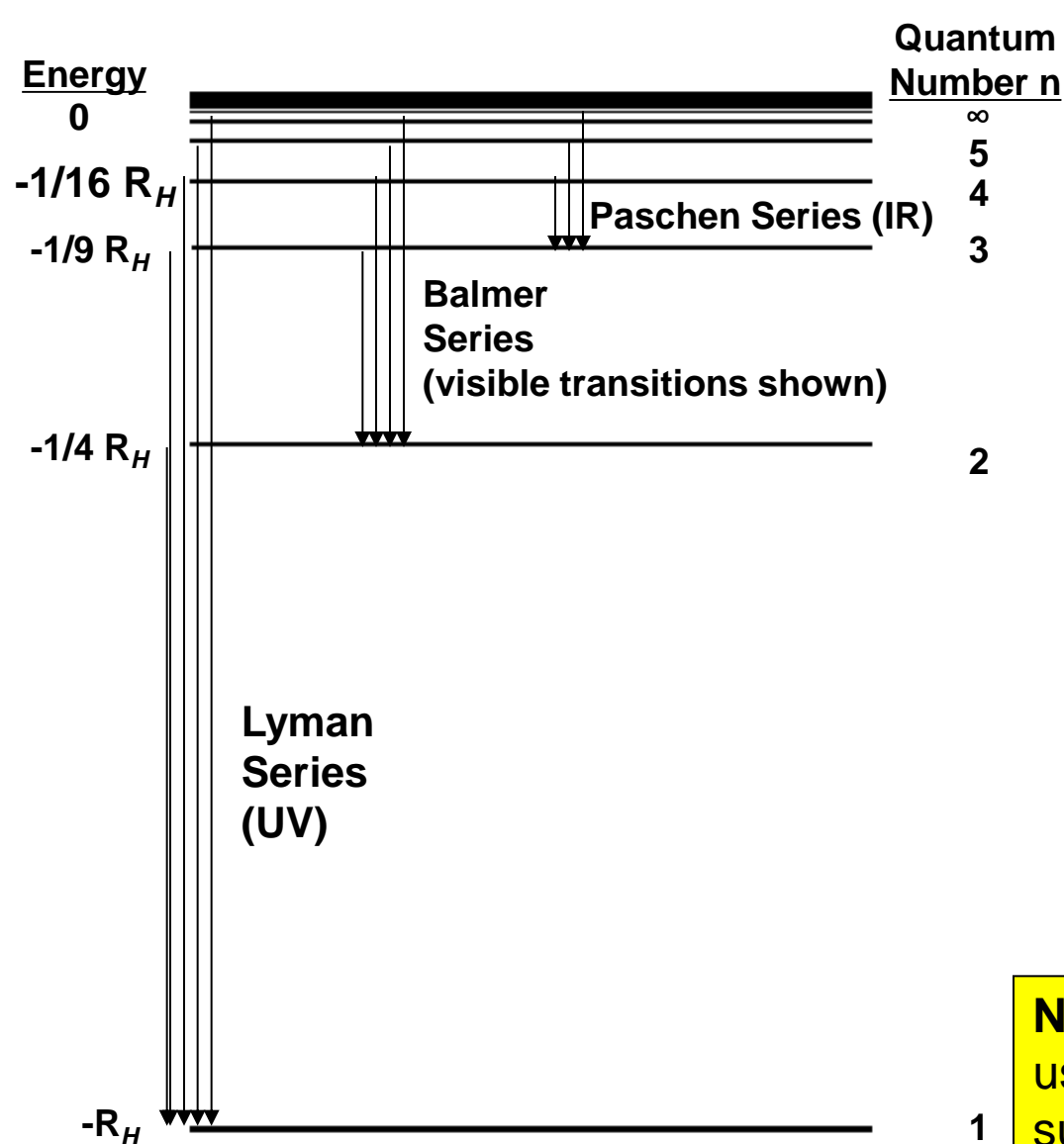
$$\nu_n = R(1/2^2 - 1/n^2)$$

where ν_n is the n th Balmer line and R is the universal Rydberg constant for frequency, named in honour of the Swedish spectroscopist Johannes Rydberg, who generalized Balmer's formula to apply to elements beyond hydrogen.

Each level can accommodate
 $2n^2$ electron:
Periodic Table Rows

The Hydrogen Atom Spectrum and Energy Levels





For Hydrogen:

$$E = \frac{-R_H}{n^2}$$

Rydberg constant for hydrogen, R_H

$$R_H = \frac{m_e e^4}{8 \epsilon_0^2 h^2} = 2.179 \times 10^{-18} \text{ J}$$

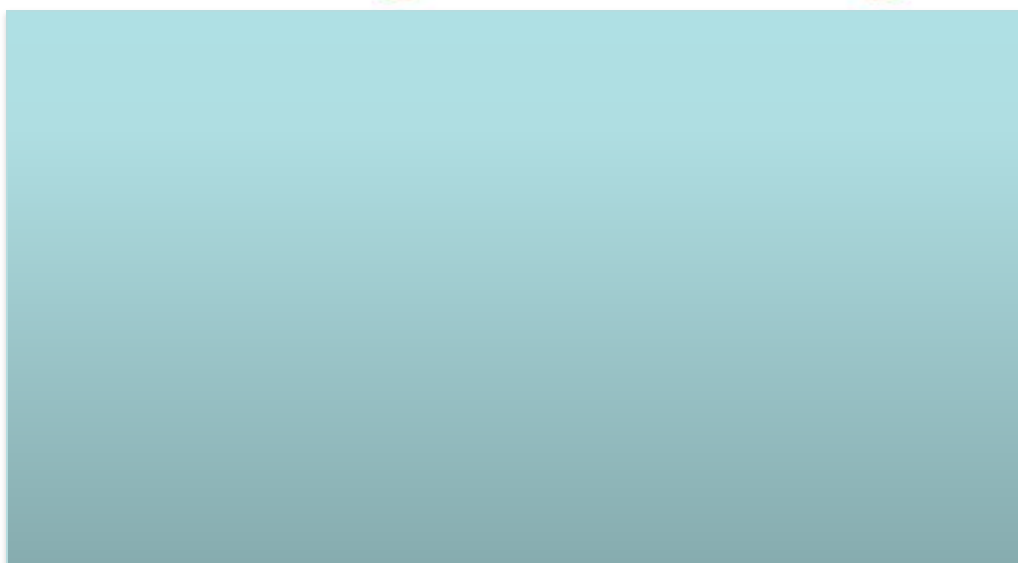
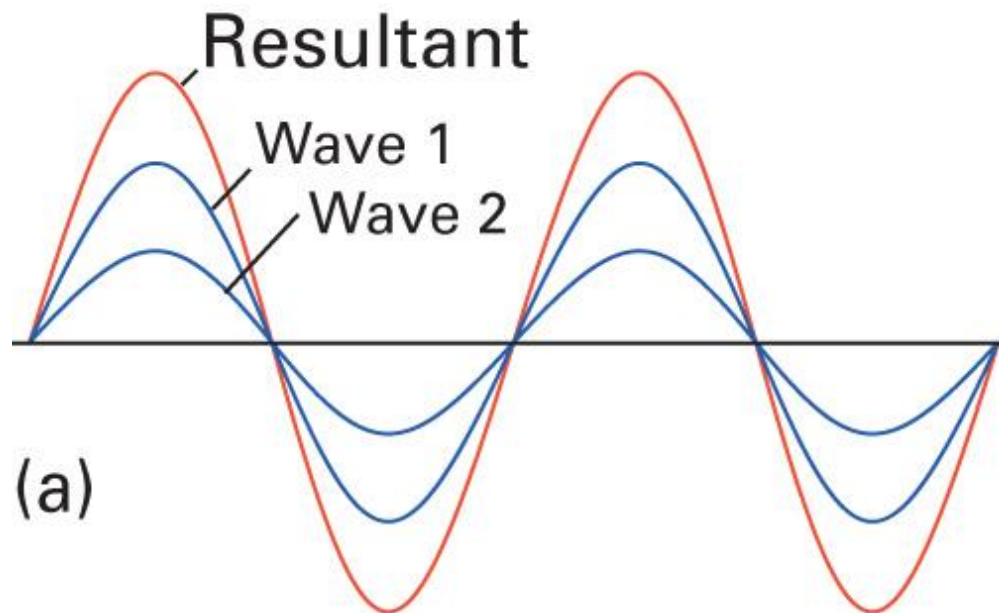
$$= 13.6 \text{ eV}$$

General equation for Rydberg constant for any element

$$R = \frac{-\mu Z^2 e^4}{8 \epsilon_0^2 h^2}$$

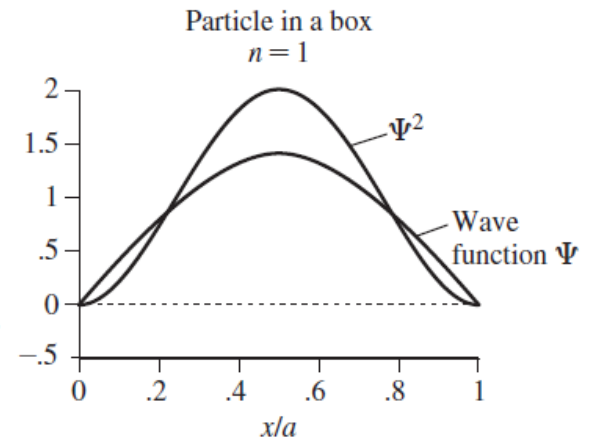
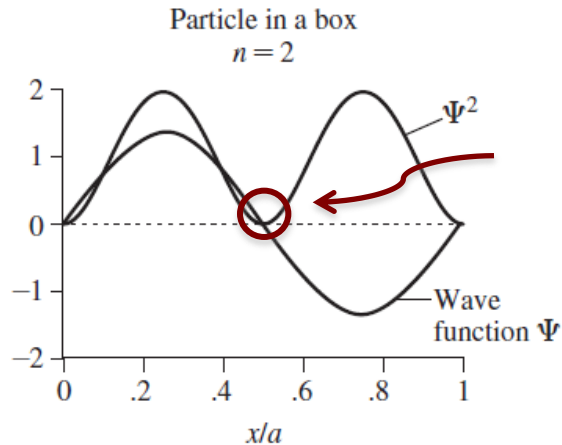
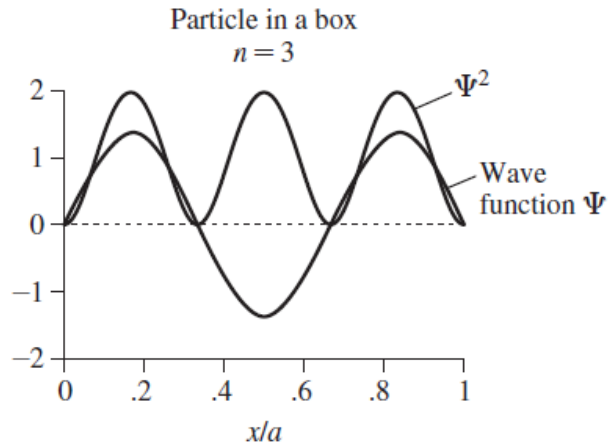
Note: The predicted emission spectra using the Rydberg constant was only successful for simple elements such as H and failed for heavier atoms due to the limitations of the Bohr view of the atom. ***This led to the foundations of quantum mechanics.***

