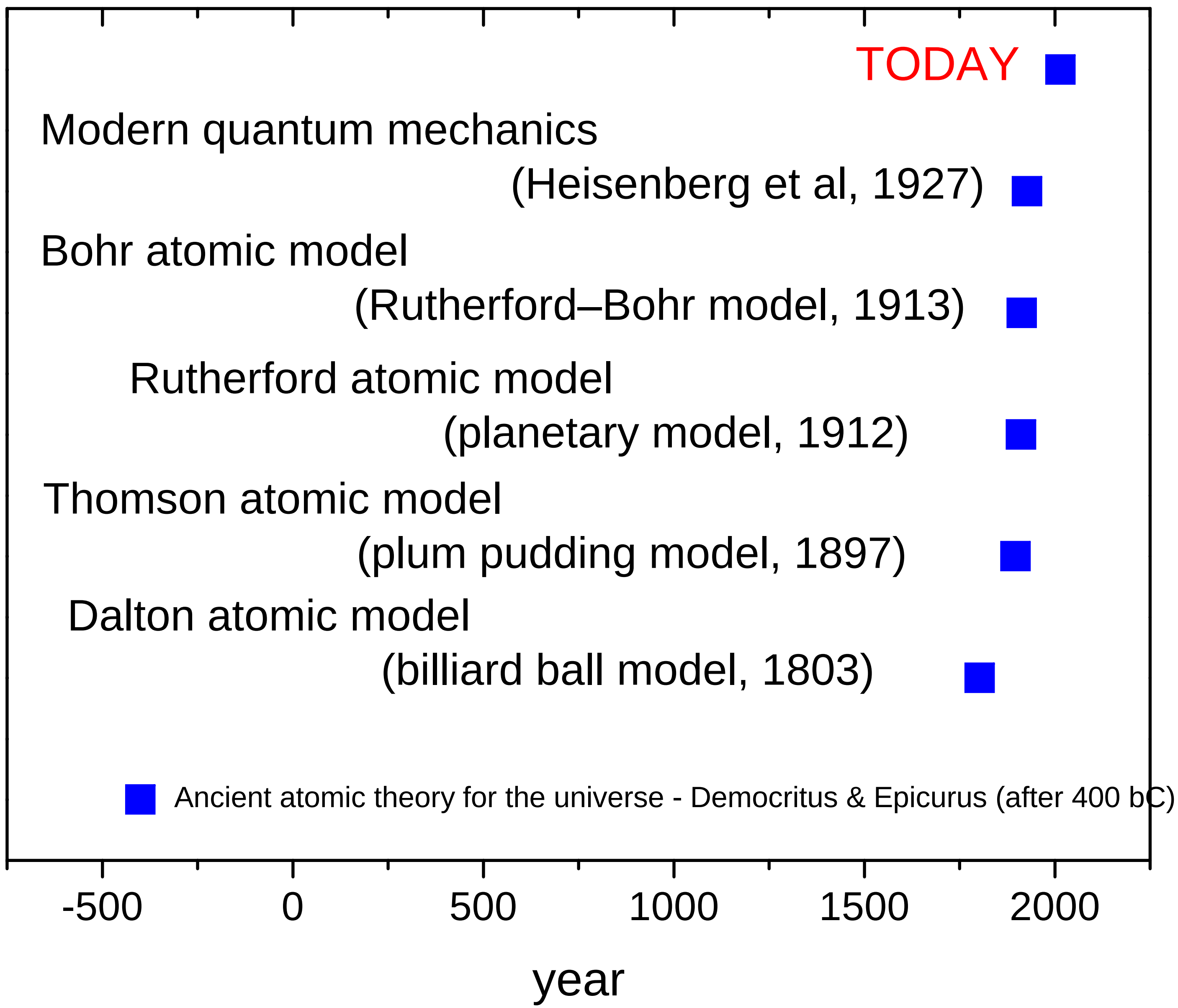
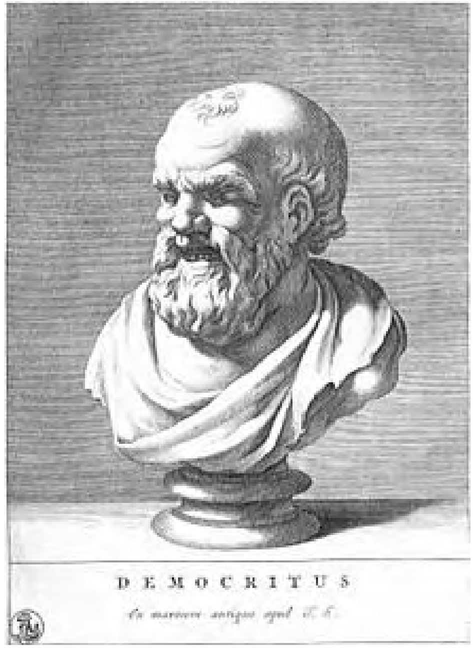
Timeline of Atomic Models [3]

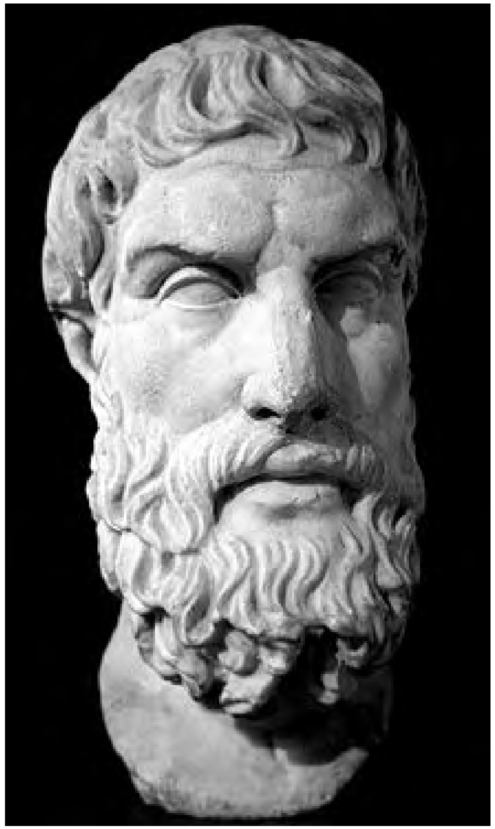


Timeline of Atomic Models



Democritus (460 b.C. – 370 b.C.):
“Matter could not be divided into smaller and smaller pieces forever, eventually the smallest possible piece would be indivisible.”
The smallest piece of matter “**atomos**”, meaning “not to be cut.”
Pioneer of **atomism.**

http://en.wikipedia.org/wiki/Democritus



Epicurus (341 b.C. – 270 b.C.):
“Everything that occurs is the result of the atoms colliding, rebounding, and becoming entangled with one another, with no purpose or plan behind their motions.”

http://en.wikipedia.org/wiki/Epicurus

Timeline of Atomic Models

- **To the Atomists**, atoms were small, hard particles that were all made of the same material but were different shapes and sizes. Atoms were infinite in number, always moving and capable of joining together.

