



The structure of the atom



1. Rutherford's model of the atom

2. Quantum-mechanics model of the atom

- **The wave nature of microparticles motion**
 - **The electron cloud**
 - **The quantum numbers**

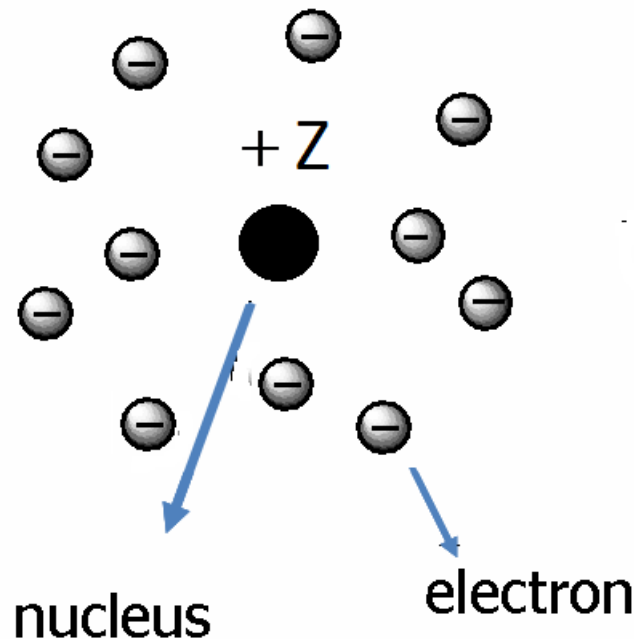


1. Rutherford's model of the atom


n The atom is a complicated microsystem consisting of the moving elementary particles

Rutherford's experiment (1911) showed that the nucleus of the atom contains the protons and the neutrons

and is very small compared to the atom itself



The positive charge of the nucleus is completely neutralized by electrons



• *The number of protons (Z)* in the nucleus identifies the charge of the nucleus and its belonging to
a given chemical element

- Another important characteristic of the nucleus is *the mass number (A)* of the atom which is equal to the total number of *protons (Z) and neutrons (N)* in it as:

$$A = Z + N$$

- Atoms with the same number of protons and with the different mass number are called *isotopes*





2. Quantum-mechanics model of the atom

n *Quantum mechanics* or *wave mechanics*
studies motion laws that govern the behavior
of small particles

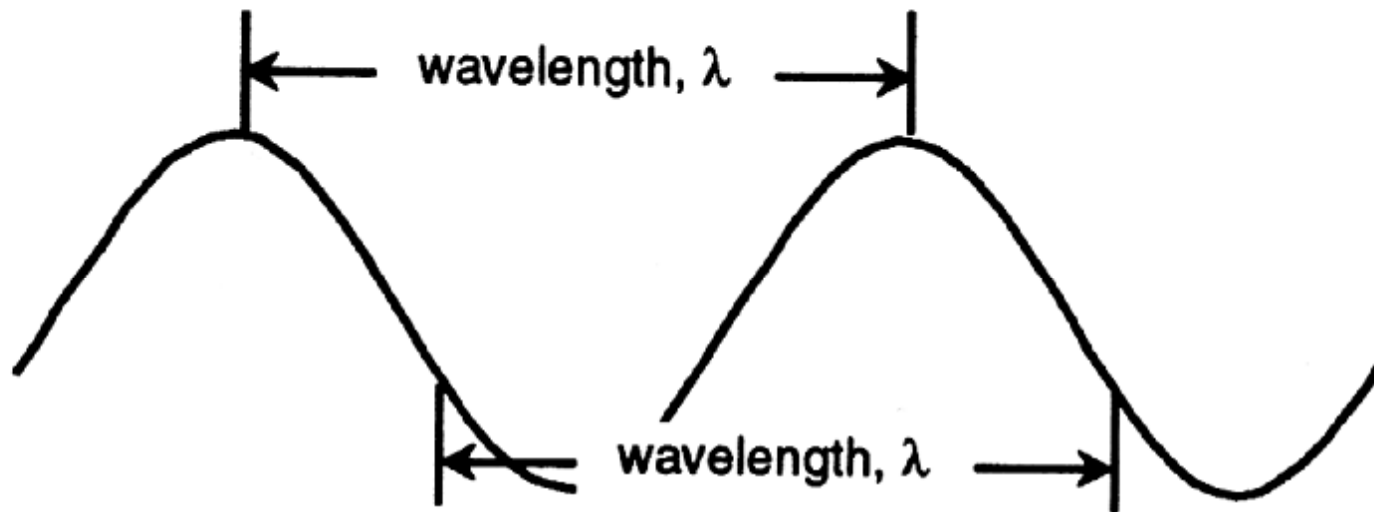


The wave nature of microparticles motion


- In 1924, Louis de Broglie proposed that an electron and other particles of comparable mass could be described by the physics of waves
- **The motion of any microparticle (electrons, *protons*) is regarded as a wave process**