Properties of waves: Addition for reinforcement or cancellation



Properties of waves: Squared = amplitude

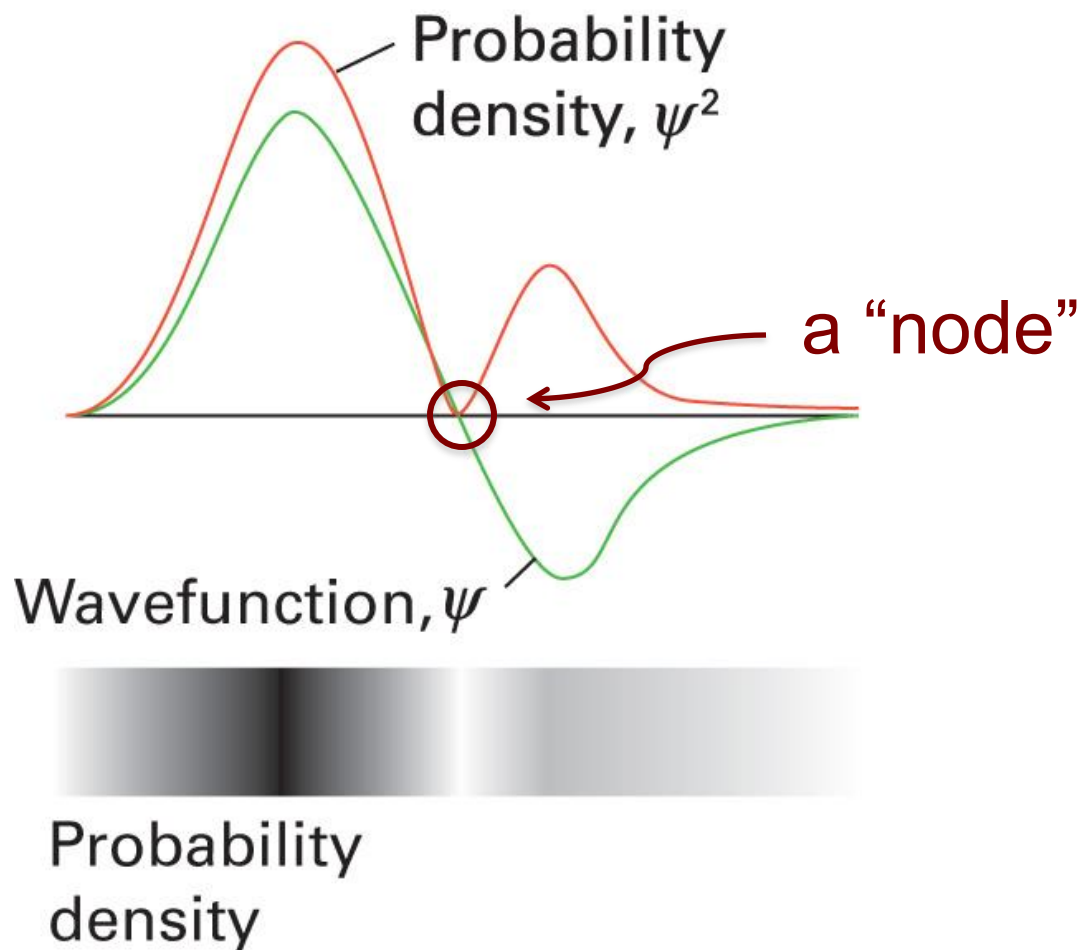
Boundaries => Restrictions on values



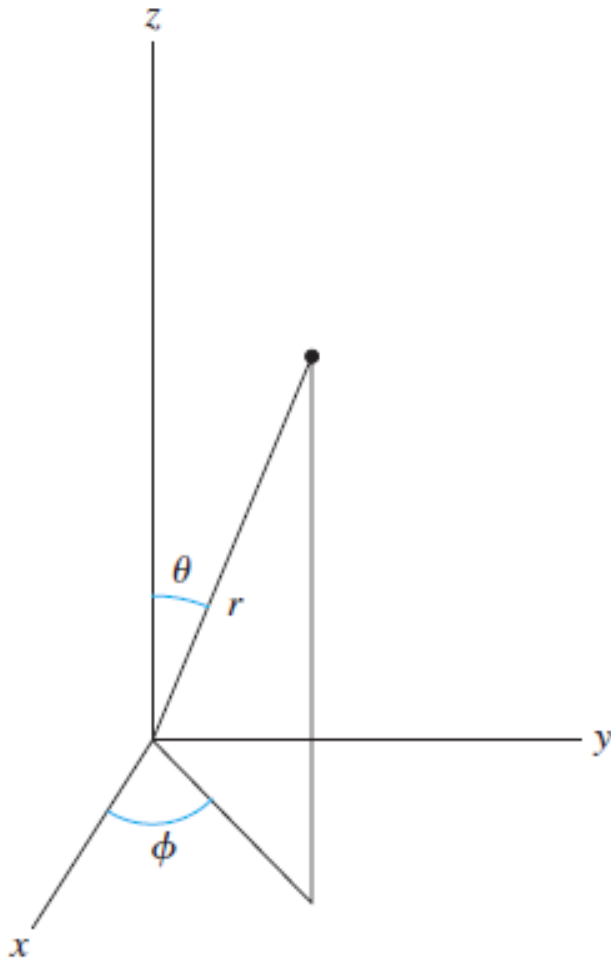
a "node"

Time-independent Schrödinger equation (general—one dimension)

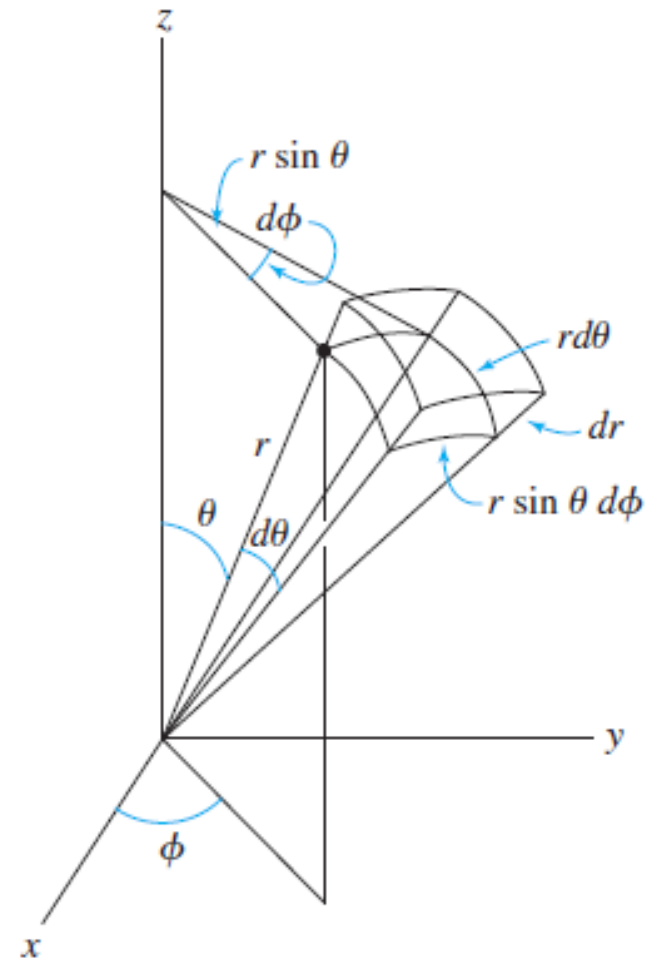
$$\boxed{E} \psi = H \psi$$



Need for Spherical Coordinates and Volume Elements



Spherical coordinates



Volume element

Need both radial and angular functions

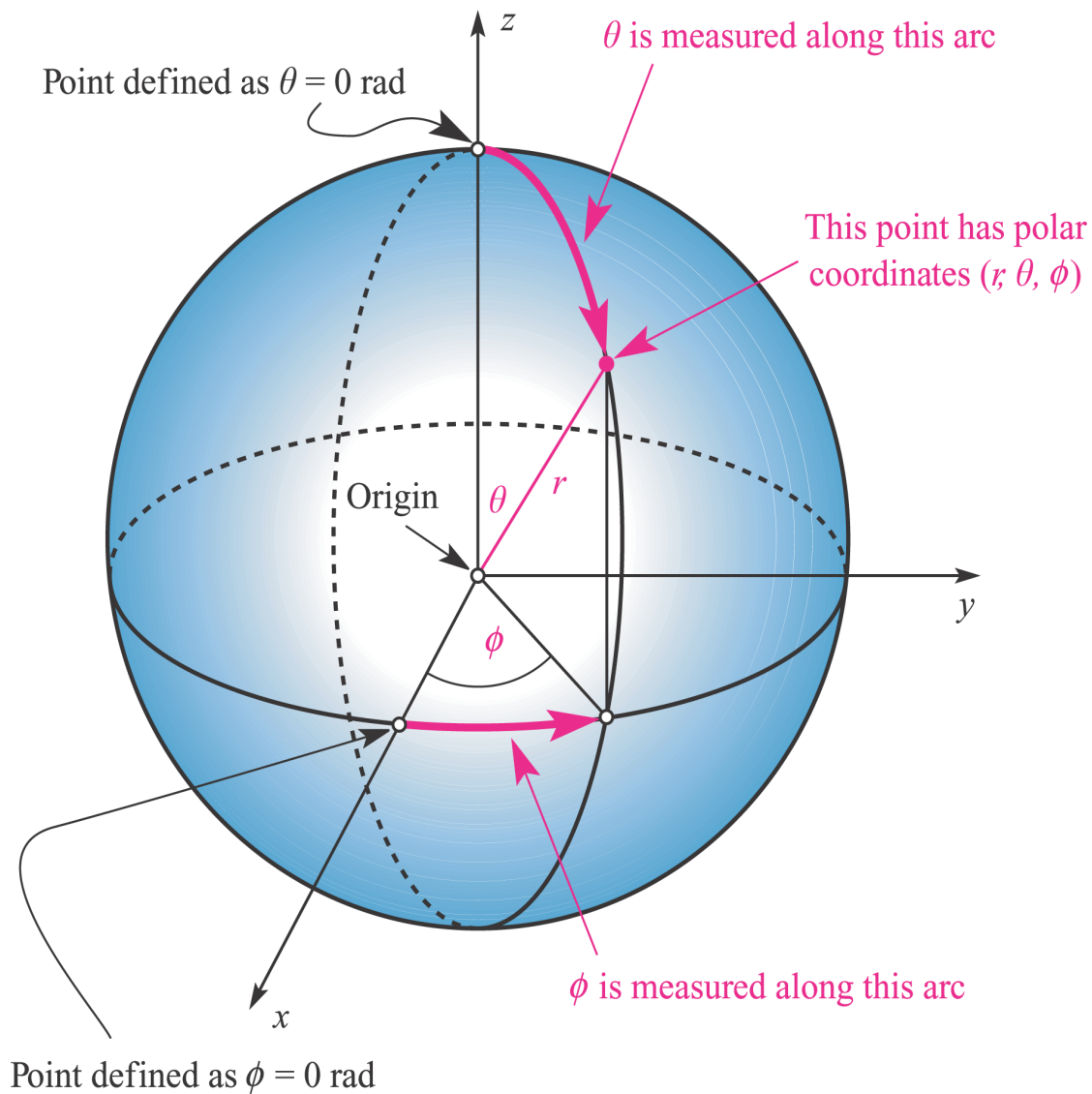


Fig. 1.4 Definition of the polar coordinates (r, θ, ϕ) for a point shown here in pink; r is the radial coordinate and θ and ϕ are angular coordinates. θ and ϕ are measured in radians (rad). Cartesian axes (x , y and z) are also shown.

Summarizing: Solutions Required Quantum Numbers

Quantum Numbers

Atomic orbital	n	l	m_l	Radial part of the wavefunction, $R(r)^\dagger$	Angular part of wavefunction, $A(\theta, \phi)$
$1s$	1	0	0	$2e^{-r}$	$\frac{1}{2\sqrt{\pi}}$
$2s$	2	0	0	$\frac{1}{2\sqrt{2}}(2-r)e^{-r/2}$	$\frac{1}{2\sqrt{\pi}}$
$2p_x$	2	1	+1	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\cos\phi)}{2\sqrt{\pi}}$
$2p_z$	2	1	0	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\cos\theta)}{2\sqrt{\pi}}$
$2p_y$	2	1	-1	$\frac{1}{2\sqrt{6}}re^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\sin\phi)}{2\sqrt{\pi}}$

[†] For the $1s$ atomic orbital, the formula for $R(r)$ is actually $2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}e^{-Zr/a_0}$ but for the hydrogen atom, $Z = 1$ and $a_0 = 1$ atomic unit. Other functions are similarly simplified.

Table 1.2 Solutions of the Schrödinger equation for the hydrogen atom which define the $1s$, $2s$ and $2p$ atomic orbitals. For these forms of the solutions, the distance r from the nucleus is measured in atomic units.

Quantum Numbers

n is the principal quantum number, indicates the size of the orbital, has all positive integer values of 1 to ∞ (infinity)

ℓ is the angular momentum quantum number, represents the shape of the orbital, has integer values of $(n - 1)$ to 0

m_ℓ is the magnetic quantum number, represents the spatial direction of the orbital, can have integer values of $-\ell$ to 0 to ℓ

m_s is the spin quantum number, has little physical meaning, can have values of either $+1/2$ or $-1/2$

Pauli Exclusion principle: no two electrons can have all four of the same quantum numbers in the same atom (Every electron has a unique set.)

Hund's Rule: when electrons are placed in a set of degenerate orbitals, the *ground state* has as many electrons as possible in different orbitals, and with *parallel spin*.

Aufbau (Building Up) Principle: the ground state electron configuration of an atom can be found by putting electrons in orbitals, starting with the lowest energy and moving progressively to higher energy.