- Others philosophers, as **Aristotle** and **Plato**, state a (wrong) theory that the nature of matter was composed by four elements – **Earth** (solid), **Water** (liquid), **Air** (gas), **Fire** (heat). **Aether** could be considered a fifth element. This theory of the four elements became the standard dogma for the **next two thousand years.**

http://en.wikipedia.org/wiki/Empedocles
http://en.wikipedia.org/wiki/Aristotle#Physics

John Dalton atomic model (billiard ball model, 1803):

John Dalton (1766-1844)

- Dalton states that all elements are composed of atoms, which are indivisible and indestructible particles.

- Atoms of the same element are exactly alike and those from different elements are different.

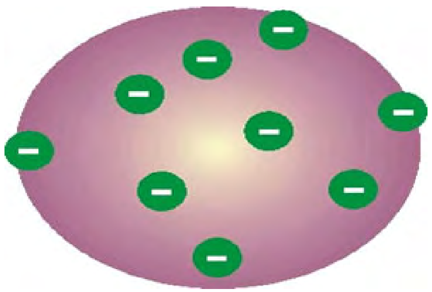
- Chemical compounds, as water, are formed by the joining of atoms of two or more elements.

http://en.wikipedia.org/wiki/John_Dalton

Timeline of Atomic Models

➢ Thomson atomic model (plum pudding model, 1897):

Joseph John Thomson
(1856-1940)



- Thomson studied the passage of an electric current through a gas.

- In 1897 Lord Kelvin proved that an atom is made of even smaller electrical charged particles (electrons).

- Thomson proposed that atoms were made from a positively charged particles/ substance with negatively charged electrons scattered inside, like raisins in a pudding.

- But he could never find them.

http://en.wikipedia.org/wiki/J._J._Thomson

Timeline of Atomic Models

➢ Rutherford atomic model (planetary model, 1912):

Ernest_Rutherford
(1871-1937)

• In 1908, Rutherford's experiment involved firing a stream of tiny positively charged particles at a thin sheet of gold foil (2000 atoms thick).

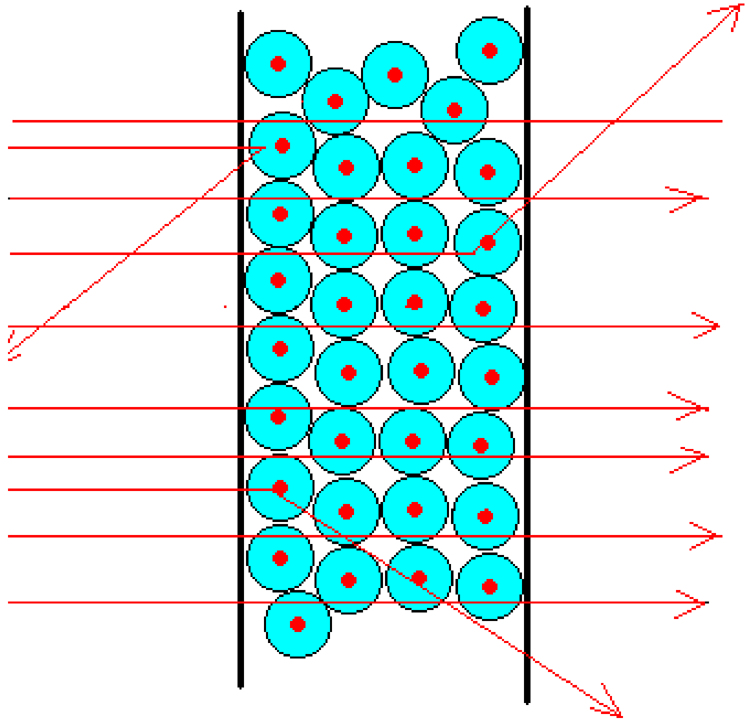
• Most of the positively charges passed right through the sheet of gold foil but some of the them did bounce away from the gold sheet as if they had hit something solid. He knew that positive charges repel positive charges.

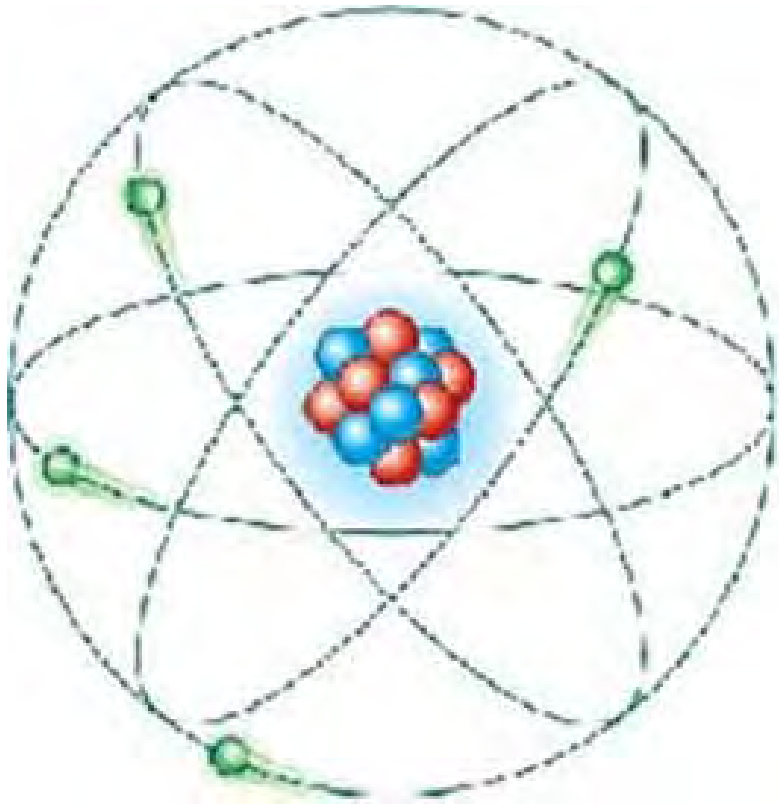
• Rutherford concluded that an atom had a small, dense, positively charged center (nucleus) that repelled his positively charged "bullets."

http://en.wikipedia.org/wiki/Ernest_Rutherford

Timeline of Atomic Models

- **Rutherford atomic model (planetary model, 1912):**





• Rutherford reasoned that all of an atom’s positively charged particles were contained in the nucleus. The negatively charged particles were scattered outside the nucleus around the atom’s edge.