Properties of a wave:
wavelength (λ), frequency (ν), velocity of a wave (v)



The distance between the corresponding points in the wave - **the wavelength**



n The waves can be described by the amount of time that passes between successive waves - ***the frequency, ν*** , of the waves and has the units of 1/time or, in SI units, 1/s

velocity of a wave: $v = \nu \lambda$




De Broglie equation

$$\lambda = h / m v$$

Where **m** – a mass of a particle,
v - a velocity,
l - a wavelength,
h is the Planck's constant ($6,626 \cdot 10^{-34}$ J·s)

- According to the equation a particle of **mass (m)** moving at **a velocity (v)** has a certain **wavelength (l)**

- 
- n According to the de Broglie equation the motion of **an electron** with the mass equal to **$9.1 \times 10^{-31} \text{ kg}$** and the velocity equal to **10^8 m/s** is associated with a wavelength equal to **10^{-10} meters**
 - n The wavelength approximately equals to the atom's size
 - n De Broglie's hypothesis was proved experimentally by the discovery of diffraction and interference effects in a stream of electrons



The uncertainty principle


- n In 1927, Werner Heisenberg
- n It is impossible to determine accurately both *the position* (or coordinates) and *the velocity* of motion of a microparticle simultaneously



Werner Heisenberg

(1901—1976)

earned a PhD in theoretical physics at the University of Munich (Germany). He received the Nobel Prize in physics in 1932



n Thus the state of an electron in an atom cannot be represented as the motion of a material particle along the orbit

n Quantum mechanics uses the idea of ***a statistical probability of finding the electron*** at a definite point in space around the nucleus

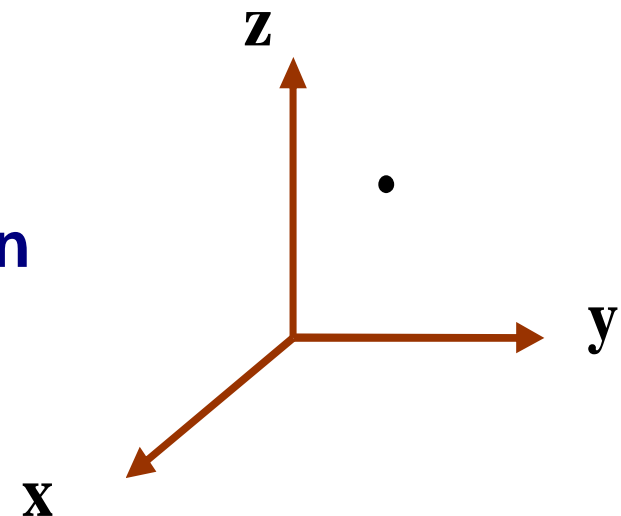
The electron cloud

n The model of an electron in an atom accepted in quantum mechanics is the idea of

the electron cloud

Let us assume that we have photographed the position of an electron at some moment of time in the three-dimensional space around the nucleus