ℓ (angular momentum)	orbital
0	s
1	p
2	d
3	f

Other terms: electron configuration, noble gas configuration, valence shell

**While n is the principal energy level,
the l value also has an effect**

**Heavier elements, more chances
For close energy levels**

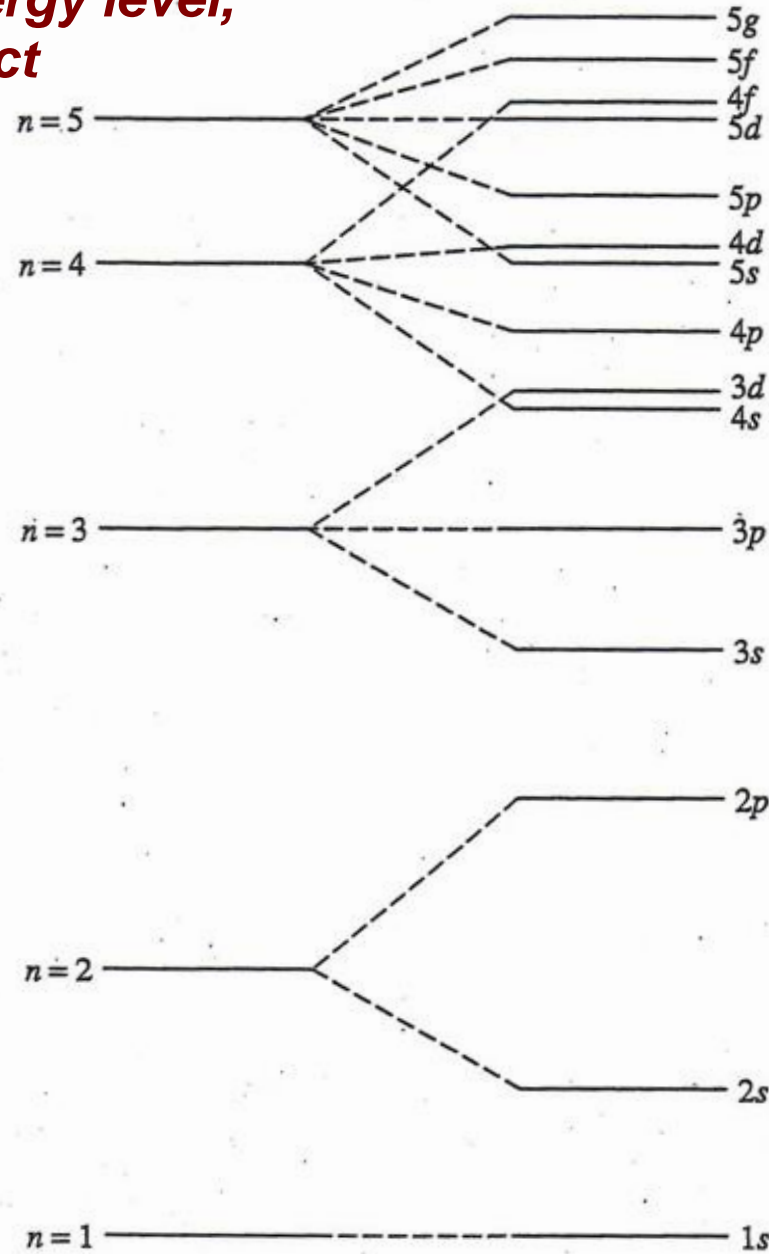
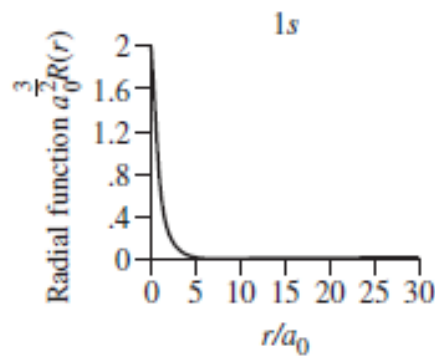
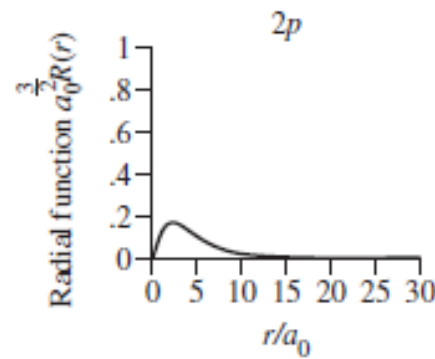
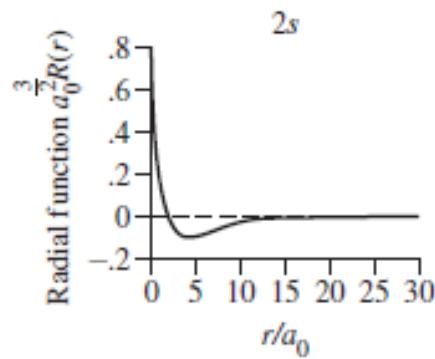
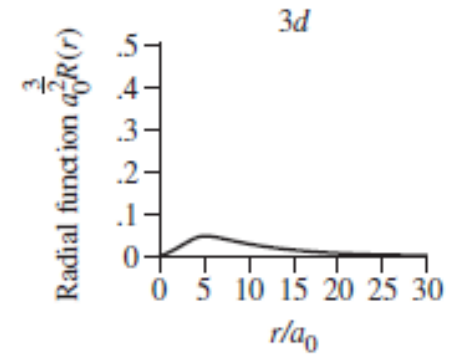
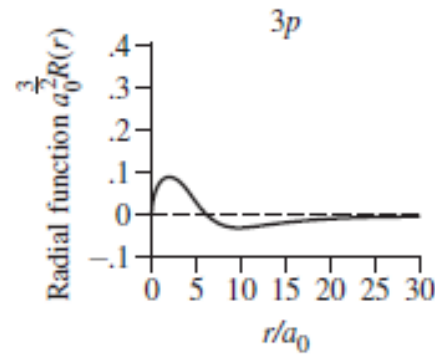
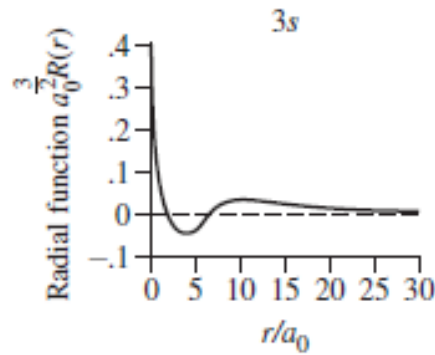


FIGURE 2-10 Energy Level Splitting and Overlap. The differences between the upper levels are exaggerated for easier visualization.

Radial Wave Functions and Nodes

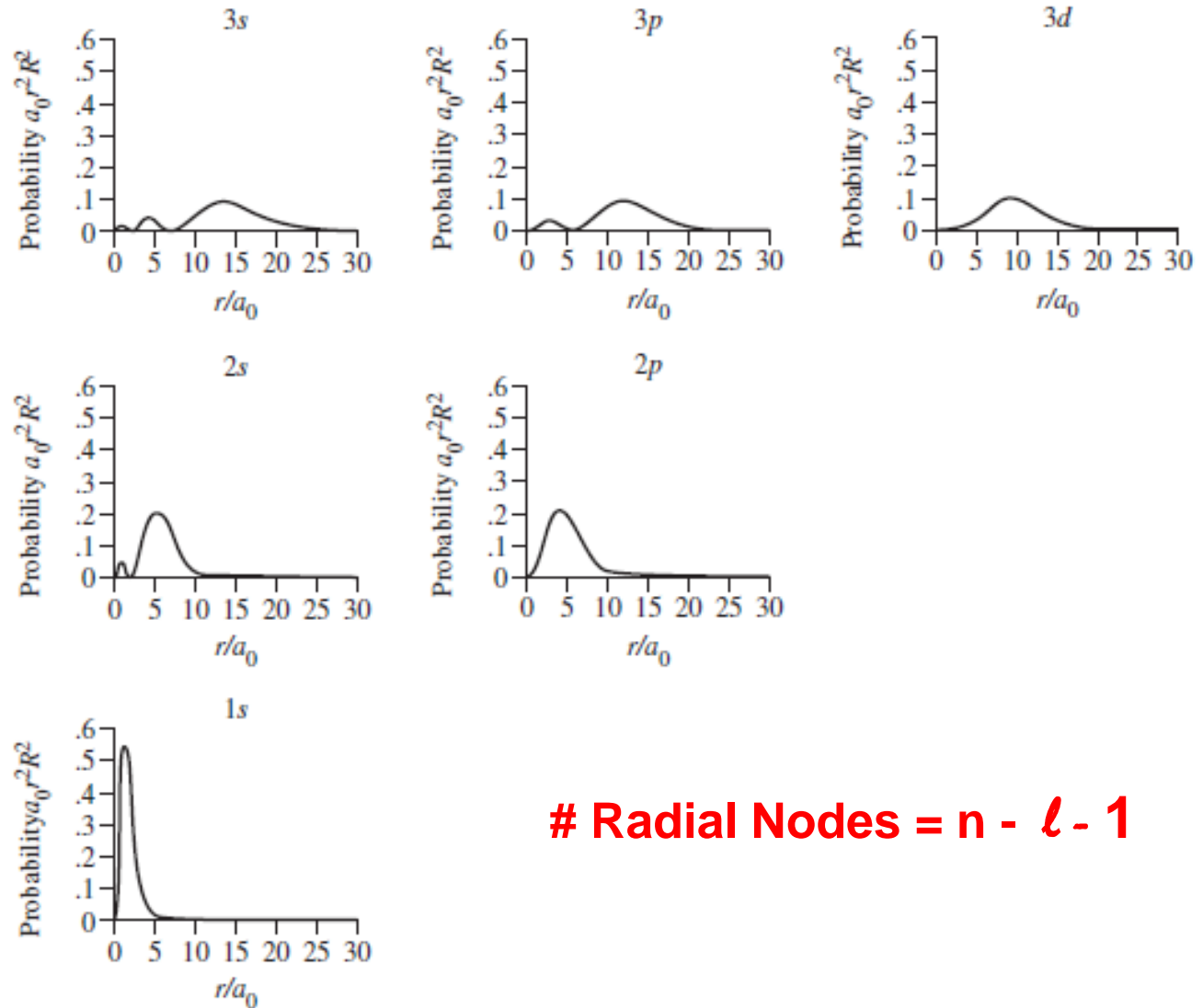
Radial Wave Functions



Radial Nodes = $n - \ell - 1$

Radial Probability Functions and Nodes

Radial Probability Functions



Radial Nodes = $n - \ell - 1$

FIGURE 2.7 Radial Wave Functions and Radial Probability Functions.

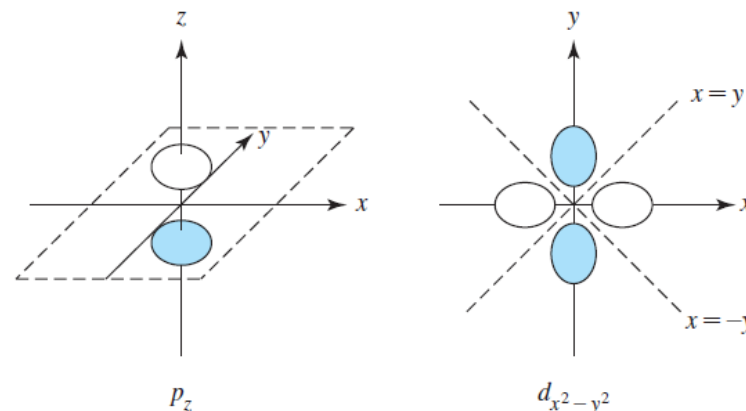
TABLE 2.5 Nodal Surfaces

Angular Nodes [$Y(\theta, \phi) = 0$]	
Examples (number of angular nodes)	
s orbitals	0
p orbitals	1 plane for each orbital
d orbitals	2 planes for each orbital except d_{z^2} 1 conical surface for d_{z^2}

Radial Nodes [$R(r) = 0$]					
Examples (number of radial nodes)					
$1s$	0	$2p$	0	$3d$	0
$2s$	1	$3p$	1	$4d$	1
$3s$	2	$4p$	2	$5d$	2

Radial Nodes = $n - \ell - 1$

Angular Nodes = ℓ



Summary:

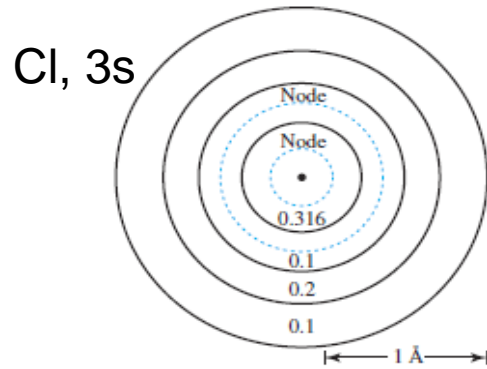
Radial Nodes = $n - \ell - 1$

Angular Nodes = ℓ

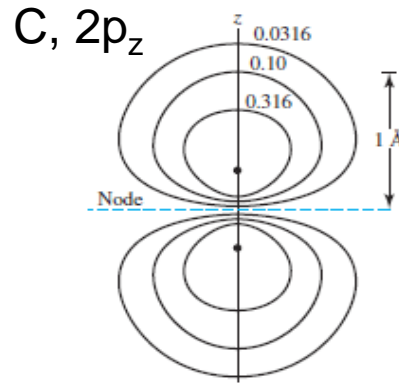
Total # Nodes = $n - 1$

Where are the nodes in orbitals???