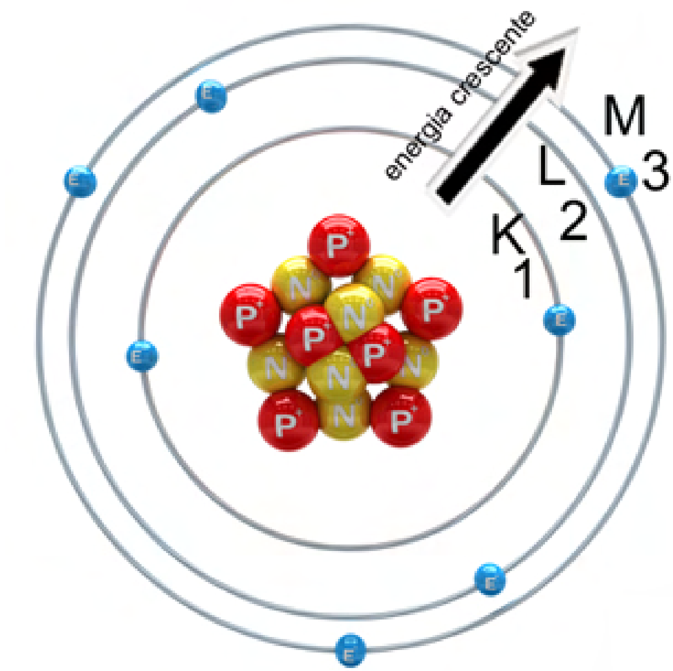
Timeline of Atomic Models

➢ Bohr atomic model (1913):

Niels_Bohr (1885-1962)

• In 1913, the Danish scientist **Niels Bohr** proposed a model where he placed each electron in a specific orbit (energy level) around the nucleus.

• These orbits, or energy levels, are located at specific distances (radius) from the nucleus.



http://en.wikipedia.org/wiki/Niels_Bohr

Timeline of Atomic Models

➢ Modern quantum mechanics (Heisenberg et al, 1927):

Werner_Heisenberg
(1901-1976)

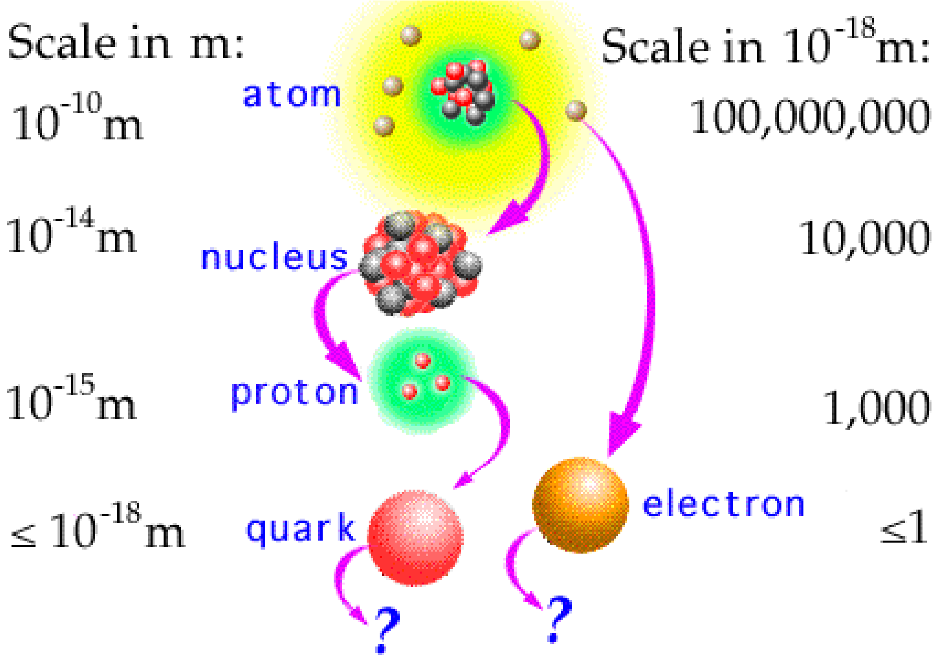
- According to the theory of wave mechanics, electrons do not move around an atom in a definite path, like the planets around the sun.

- In fact, it is impossible to determine the exact position of an electron. The probable location of an electron is based on how much energy the electron has.

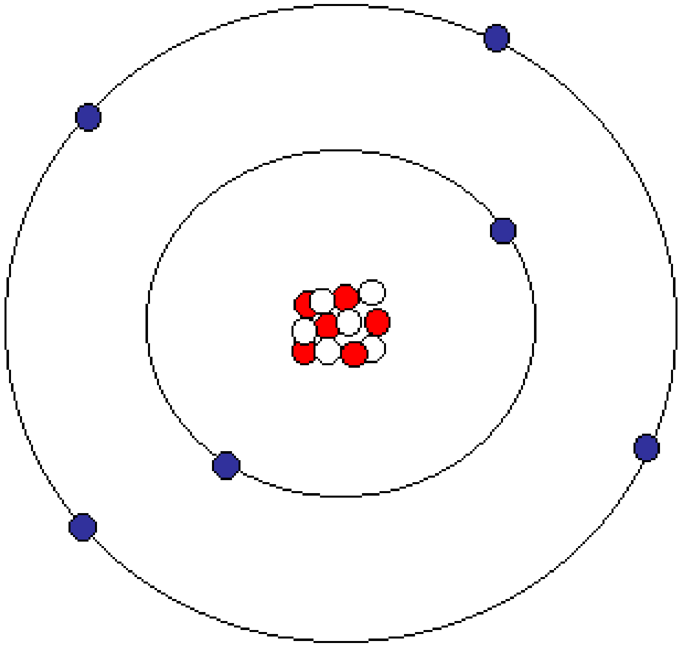
- According to the modern atomic model, at atom has a small positively charged nucleus surrounded by a large region (electron cloud) in which there are enough electrons to make an atom electrically neutral.