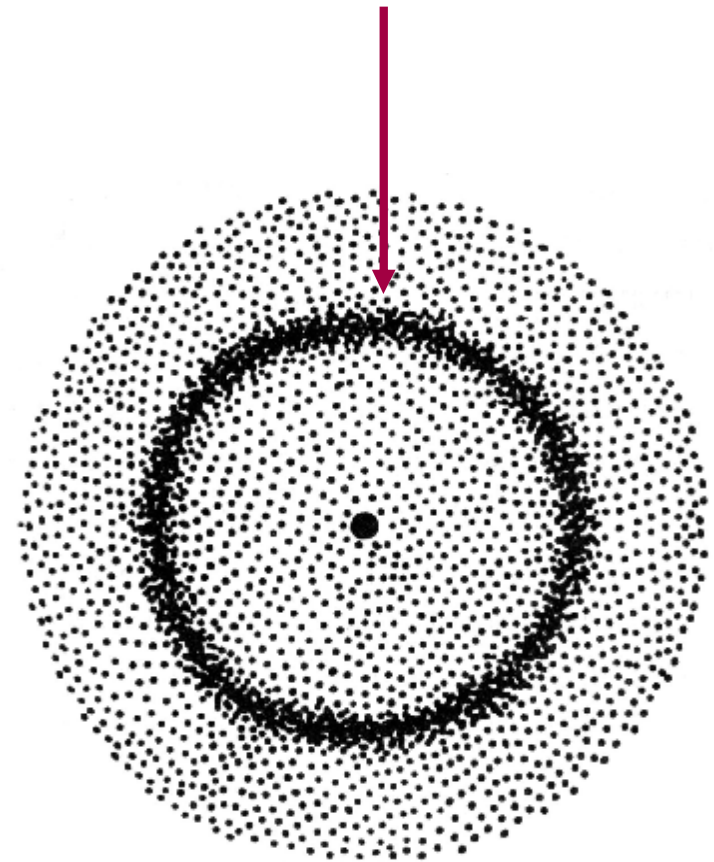
The position of an electron is shown on the photographs as a dot



n If we repeat the experience thousands of times, the new photos taken at short intervals, will discover the electron in new positions

n When all the photos are superimposed on one another, we will get a picture resembling **a cloud**

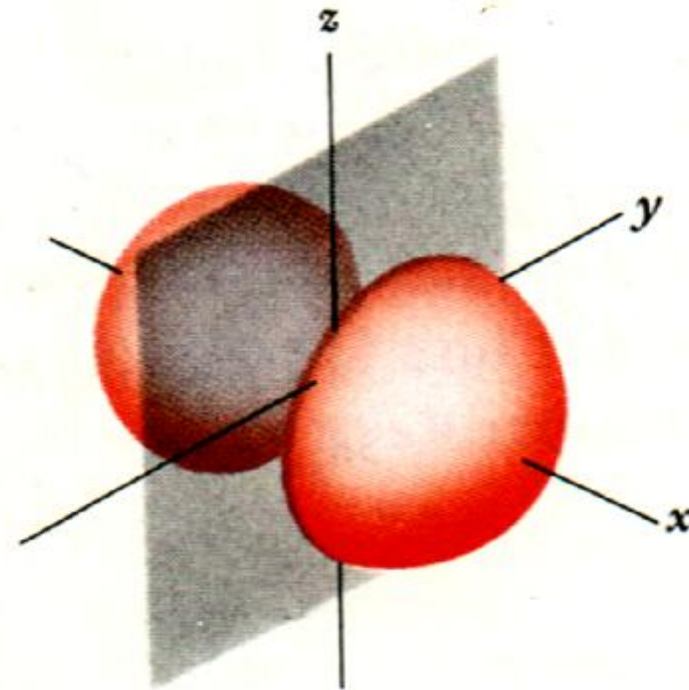
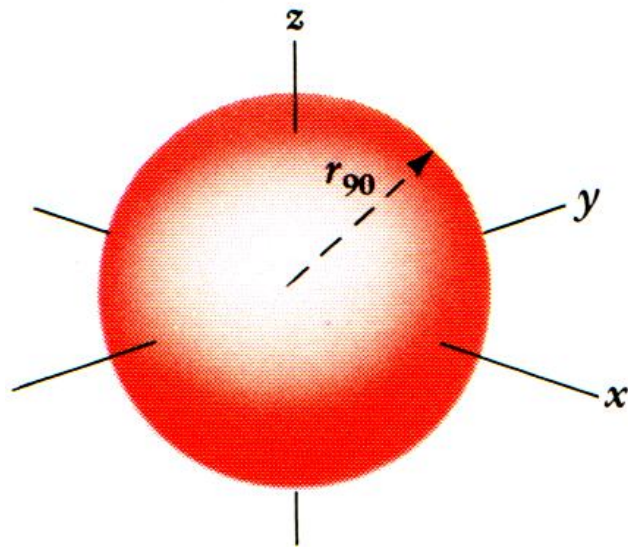
n The space around the nucleus in which the probability of finding the electron is the highest is called ***the orbital***