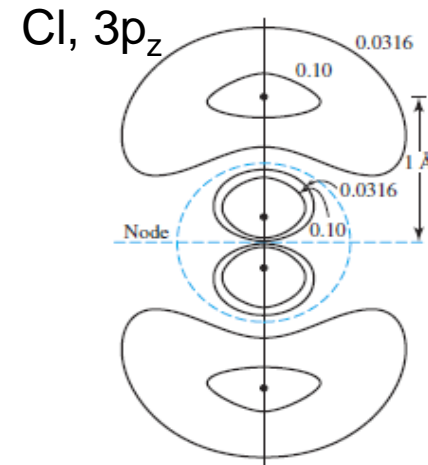
(MFT, Figure 2.8 shows both radial and angular)



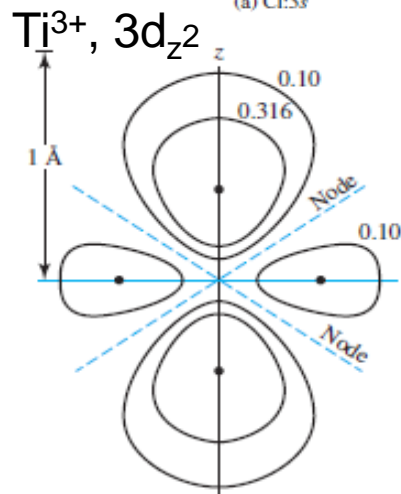
(a) Cl:3s



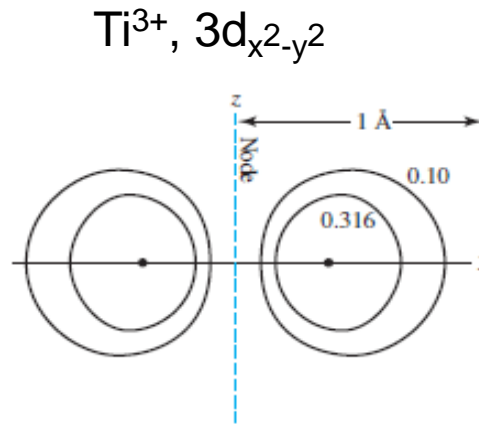
(b) C:2p



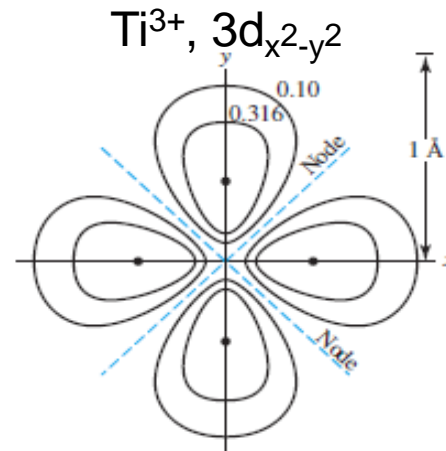
(c) Cl:3p



(d) Ti³⁺:3d_{z²}



(e) Ti³⁺:3d_{x²-y²}

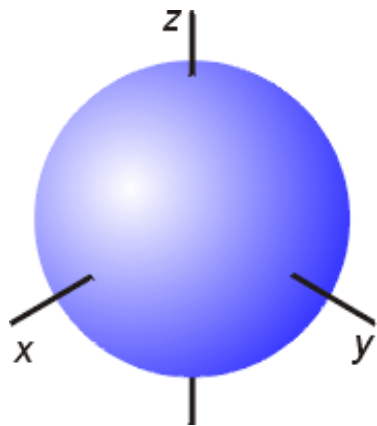
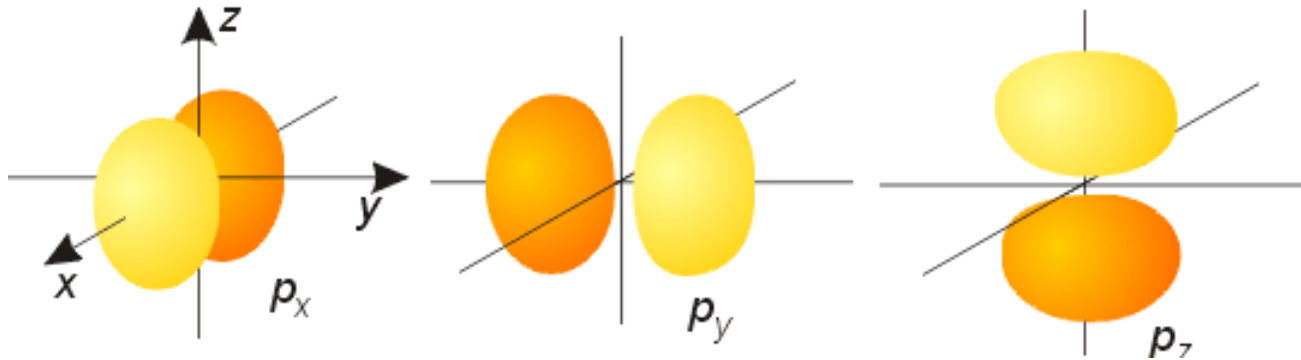


(f) Ti³⁺:3d_{x²-y²}

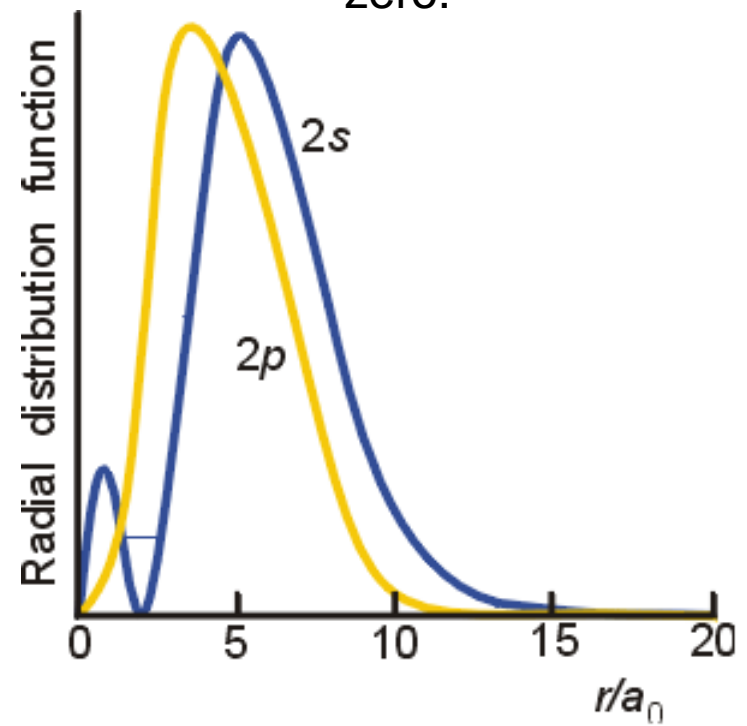
Orbitals and Shapes/Electron Distribution

Each p-orbital has two lobes with positive and negative values (**phases**) of the wavefunction either side of the nucleus separated by a **nodal plane** where the wavefunction is zero.

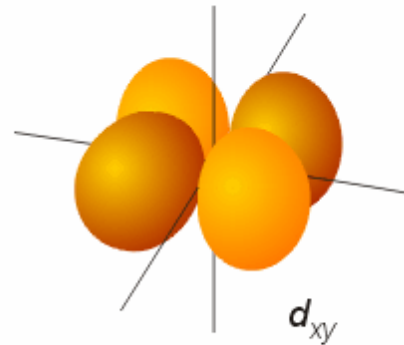
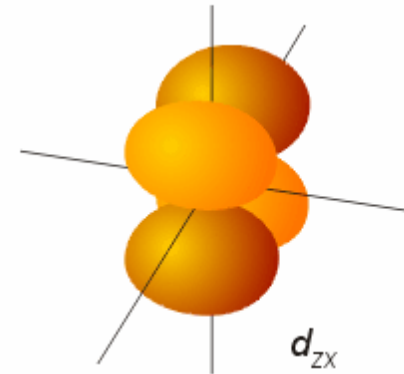
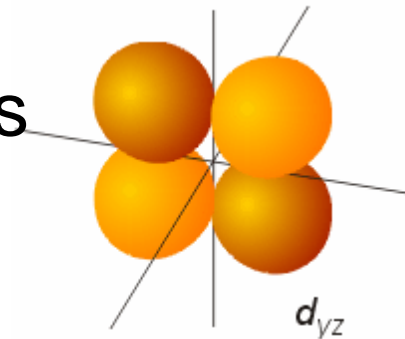
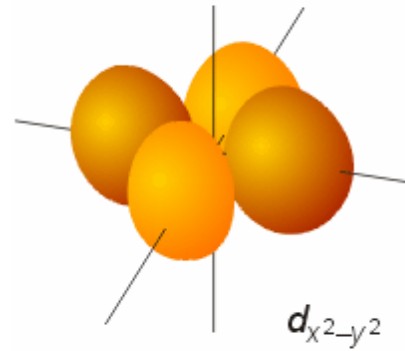
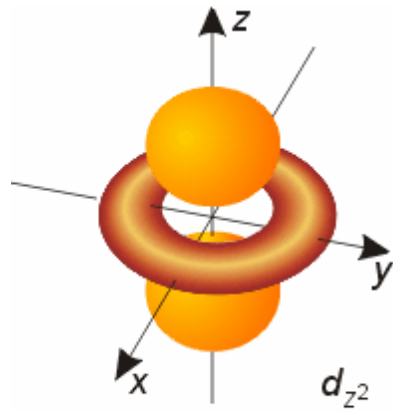
The p-orbitals



The s-orbital

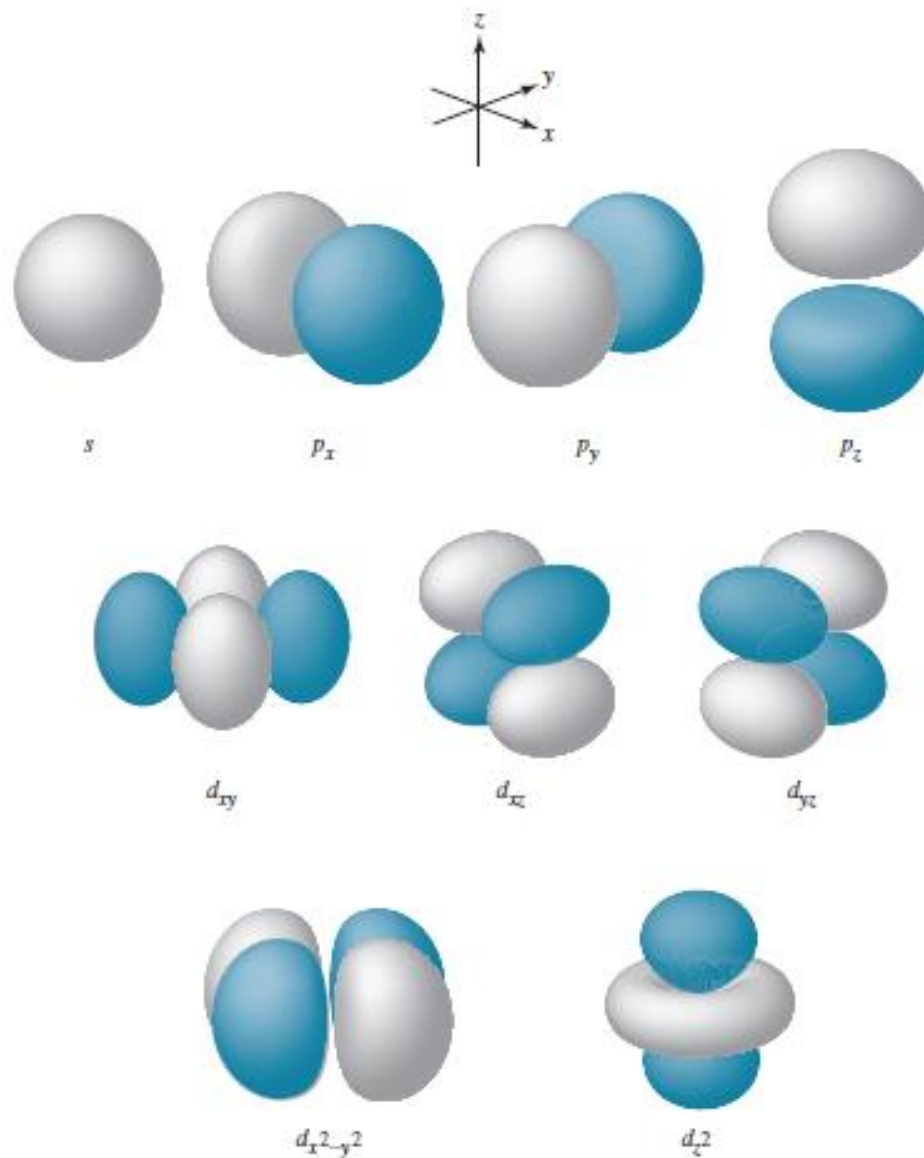


The d-orbitals



Two angular nodes

As pictured in MFT, Figure 2.6



Quantum Numbers

n is the principal quantum number, indicates the size of the orbital, has all positive integer values of 1 to ∞ (infinity)

l is the angular momentum quantum number, represents the shape of the orbital, has integer values of $n-1$ to 0

m_l is the magnetic quantum number, represents the spatial direction of the orbital, can have integer values of $-l$ to 0 to l

m_s is the spin quantum number, has little physical meaning, can have values of either $+1/2$ or $-1/2$

Pauli Exclusion principle: no two electrons can have all four of the same quantum numbers in the same atom

Hund's Rule: when electrons are placed in a set of degenerate orbitals, the *ground state* has as many electrons as possible in different orbitals, and with *parallel spin*.