http://en.wikipedia.org/wiki/Werner_Heisenberg

The free atom



- nucleus: protons (+) and neutrons
- electrosphere: electrons (-)
- electrical
- electrical charge: 1.60×10^{-19} C
- mass of proton: 1.67×10^{-24} g
- mass of electron: 9.11×10^{-28} g
- **atomic number Z** :
  number of electrons or protons
- **atomic mass M** :
  average number of protons and neutrons in NA atoms
- **Avogadro number NA** :
  6.02×10^{23} atoms/mol
- **atomic radii R** :
  typical distance from the nucleus to the boundary of the surrounding cloud of electrons

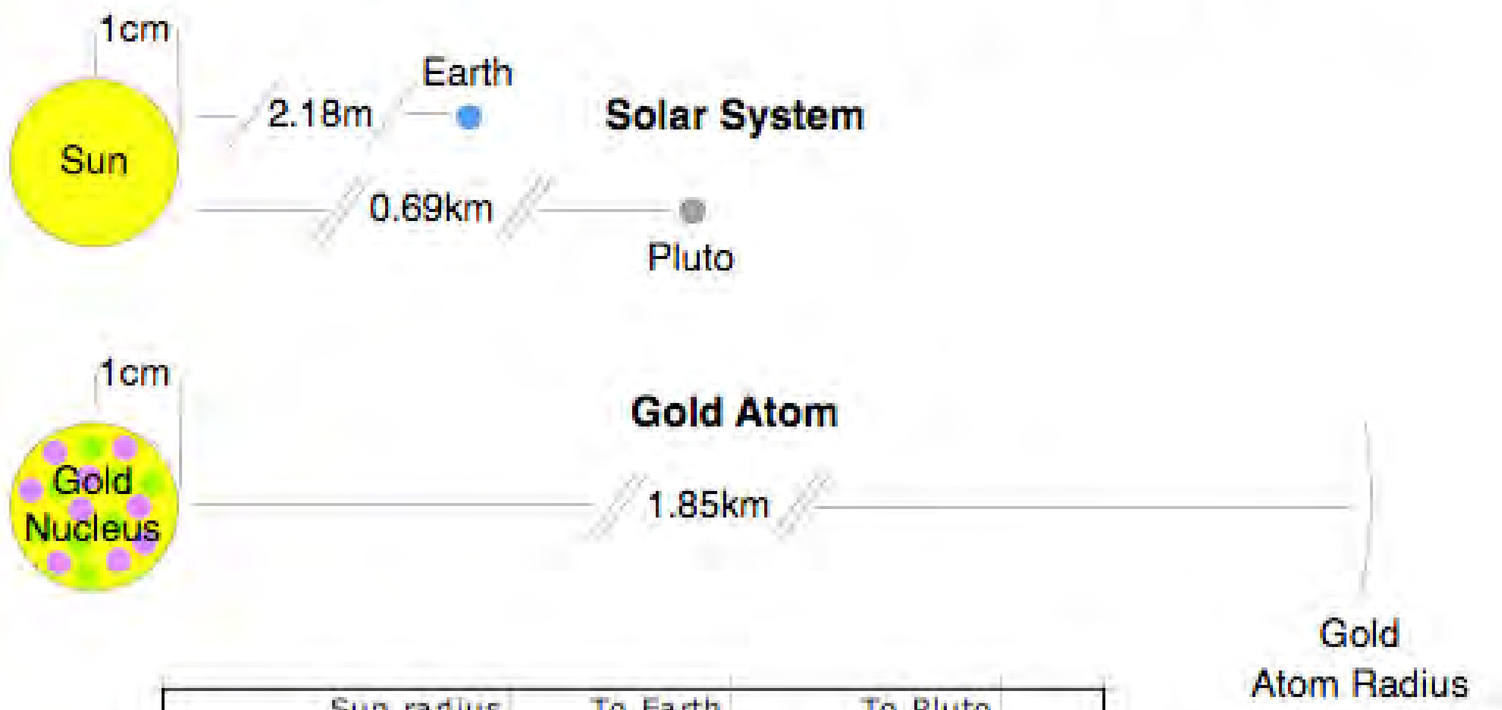


Carbon atom

Z=6
M=12.01 g/mol
R=70 pm

The free atom

Comparison of the Size of the Sun to the Solar System with the Size of the Gold Atomic Nucleus to the Gold Atom



Sun radius	To Earth	To Pluto	
6.96E+08	1.52E+11	4.77E+12	m

Gold Nucleus radius	Atomic radius	
7.30E-15	1.35E-10	m

http://www.meta-synthesis.com/webbook/34_qn/qn_to_pt.html

The Electronic Structure of the Atom

- **Quantum numbers of electrons:**

Defined as "The sets of numerical values which give acceptable solutions to the Schrödinger wave equation for the Hydrogen atom". From: http://en.wikipedia.org/wiki/Quantum_number

- **Principal quantum number (n):** n = 1 (K), 2 (L), ..

- **Azimuthal (orbital) quantum number (ℓ):**

"ℓ = 0" - **S**harp orbital, "ℓ = 1" - **P**rimitive orbital,
"ℓ = 2" - **D**iffuse orbital, and "ℓ = 3" - **F**undamental orbital.

- **Magnetic quantum number (m):**

“m = 0” – s orbital; “m = -1,0,1” – p orbital;
“m = -2,-1,0,1,2” – d orbital

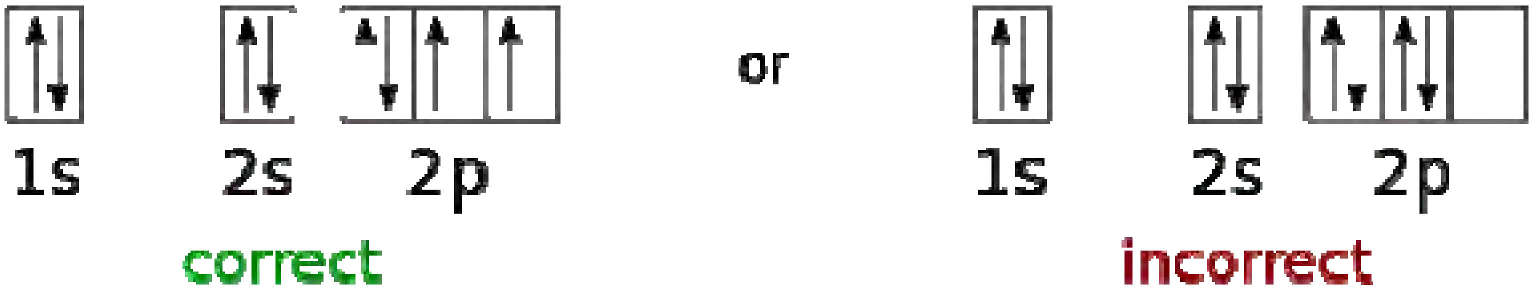
- **Spin quantum number (s):** s = - ½ or s = + ½