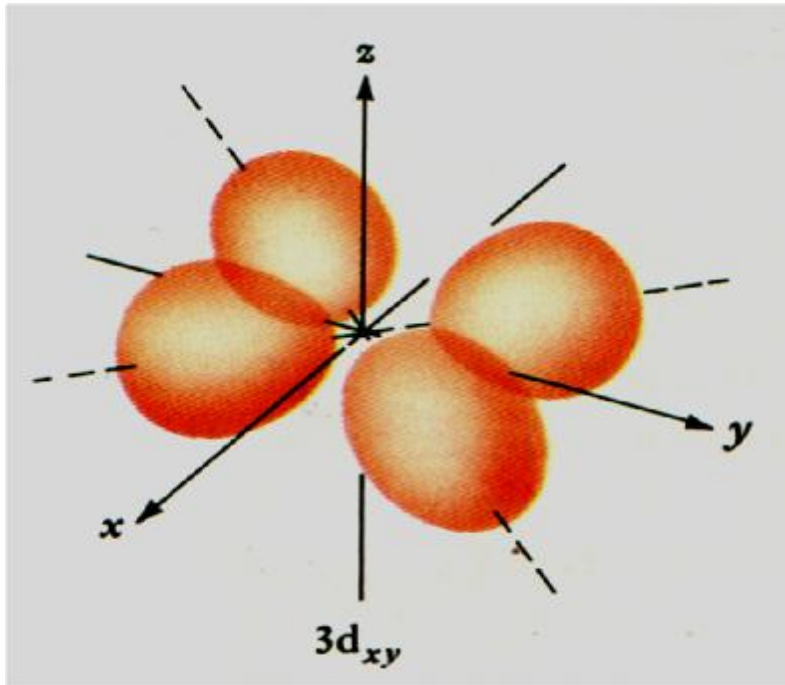
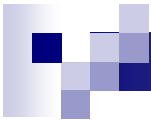
The shapes of atomic orbitals

s - orbital

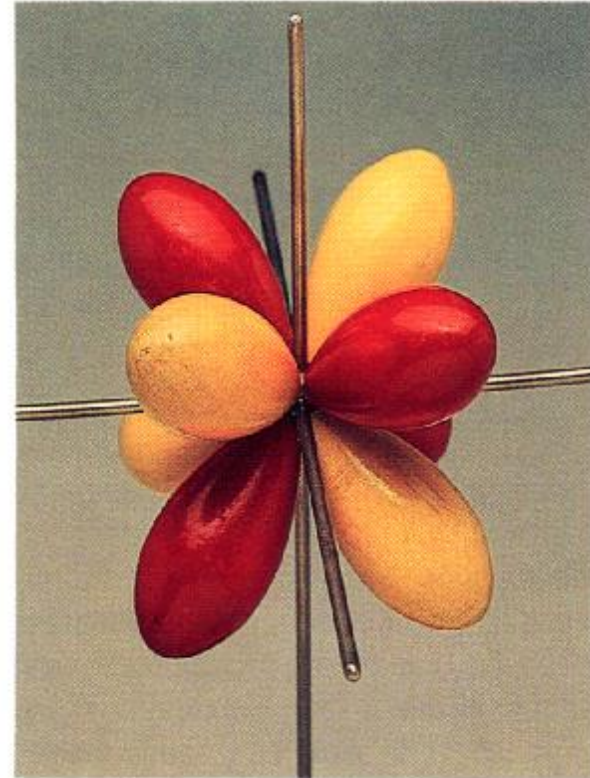
- the surface of the sphere within which the electron is found 90% of the time