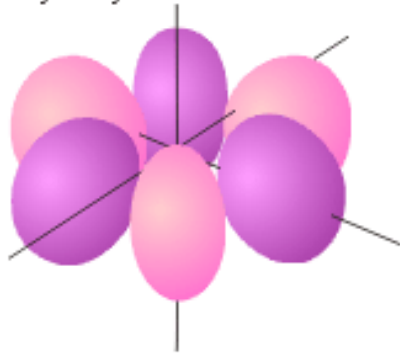
Aufbau (Building Up) Principle: the ground state electron configuration of an atom can be found by putting electrons in orbitals, starting with the lowest energy and moving progressively to higher energy.

l (angular momentum)	orbital
0	s
1	p
2	d
3	f

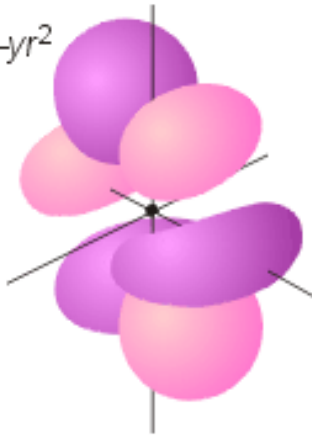
Other terms: electron configuration, noble gas configuration, valence shell

The f-orbitals

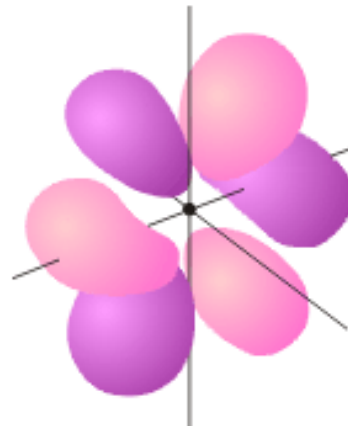
$$4f_{y^3-3yx^2}$$



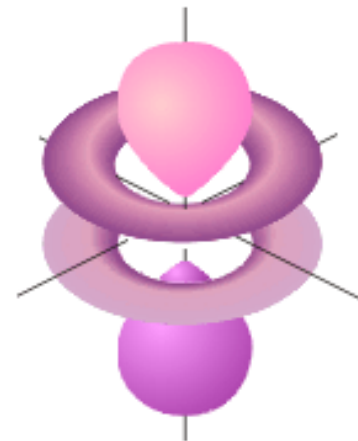
$$4f_{5yz^2-yr^2}$$



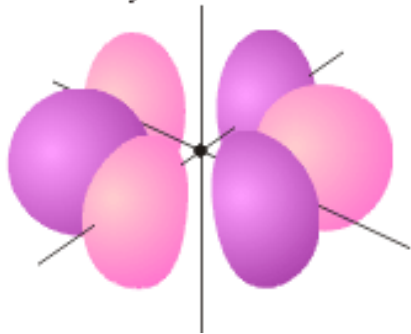
$$4f_{5xz^2-3xr^2}$$



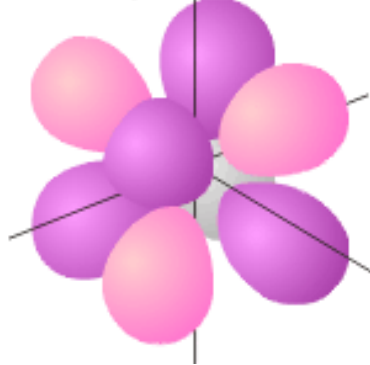
$$4f_{5z^3-3zr^2}$$



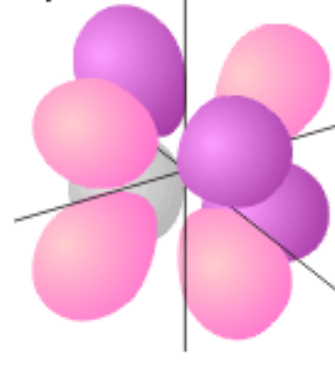
$$4f_{x^3-3xy^2}$$



$$4f_{zx^2-zy^2}$$



$$4f_{xyz}$$



Quantum Numbers

n is the principal quantum number, indicates the size of the orbital, has all positive integer values of 1 to ∞ (infinity)

l is the angular momentum quantum number, represents the shape of the orbital, has integer values of $n-1$ to 0

m_l is the magnetic quantum number, represents the spatial direction of the orbital, can have integer values of $-l$ to 0 to l

m_s is the spin quantum number, has little physical meaning, can have values of either $+1/2$ or $-1/2$

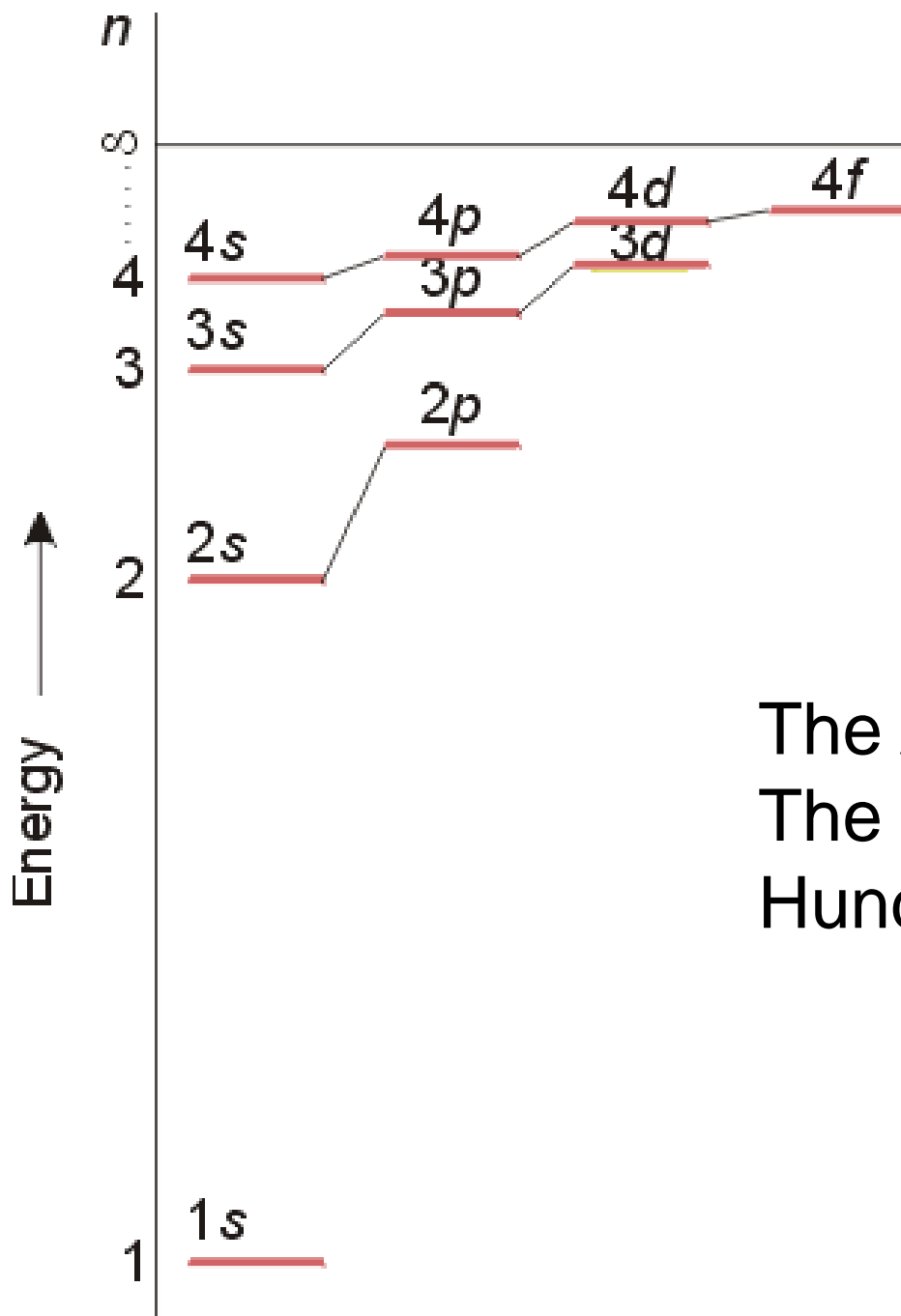
Pauli Exclusion principle: no two electrons can have all four of the same quantum numbers in the same atom

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Aufbau (Building Up) Principle: the ground state electron configuration of an atom can be found by putting electrons in orbitals, starting with the lowest energy and moving progressively to higher energy.

l (angular momentum)	orbital
0	s
1	p
2	d
3	f

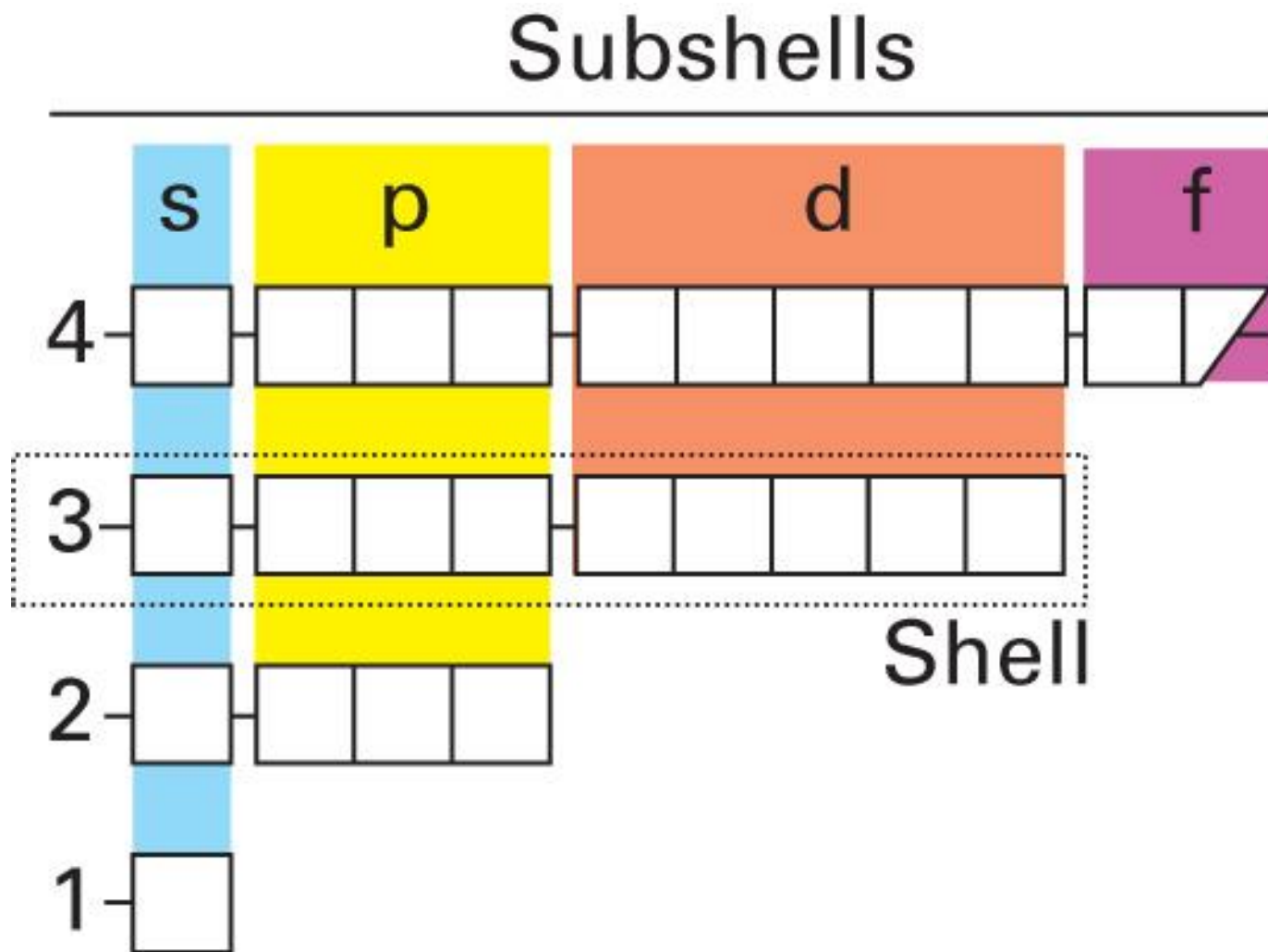
Other terms: electron configuration, noble gas configuration, valence shell