The Electronic Structure of the Atom

- **Electrons enter and fill orbitals according to four rules:**

Pauli Exclusion Principal	Orbitals can contain a maximum of two electrons which must be of opposite spin.
Aufbau or **Build-up Principle**	Electrons enter and fill lower energy orbitals before higher energy orbitals.
Hund's Rule	When there there are degenerate (equal energy) orbitals available, electrons will enter the orbitals one-at-a-time to maximise degeneracy, and only when all the orbitals are half filled will pairing-up occur. This is the rule of maximum multiplicity.
Madelung's Rule	Orbitals fill with electrons as *n* + *l*, where *n* is the principal quantum number and *l* is the subsidiary quantum number. This rule 'explains' why the 4s orbital has a lower energy than the 3d orbital, and it gives the periodic table its characteristic appearance.

- **Hund's Rule:**

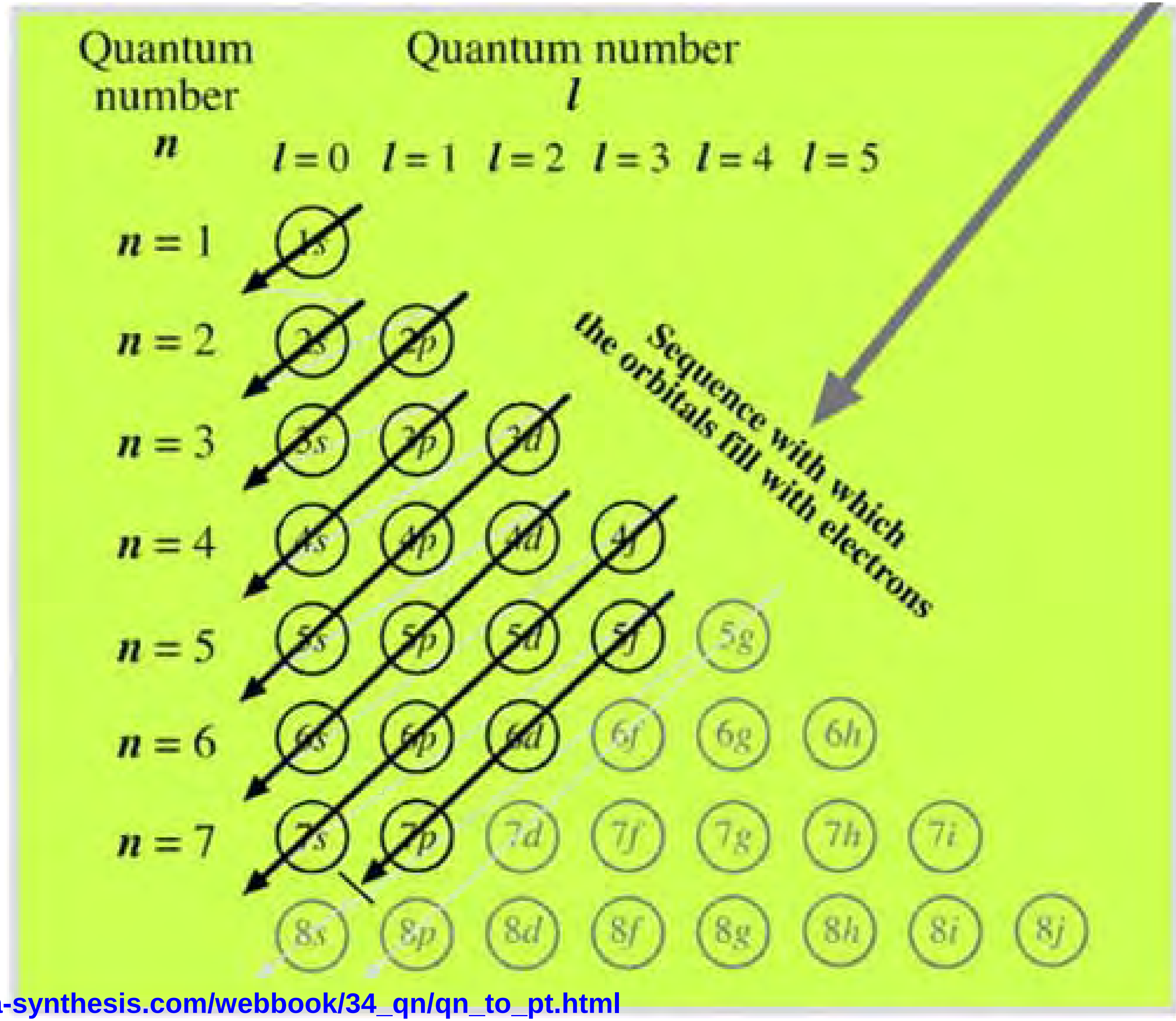


From: http://www.meta-synthesis.com/webbook/34_qn/qn_to_pt.html

The Electronic Structure of the Atom

- **Madelung's Rule:**

K (2)
L (8)
M (18)
N (32)
O (32)
P (18)
Q (8)



From: http://www.meta-synthesis.com/webbook/34_qn/qn_to_pt.html

The Electronic Structure of the Atom

➢ Expected Electron Configurations:

C: $1s^2\ 2s^2\ 2p^2$

Na: $1s^2\ 2s^2\ 2p^6\ 3s^1$

Cl: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

Fe: $1s^2\ 2s^2\ 2p^6$
$3s^2\ 3p^6\ 3d^6\ 4s^2$

Element	*Symbol*	*Atomic Number*	*Electron Configuration*
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^22s^1$
Beryllium	Be	4	$1s^22s^2$
Boron	B	5	$1s^22s^22p^1$
Carbon	C	6	$1s^22s^22p^2$
Nitrogen	N	7	$1s^22s^22p^3$
Oxygen	O	8	$1s^22s^22p^4$
Fluorine	F	9	$1s^22s^22p^5$
Neon	Ne	10	$1s^22s^22p^6$
Sodium	Na	11	$1s^22s^22p^63s^1$
Magnesium	Mg	12	$1s^22s^22p^63s^2$
Aluminum	Al	13	$1s^22s^22p^63s^23p^1$
Silicon	Si	14	$1s^22s^22p^63s^23p^2$
Phosphorus	P	15	$1s^22s^22p^63s^23p^3$
Sulfur	S	16	$1s^22s^22p^63s^23p^4$
Chlorine	Cl	17	$1s^22s^22p^63s^23p^5$
Argon	Ar	18	$1s^22s^22p^63s^23p^6$
Potassium	K	19	$1s^22s^22p^63s^23p^64s^1$
Calcium	Ca	20	$1s^22s^22p^63s^23p^64s^2$
Scandium	Sc	21	$1s^22s^22p^63s^23p^63d^14s^2$
Titanium	Ti	22	$1s^22s^22p^63s^23p^63d^24s^2$
Vanadium	V	23	$1s^22s^22p^63s^23p^63d^34s^2$
Chromium	Cr	24	$1s^22s^22p^63s^23p^63d^54s^1$
Manganese	Mn	25	$1s^22s^22p^63s^23p^63d^54s^2$
Iron	Fe	26	$1s^22s^22p^63s^23p^63d^64s^2$
Cobalt	Co	27	$1s^22s^22p^63s^23p^63d^74s^2$
Nickel	Ni	28	$1s^22s^22p^63s^23p^63d^84s^2$
Copper	Cu	29	$1s^22s^22p^63s^23p^63d^{10}4s^1$
Zinc	Zn	30	$1s^22s^22p^63s^23p^63d^{10}4s^2$

The Electronic Structure of the Atom

- **Deviations from Expected Electronic Structures:**

Fe (expected): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^8$

Fe (actual): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \boxed{3d^6\ 4s^2}$

The unfilled 3d level causes the magnetic behavior of iron.

- **Valence:** number of electrons in an atom that participate in bonding or chemical reactions. Valence also depends on the immediate environment surrounding the atom or the neighboring atoms available for bonding.

Na: $1s^2\ 2s^2\ 2p^6\ 3s^1$	V = 1
Mg: $1s^2\ 2s^2\ 2p^6\ 3s^2$	V = 2
Al: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$	V = 3
Cl: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$	V = 7
Ar: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$	V = 0

The Electronic Structure of the Atom

- **Electronegativity:** describes the tendency of an atom to gain an electron.

readly accept

electrons

give up

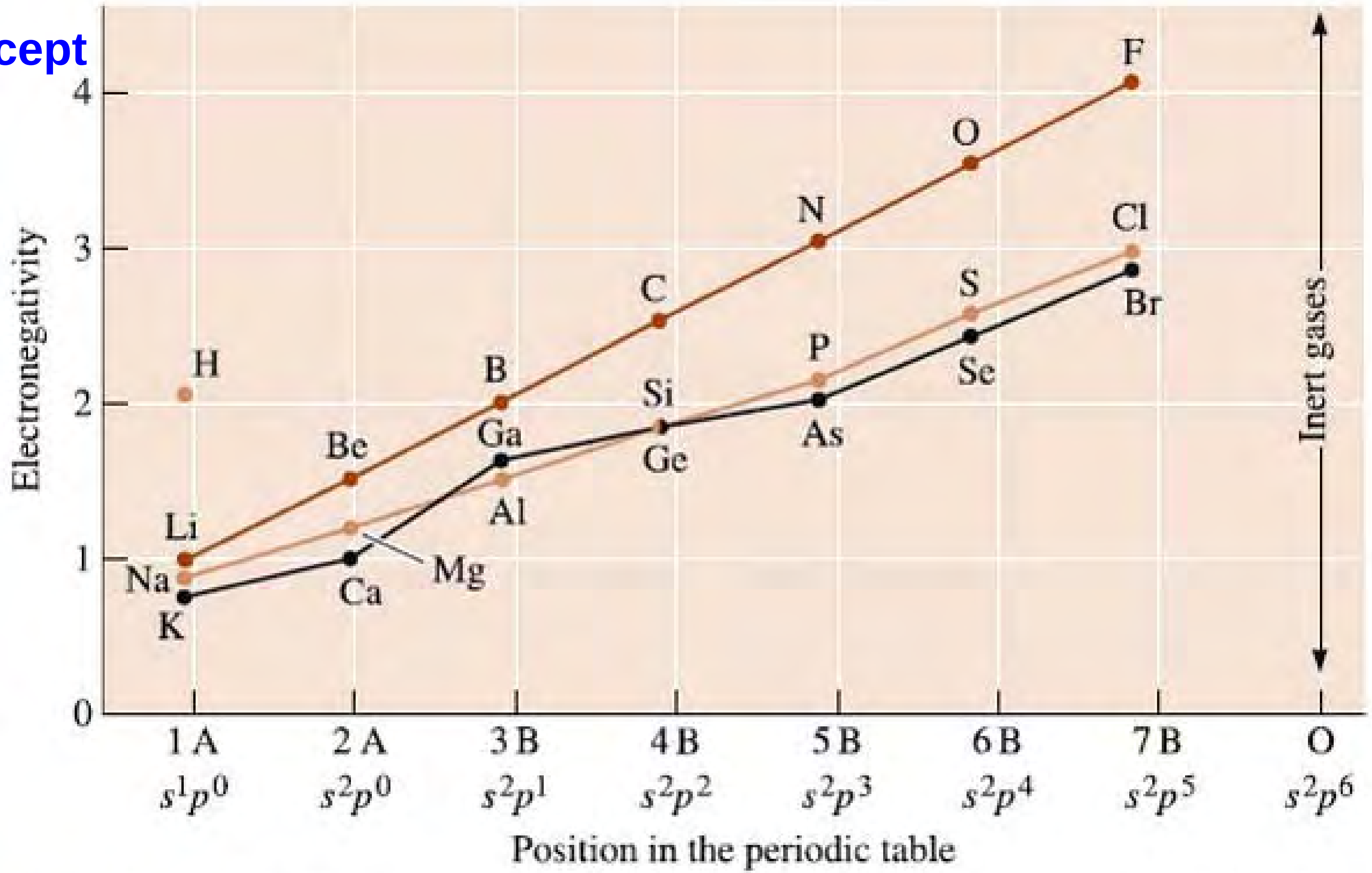


Figure 2-8 The electronegativities of selected elements relative to the position of the elements in the periodic table.