Energy Levels for Electron Configurations

The Aufbau Principle
 The Pauli Exclusion Principle
 Hund's Rules

Box Diagrams



While n is the principal energy level, the ℓ value also has an effect

Heavier elements, more chances
For close energy levels

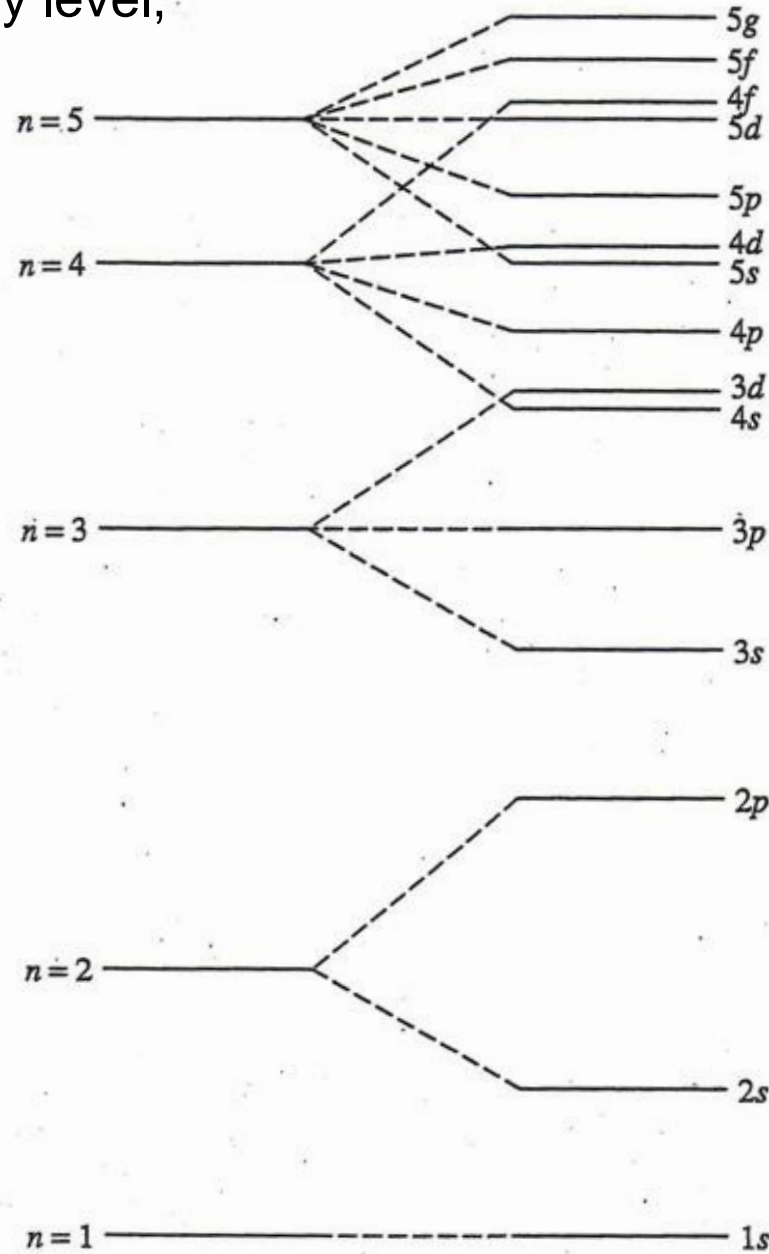
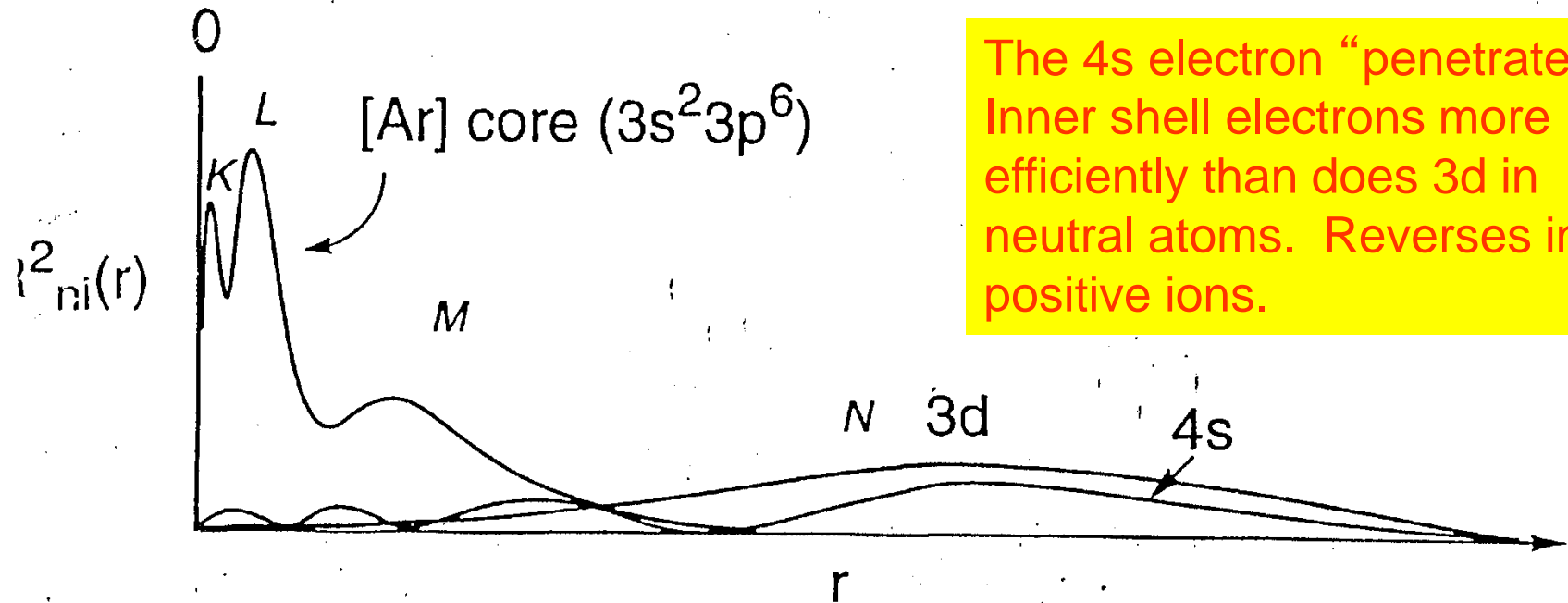


FIGURE 2-10 Energy Level Splitting and Overlap. The differences between the upper levels are exaggerated for easier visualization.

Screening:

Interpenetration of 4s and 3d orbitals at K:

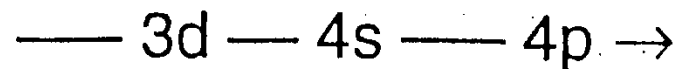


The 4s electron “penetrates”
Inner shell electrons more
efficiently than does 3d in
neutral atoms. Reverses in
positive ions.

order of orbital filling, $Z = 19-36$, for neutral atoms:



for positive ions, the order of 4s and 3d is reversed:



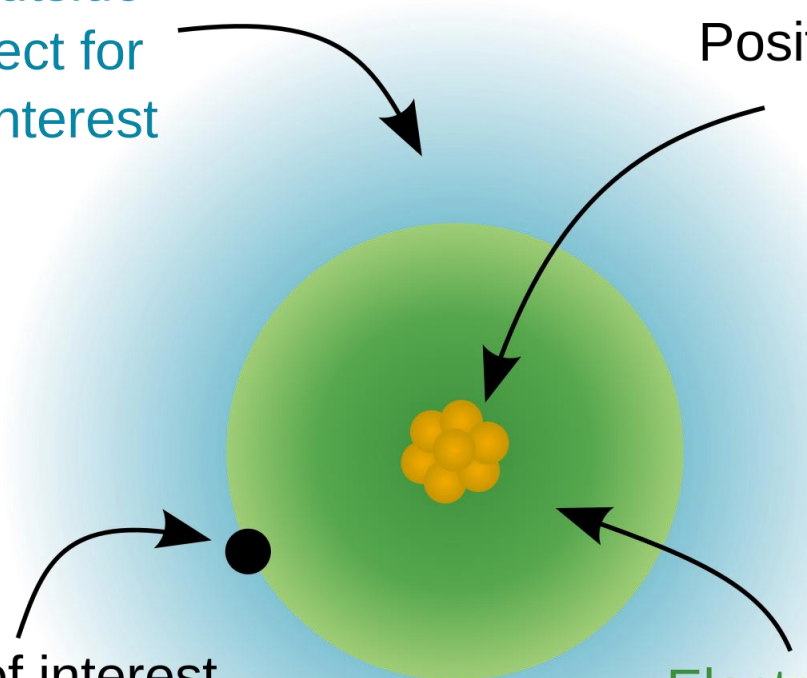
How to handle atoms larger than H? Effective Nuclear Charge or Z_{eff}

Electrons outside
have no effect for
electron of interest

Positively charged
nucleus

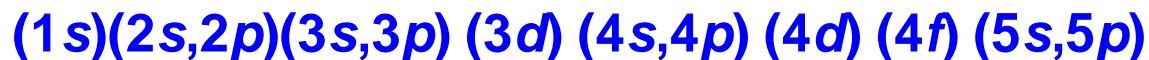
Electron of interest

Electrons in between
cancel some of
the nuclear charge



Slater's Rules for Calculating Z_{eff}

1) Write the electron configuration for the atom as follows:



2) Any electrons to the right of the electron of interest contributes no shielding. (Approximately correct statement.)

3) All other electrons in the same group as the electron of interest shield to an extent of 0.35 nuclear charge units

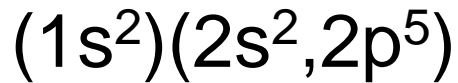
4) If the electron of interest is an *s* or *p* electron: All electrons with one less value of the principal quantum number shield to an extent of 0.85 units of nuclear charge. All electrons with two less values of the principal quantum number shield to an extent of 1.00 units.

5) If the electron of interest is an *d* or *f* electron: All electrons to the left shield to an extent of 1.00 units of nuclear charge.

6) Sum the shielding amounts from steps 2 - 5 and subtract from the nuclear charge value to obtain the effective nuclear charge.

Slater's Rules: Examples

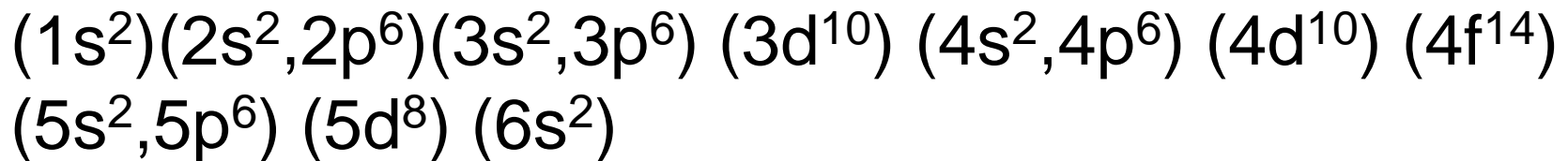
Calculate Z_{eff} for a valence electron in fluorine.



Rule 2 does not apply; therefore, for a valence electron the shielding or screening is $(0.35 \cdot 6) + (0.85 \cdot 2) = 3.8$

$$Z_{\text{eff}} = 9 - 3.8 = 5.2$$

Calculate Z_{eff} for a 6s electron in Platinum.



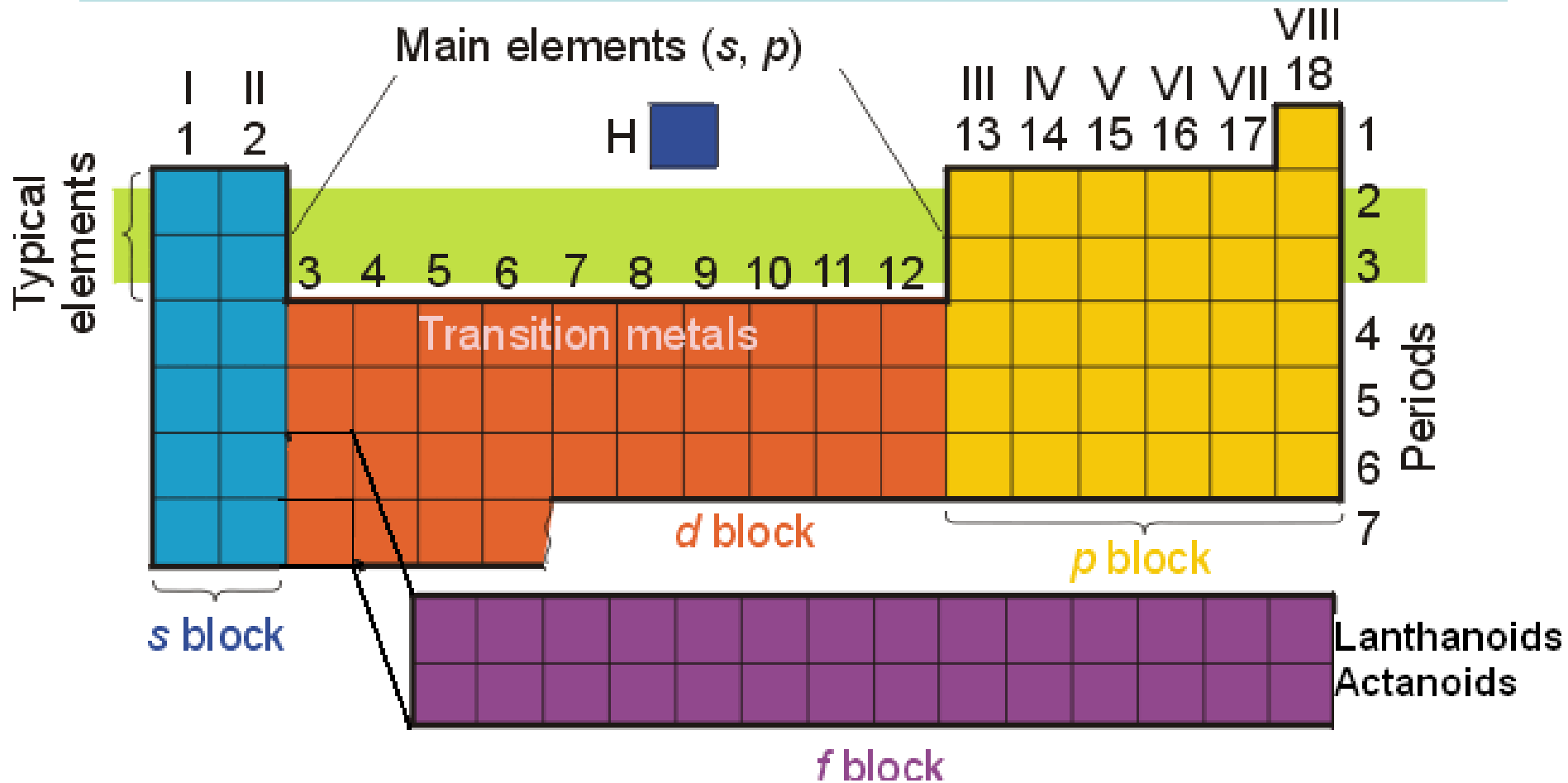
Rule 2 does not apply, and the shielding is:

$$(0.35 \cdot 1) + (0.85 \cdot 16) + (60 \cdot 1.00) = 73.95$$

Table 1.2 Effective nuclear charge, 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	

The Periodic Table



Special Names

- Group 1: Alkali Metals
- Group 2: Alkaline-earth metals
- Group 16: Chalcogens
- Group 17: Halogens
- Group 18: Noble gases

<http://www.youtube.com/watch?v=SmwlzwGMMwc>

Electron Configurations and Screening

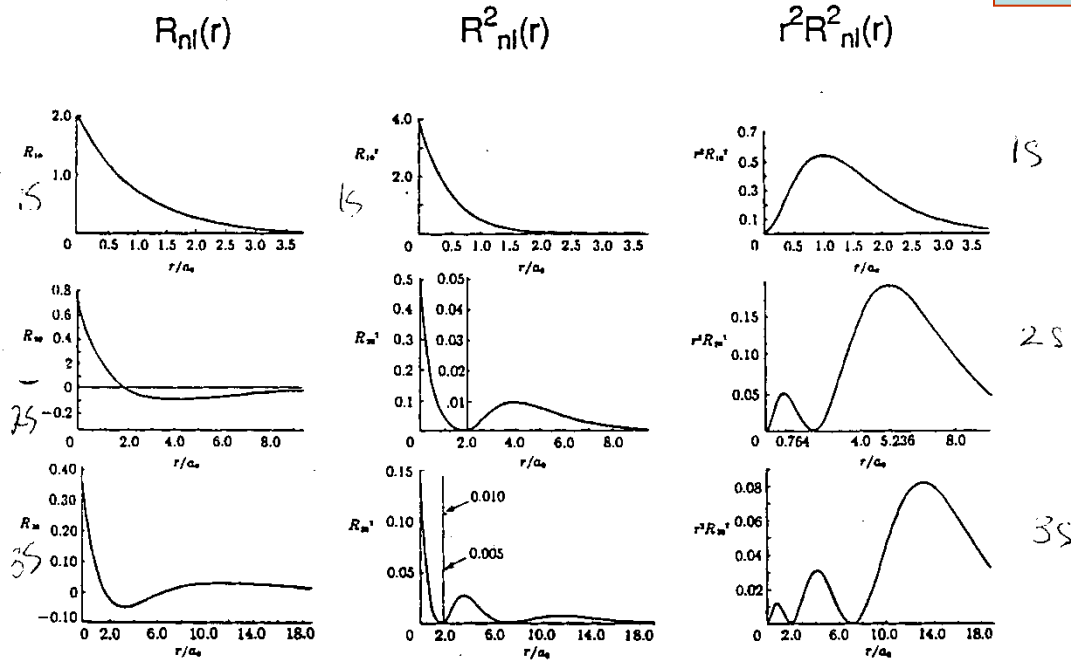
H → Ar energy order:

1s < 2s < 2p < 3s < 3p

I'd like to make two points:



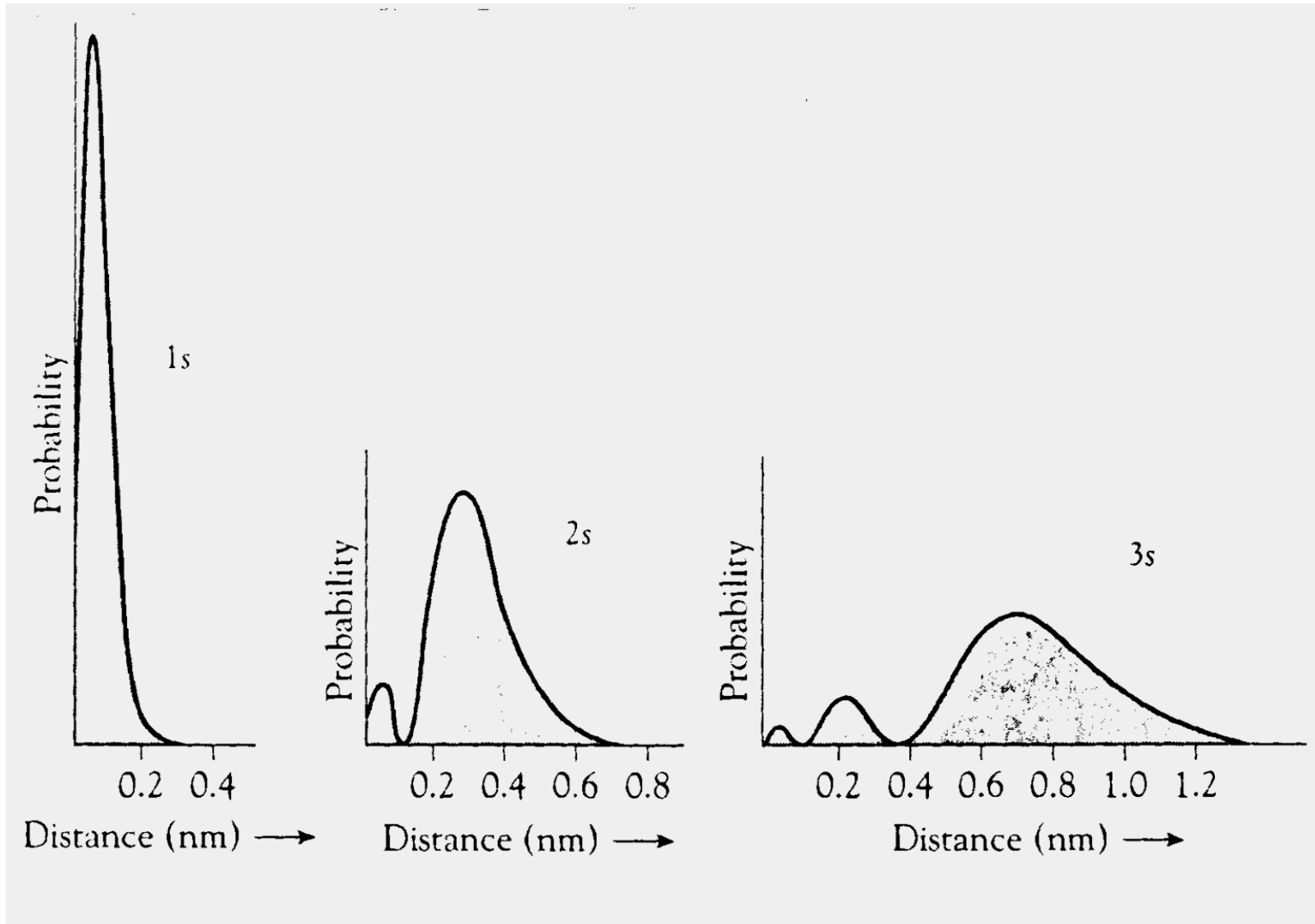
Radial Wave Functions (hydrogenic)



$R_{nl}^2(r)$: radial probability function

- s orbitals ($l = 0$) have non-zero probability at nucleus
- node: distance at which, or surface on which, the electron described by that orbital is not found

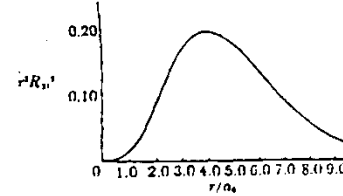
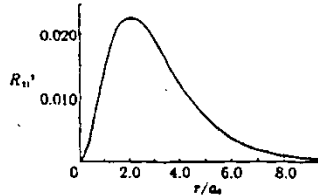
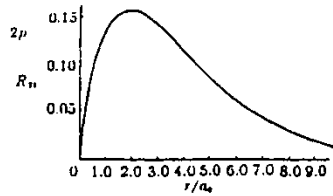
Figure 1.7 The variation of the radial density distribution function with distance from the nucleus for electrons in the 1s, 2s, and 3s orbitals of a hydrogen atom.





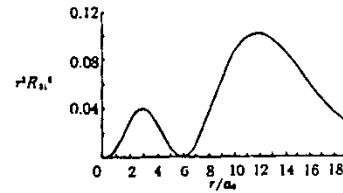
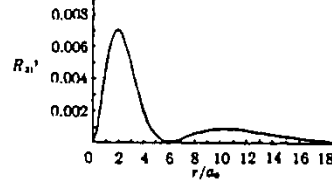
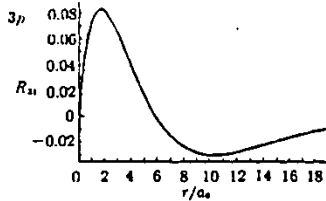
Radial Wave Functions (hydrogenic)

2p



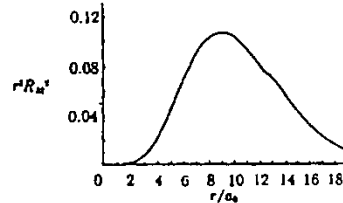
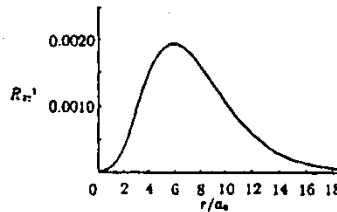
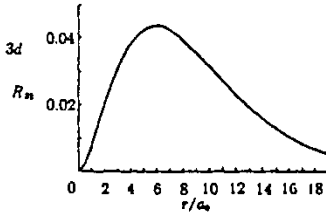
2p

3p



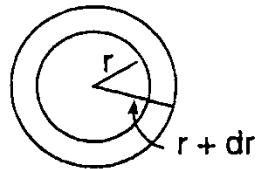
3p

3d



3d

sphere of radius r



$$V = \frac{4}{3} \pi r^3$$

$$dV = \underbrace{4\pi r^2}_{\text{surface area}} dr$$

$$R_{nl}^2(r) dV = 4\pi r^2 R_{nl}^2(r) dr = \underline{\underline{S(r)}}$$

S(r): surface density function

- gives the probability of finding e^-_{nl} in a spherical shell of thickness dr at a distance r from the nucleus

<http://www.youtube.com/watch?v=IhTSfOZUNLo>

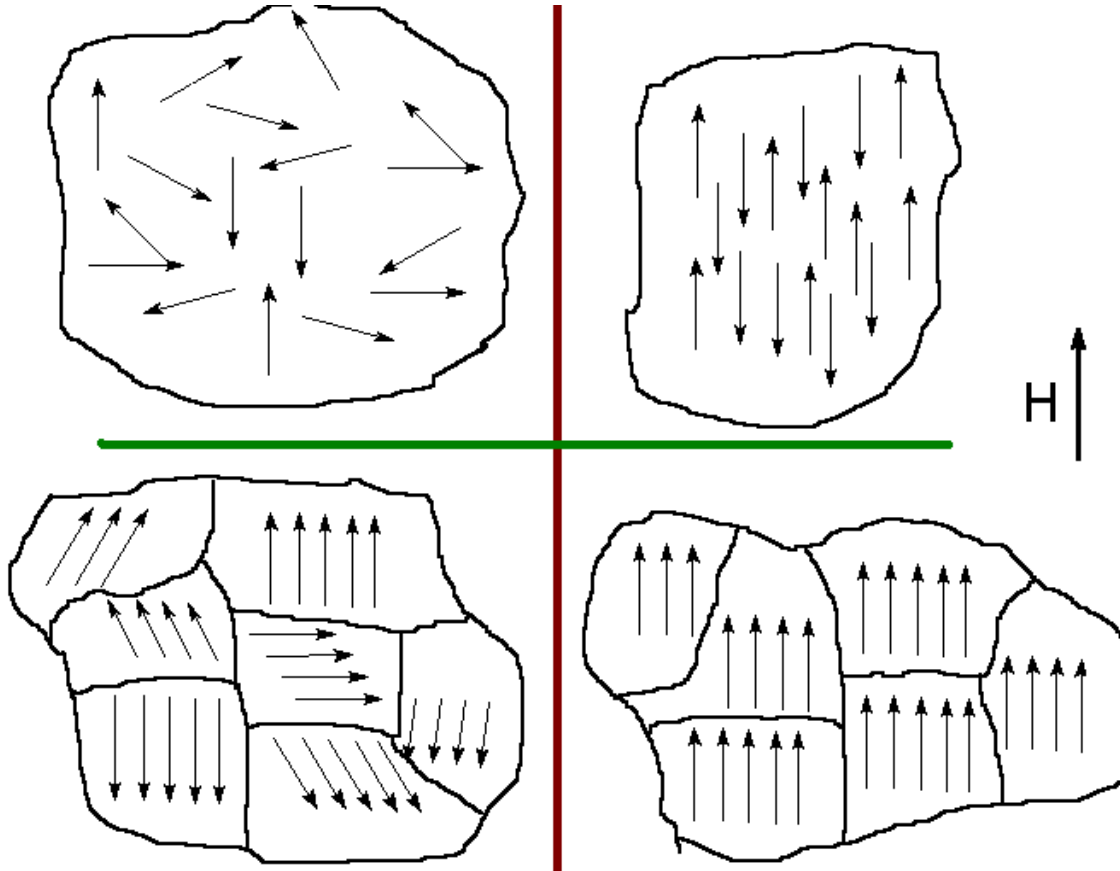
Three types of Magnetic Behavior

Paramagnetism: atoms, molecules, and solids with unpaired electrons are attracted in a magnetic field

Diamagnetic: substances with no unpaired electrons which are weakly repelled in a magnetic field

Ferro-magnetism: the unpaired electrons are aligned with their neighbors even in the absence of a magnetic field

Magnetic domains: the groups of mutually aligned spins in a ferromagnetic substance



Ferro-magnet
In the absence
of a magnetic
field

Ferro-magnet
In the
presence of a
magnetic field

Figure 1.4 The possible sets of quantum numbers for $n = 1$ and $n = 2$.