From: Askeland & Fulay (2009)

Periodic Table

V·T·E **Periodic table** [hide]

http://en.wikipedia.org/wiki/Periodic_table#Periodic_table_legend_for_category

Group → / Period ↓	1 Alkali metals	2 Alkaline earth metals		3	4	5	6	7	8	9	10	11	12	13	14	15 Pnictogens	16 Chalco-gens	17 Halogens	18 Noble gases
1	Hydrogen 1 H																		Helium 2 He
2	Lithium 3 Li	Beryllium 4 Be												Boron 5 B	Carbon 6 C	Nitrogen 7 N	Oxygen 8 O	Fluorine 9 F	Neon 10 Ne
3	Sodium 11 Na	Magne-sium 12 Mg												Aluminium 13 Al	Silicon 14 Si	Phos-phorus 15 P	Sulfur 16 S	Chlorine 17 Cl	Argon 18 Ar
4	Potassium 19 K	Calcium 20 Ca		Scandium 21 Sc	Titanium 22 Ti	Vanadium 23 V	Chromium 24 Cr	Manga-nese 25 Mn	Iron 26 Fe	Cobalt 27 Co	Nickel 28 Ni	Copper 29 Cu	Zinc 30 Zn	Gallium 31 Ga	Germa-nium 32 Ge	Arsenic 33 As	Selenium 34 Se	Bromine 35 Br	Krypton 36 Kr
5	Rubidium 37 Rb	Strontium 38 Sr		Yttrium 39 Y	Zirconium 40 Zr	Niobium 41 Nb	Molyb-denum 42 Mo	Tech-netium 43 Tc	Ruthenium 44 Ru	Rhodium 45 Rh	Palladium 46 Pd	Silver 47 Ag	Cadmium 48 Cd	Indium 49 In	Tin 50 Sn	Antimony 51 Sb	Tellurium 52 Te	Iodine 53 I	Xenon 54 Xe
6	Caesium 55 Cs	Barium 56 Ba	*	Lutetium 71 Lu	Hafnium 72 Hf	Tantalum 73 Ta	Tungsten 74 W	Rhenium 75 Re	Osmium 76 Os	Iridium 77 Ir	Platinum 78 Pt	Gold 79 Au	Mercury 80 Hg	Thallium 81 Tl	Lead 82 Pb	Bismuth 83 Bi	Polonium 84 Po	Astatine 85 At	Radon 86 Rn
7	Francium 87 Fr	Radium 88 Ra	**	Lawren-cium 103 Lr	Ruther-fordium 104 Rf	Dubnium 105 Db	Sea-borgium 106 Sg	Bohrium 107 Bh	Hassium 108 Hs	Meitnerium 109 Mt	Darm-stadtium 110 Ds	Roent-genium 111 Rg	Coper-nicium 112 Cn	Ununtrium 113 Uut	Flerovium 114 Fl	Unun-pentium 115 Uup	Liver-morium 116 Lv	Unun-septium 117 Uus	Unun-octium 118 Uuo

*	Lanthanum 57 La	Cerium 58 Ce	Praseo-dymium 59 Pr	Neo-dymium 60 Nd	Prome-thium 61 Pm	Samarium 62 Sm	Europium 63 Eu	Gadolinium 64 Gd	Terbium 65 Tb	Dyspro-sium 66 Dy	Holmium 67 Ho	Erbium 68 Er	Thulium 69 Tm	Ytterbium 70 Yb
**	Actinium 89 Ac	Thorium 90 Th	Protac-tinium 91 Pa	Uranium 92 U	Neptunium 93 Np	Plutonium 94 Pu	Americium 95 Am	Curium 96 Cm	Berkelium 97 Bk	Californium 98 Cf	Einsteinium 99 Es	Fermium 100 Fm	Mende-levium 101 Md	Nobelium 102 No

black=solid green=liquid red=gas grey=unknown **Color of the atomic number** shows state of matter (at 0 °C and 1 atm)

Primordial From decay Synthetic **Border** shows natural occurrence of the element

Background color shows subcategory in the metal–metalloid–nonmetal trend:

Metal						Metalloid	Nonmetal			Unknown chemical properties
Alkali metal	Alkaline earth metal	Lanthanide	Actinide	Transition metal	Post-transition metal		Polyatomic nonmetal	Diatomic nonmetal	Noble gas	

Periodic Table

ELEMENTS IN METALLIC MATERIALS

1 IA	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18 VIIA
	IIA											IIIA	IVA	VA	VIA	VIIA	
3 Li	4 Be											5 B					
11 Na	12 Mg	IIIB	IVB	VB	VIB	VIIB	-----	VIII	-----	IB	IIB	13 Al					
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga					
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb			
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi			
87 Fr	88 Ra																

Shackelford & Alexander (2001)

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lw

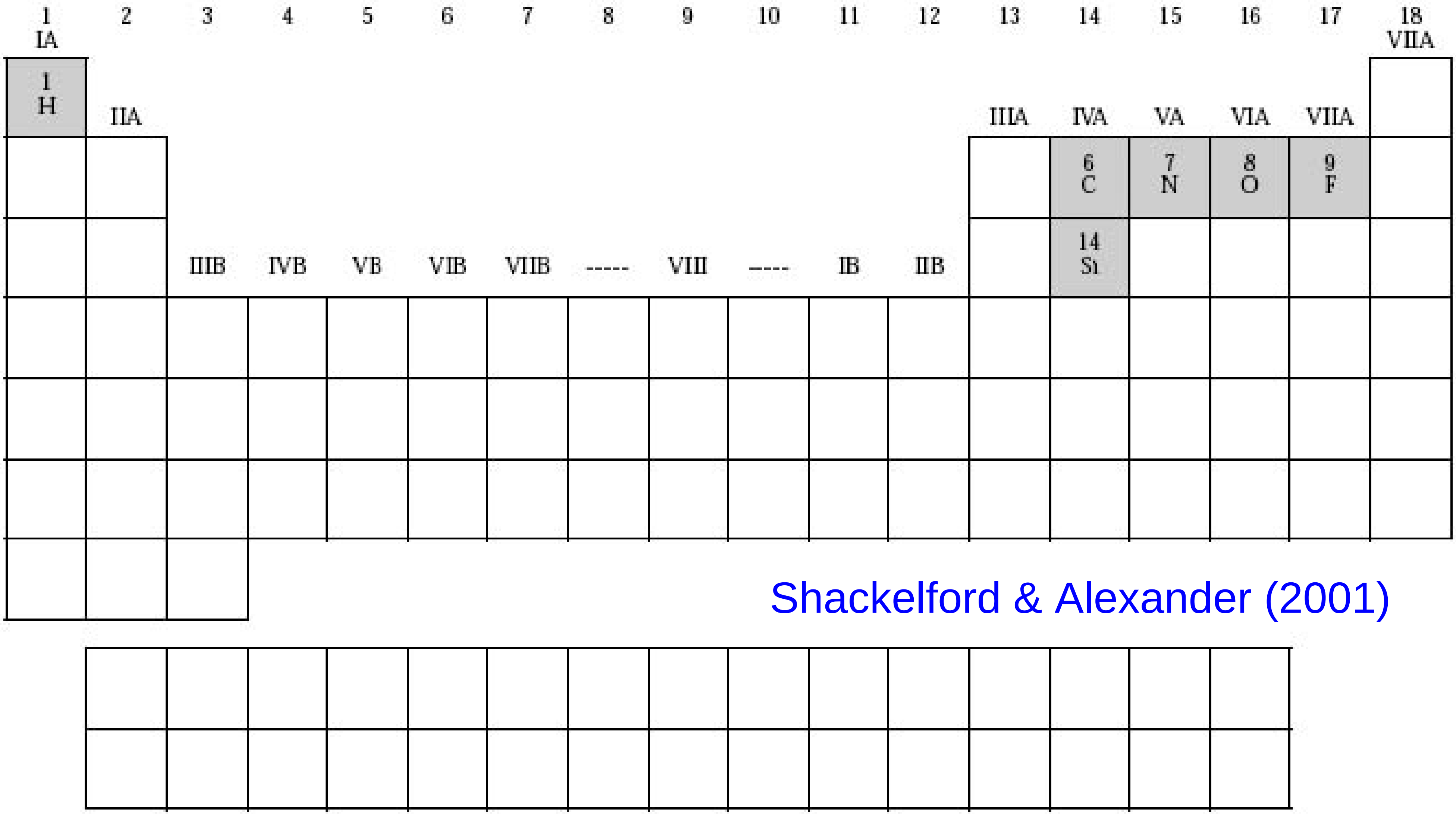
ELEMENTS IN CERAMIC MATERIALS

1 IA	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18 VIIA
	IIA											IIIA	IVA	VA	VIA	VIIA	
3 Li	4 Be											5 B	6 C	7 N	8 O		
11 Na	12 Mg	IIIB	IVB	VB	VIB	VIIB	-----	VIII	----	IB	IIB	13 Al	14 Si	15 P	16 S		
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge				
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb			
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi			
87 Fr	88 Ra																

Shackelford & Alexander (2001)

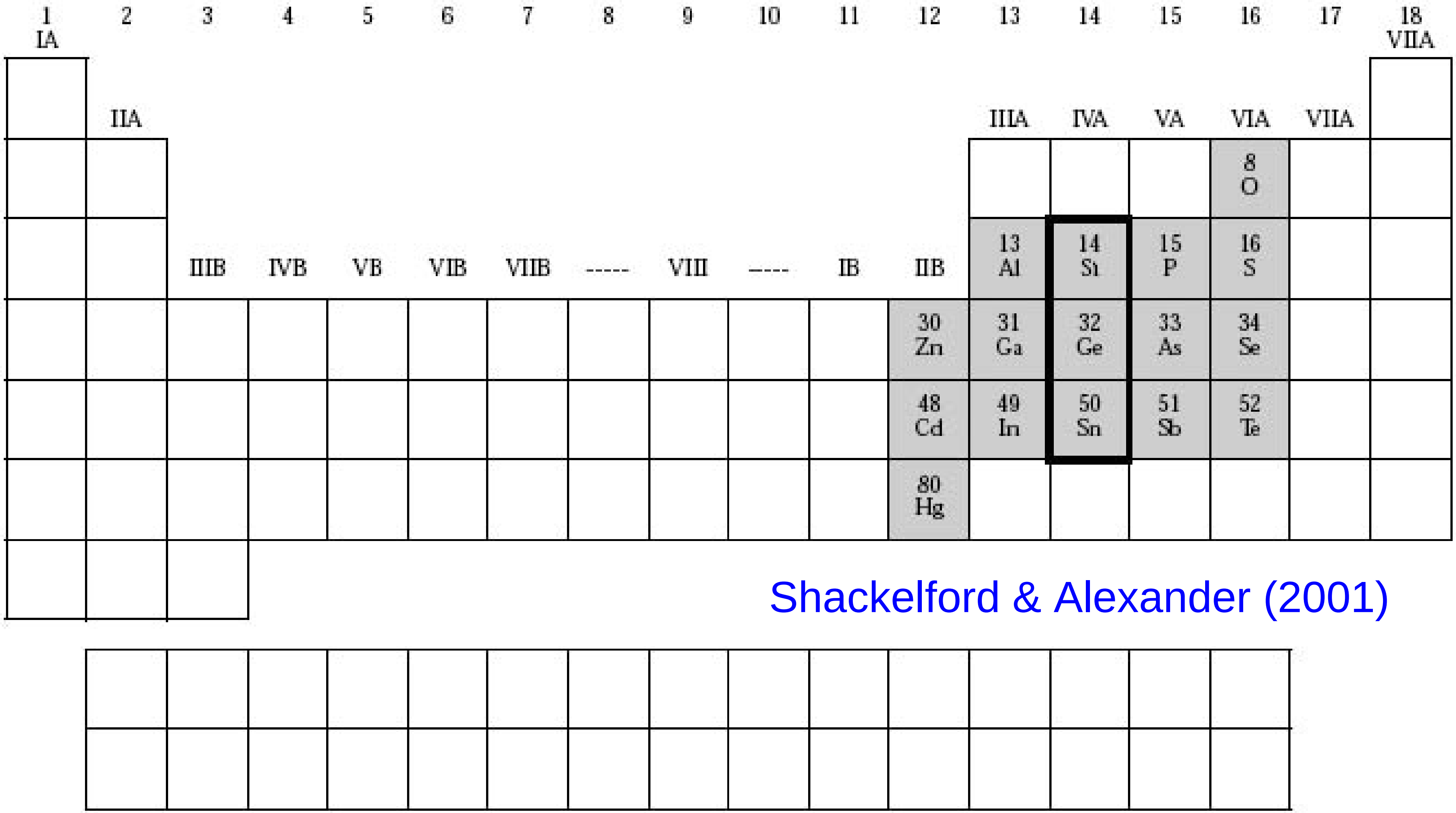
57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lw

ELEMENTS IN POLYMERIC MATERIALS



Shackelford & Alexander (2001)

ELEMENTS IN SEMICONDUCTING MATERIALS



Shackelford & Alexander (2001)

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