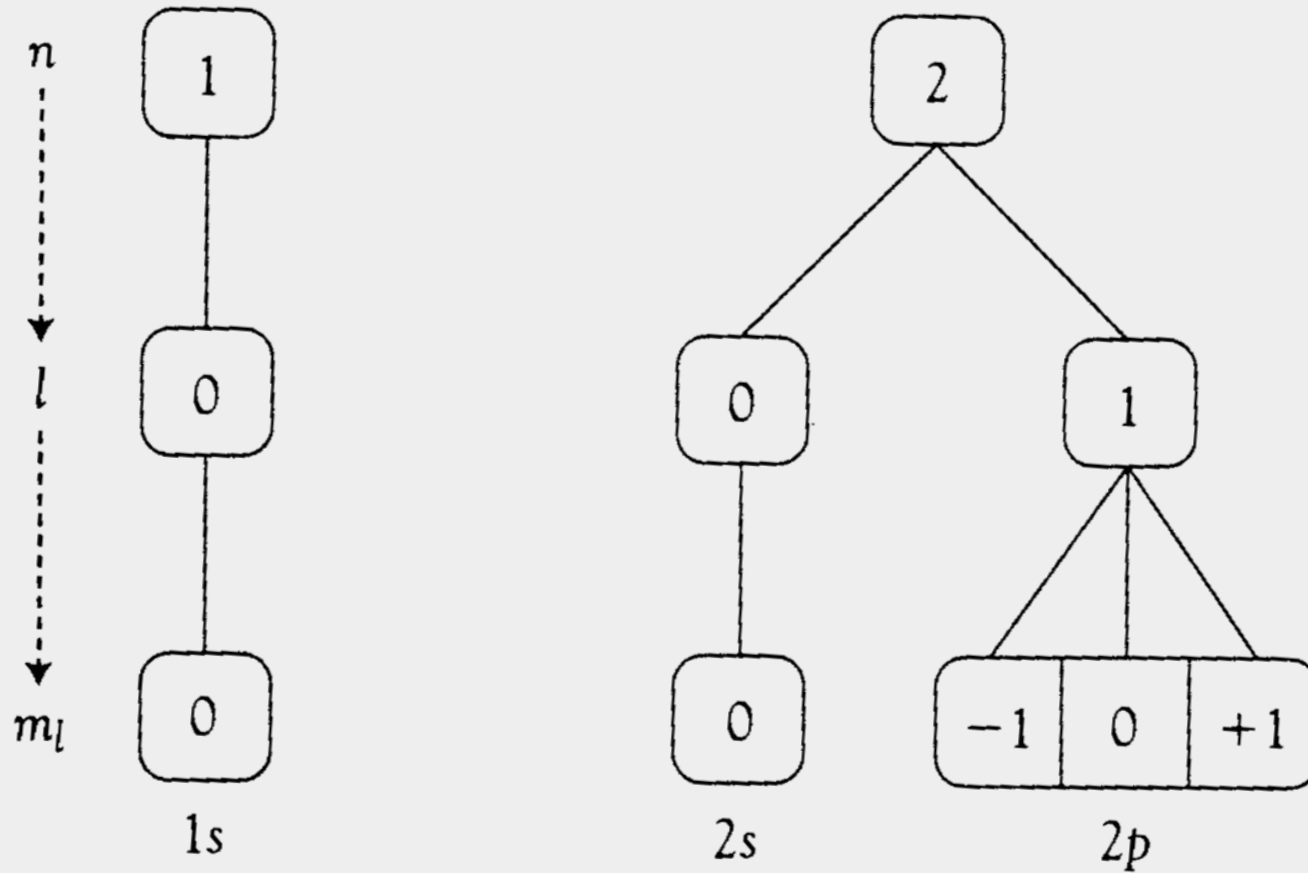


Figure 1.5 The possible sets of quantum numbers for $n = 3$.

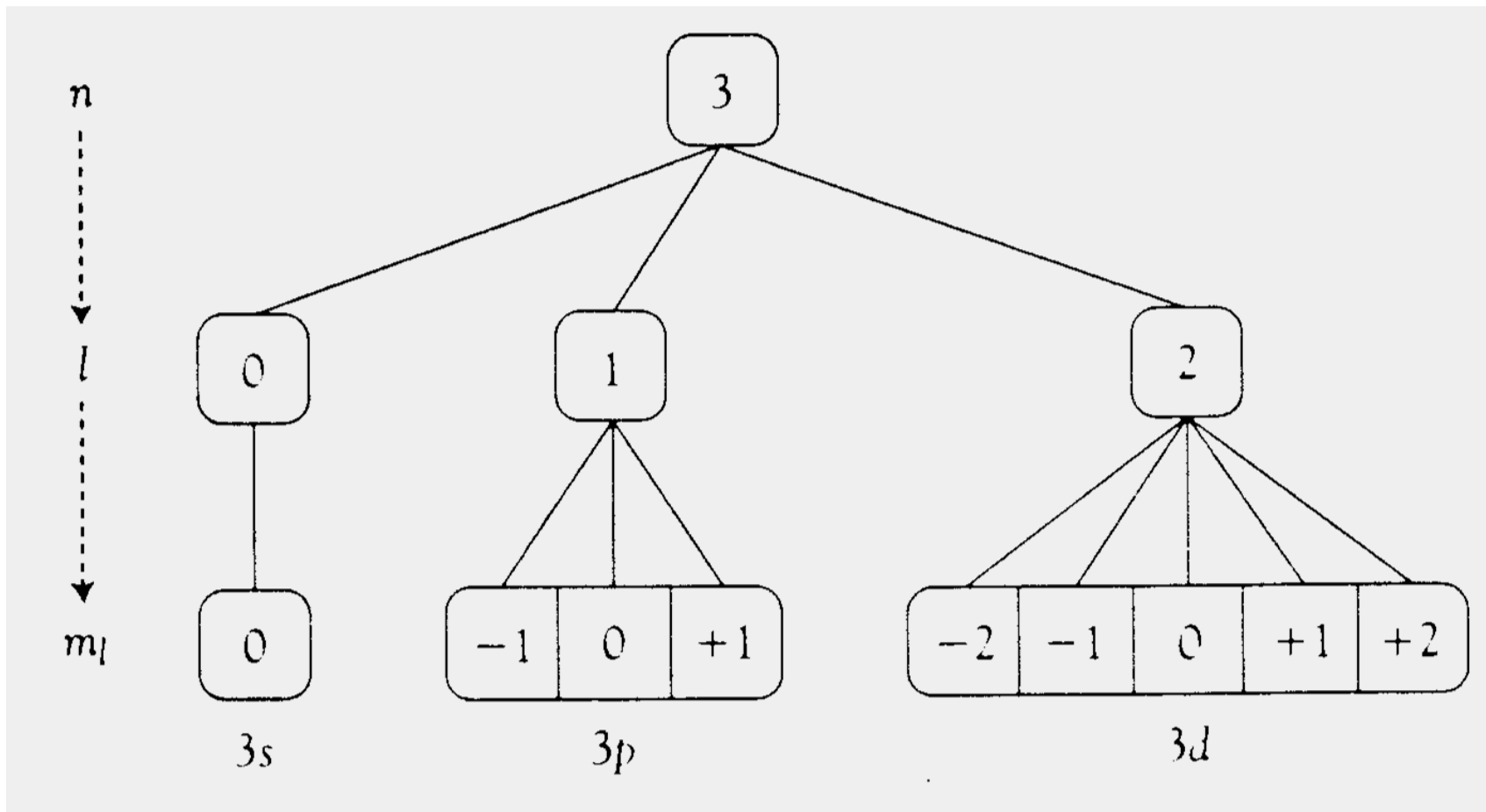
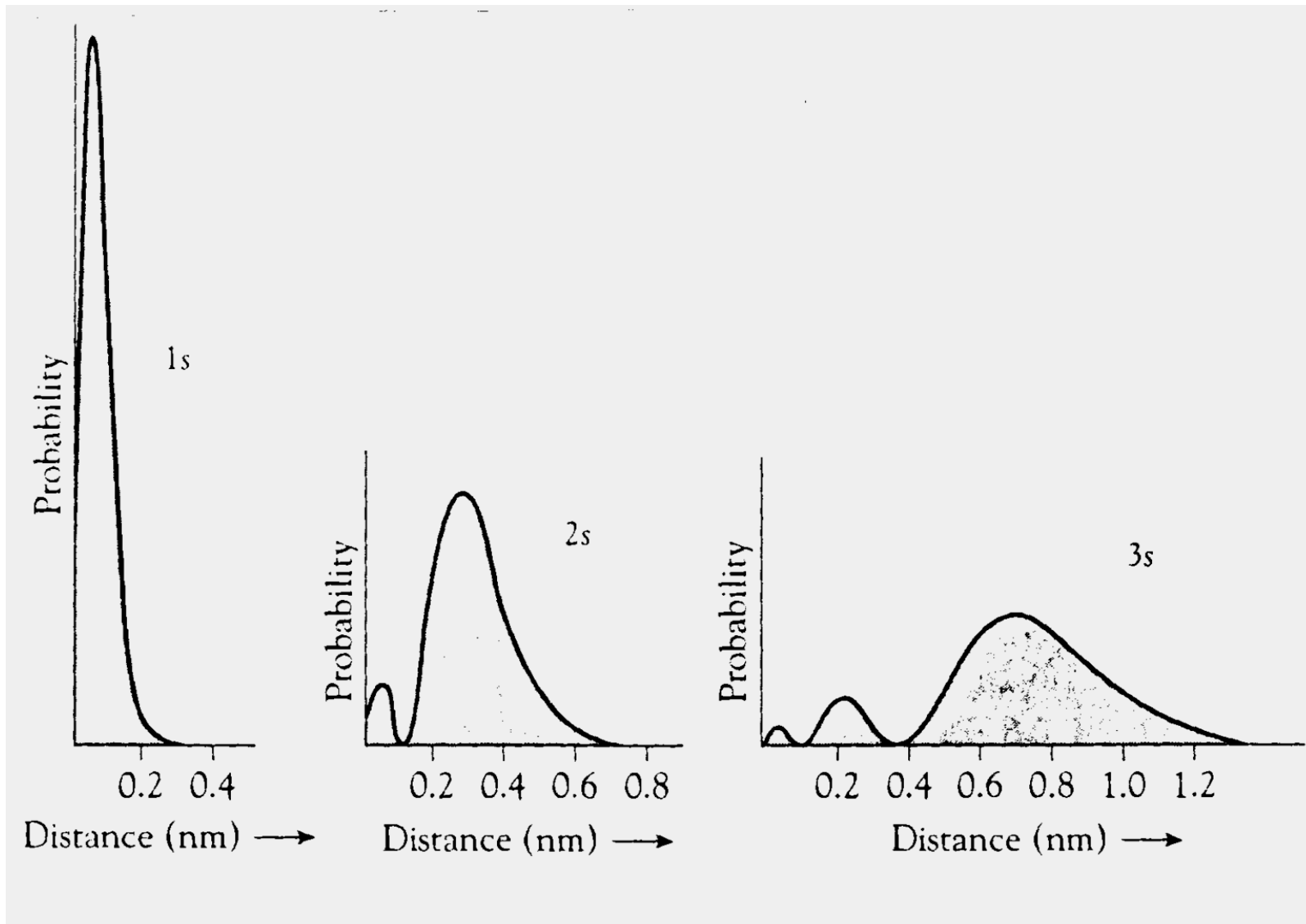


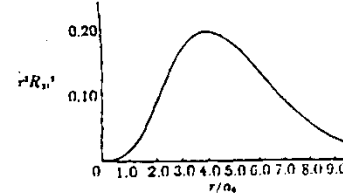
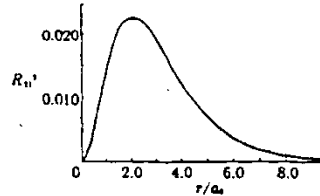
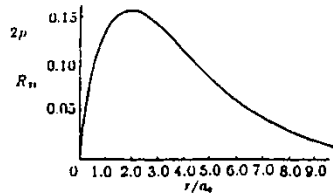
Figure 1.7 The variation of the radial density distribution function with distance from the nucleus for electrons in the 1s, 2s, and 3s orbitals of a hydrogen atom.





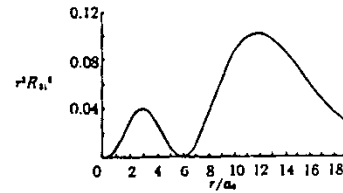
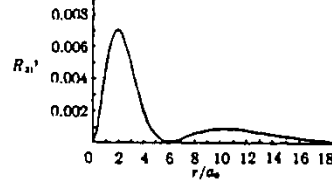
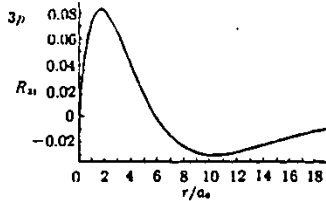
Radial Wave Functions (hydrogenic)

2p



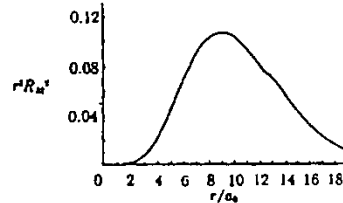
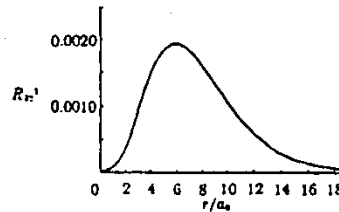
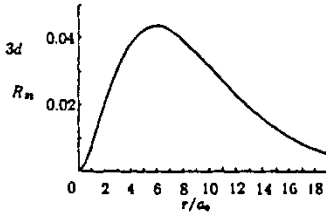
2p

3p



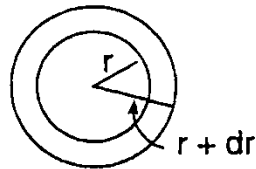
3p

3d



3d

sphere of radius r



$$V = \frac{4}{3} \pi r^3$$

$$dV = \underbrace{4\pi r^2}_{\text{surface area}} dr$$

$$R_{nl}^2(r) dV = 4\pi r^2 R_{nl}^2(r) dr = \underline{\underline{S(r)}}$$

S(r): surface density function

- gives the probability of finding e^-_{nl} in a spherical shell of thickness dr at a distance r from the nucleus