p - orbital



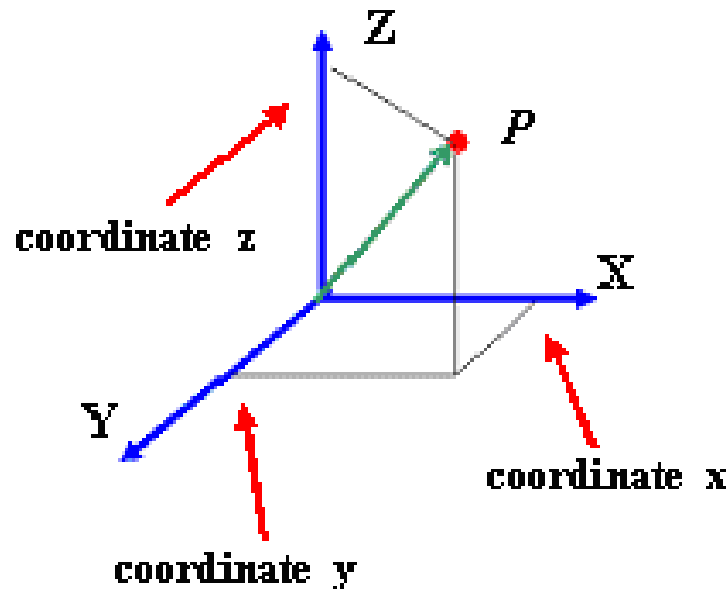
d - orbital




d - orbital

The quantum numbers

- n In a three-dimensional world, three parameters are required to describe the location of an object in space
- n The position of a point **P** in space can be specified by giving the **x**, **y**, and **z** coordinates





For the atomic electron, this requirement leads to the existence of three quantum numbers:

n , l , and m_l ,

which define **an orbital by giving the electron shell,**

the subshell,

and **the orbital within that subshell**

- 
- n ***The principal quantum number n can have any integer value from 1 to infinity:***

$$n = 1, 2, 3...$$

- n **It is the most important quantum number because its value determines **the total energy** of the electron**

- n **The value of n also gives a measure of the most probable distance of the electron from the nucleus:**

the greater the value of n , than the electron is found further from the nucleus




The angular momentum quantum number ℓ

- ℓ is related to the shape of electron orbitals, and
- the number of values of ℓ states how many different orbital types or electron subshells there are in a particular electron shell

ℓ , the angular momentum quantum number = $0, 1, 2, \dots, (n - 1)$

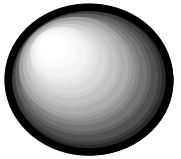

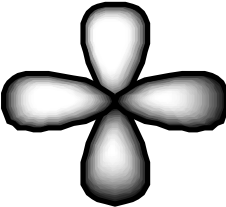
If n is 1, then there is only **one ℓ value** possible; ℓ can only be 0, and there can only be **one type of the orbital or subshell** in the $n = 1$ electron shell



n The values of the ℓ quantum number are usually coded by a letter:

Value of ℓ	Corresponding orbital label
0	s
1	p
2	d
3	f

For example, a subshell with a label of $\ell = 1$ is called a “p subshell,” and an orbital found in that subshell is called a “p orbital”

<i>l</i>	0	1	2	3	4
orbital label	s	p	d	f	g
The shapes of atomic orbitals					

$$E_s < E_p < E_d < E_f \dots$$



Magnetic quantum number, m_ℓ

n The number of m_ℓ values = the number of orbitals in a subshell

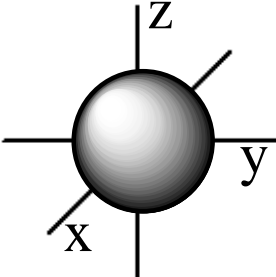
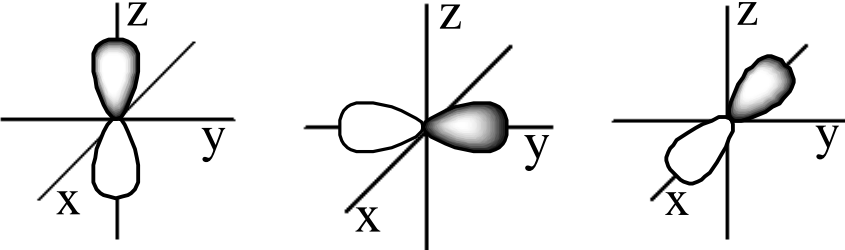
n m_ℓ values can range from $+\ell$ to $-\ell$ with 0 included:

$$m_\ell = 0, \pm 1, \pm 2, \pm 3, \dots \pm \ell$$

For example, when $\ell = 2$, m_ℓ has the five values

$$+2, +1, 0, -1, -2$$

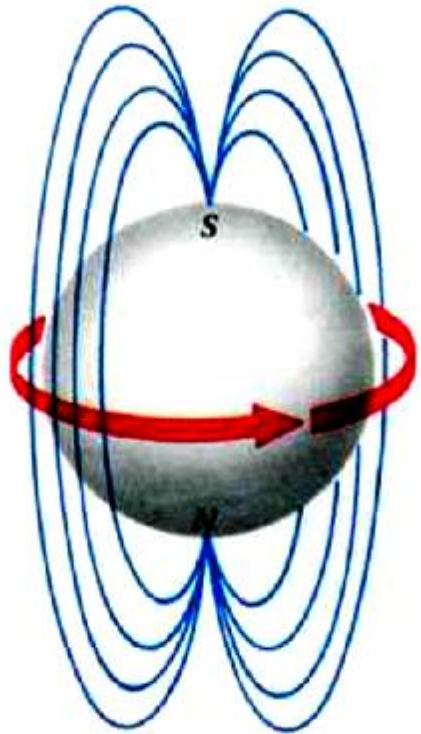
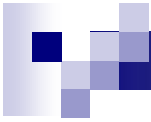
n m_ℓ is related to the spatial orientation of an orbital in a given subshell

l	m_l	The total number of AO on subshell = $= (2l+1)$	The direction in space
0 (s)	0	<input type="checkbox"/>	
1 (p)	-1 0 +1	<input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	
2 (d)	-2;-1; 0; +1;+2	<input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	complex
3 (f)	-3;-2;-1;0; +1;+2;+3	<input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>	complex




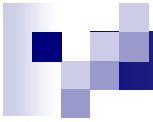
Electron spin

- n Experiments show that electrons behave like magnets, as a result of a property called *spin*
- n This spin is much like that of the earth spinning on its axis



Since the electron is electrically charged, the spinning charge generates a magnetic field with north and south magnetic poles

- 
- n There are only two possible orientations of an electron in a magnetic field, one associated with a spin quantum number, m_s , of $+1/2$ and the other with an m_s value of $-1/2$

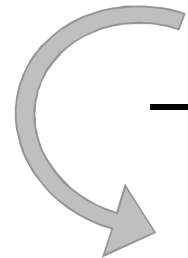
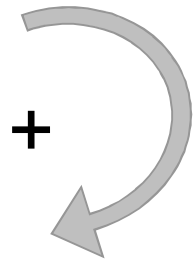


$m_s -$

to spin

$$m_s = +1/2$$

$$m_s = -1/2$$






Electron Configurations of Elements

- n The four quantum numbers lead to a complete description of an electron

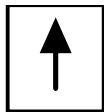


n If we consider the 1s orbital of the H atom, this orbital is defined by the set of quantum numbers:

$$n = 1, \ell = 0 \text{ and } m_\ell = 0$$

- 
- n If this orbital has an electron, the electron spin direction must also be specified
 - n The orbital is shown as a "box," and the electron spin is depicted by an arrow:

Electron in 1s orbital



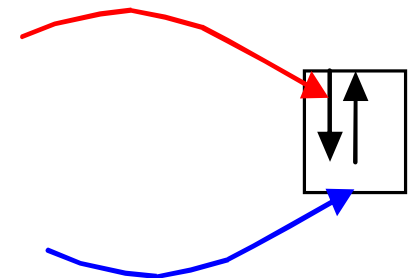
Quantum Number Set


$$n = 1, \ell = 0, m_{\ell} = 0, m_s = +1/2$$

n Two electrons in the 1s orbital of He atom:

this electron has $n = 1, \ell = 0, m_\ell = 0, m_s = -1/2$

this electron has $n = 1, \ell = 0, m_\ell = 0, m_s = +1/2$





n There are rules to help determine which values of the quantum numbers represent the most stable arrangement of electrons in an atom:

- .. The Pauli exclusion principle**
- .. The principle of the minimum of an orbital energy**
- .. The Klechkovski's rule**
- .. The Hund's rule**



The Pauli exclusion principle

n **Wolfgang Pauli, in 1925**

n **Principle:**

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

n This principle leads to yet another important conclusion, that *no atomic orbital can be assigned to (or "contain") more than two electrons*

n The Pauli exclusion principle limits the number of electrons in an orbital



The principle of the minimum of an orbital energy

n Principle:

Each successive electron is placed in the most stable orbital

n Principle determines the order in which the electrons are “added” to the orbitals in determining the ground state configuration

n Electrons are usually assigned in order of increasing orbital energy



The Klechkovski's rule


n Orbital energies of many-electron atoms depend on both n and ℓ

n *The $(n+\ell)$ rule:*

Electrons are assigned first to orbital of lower $(n + \ell)$, for two orbitals of the same $(n+\ell)$, electrons are assigned first to orbital of lower n

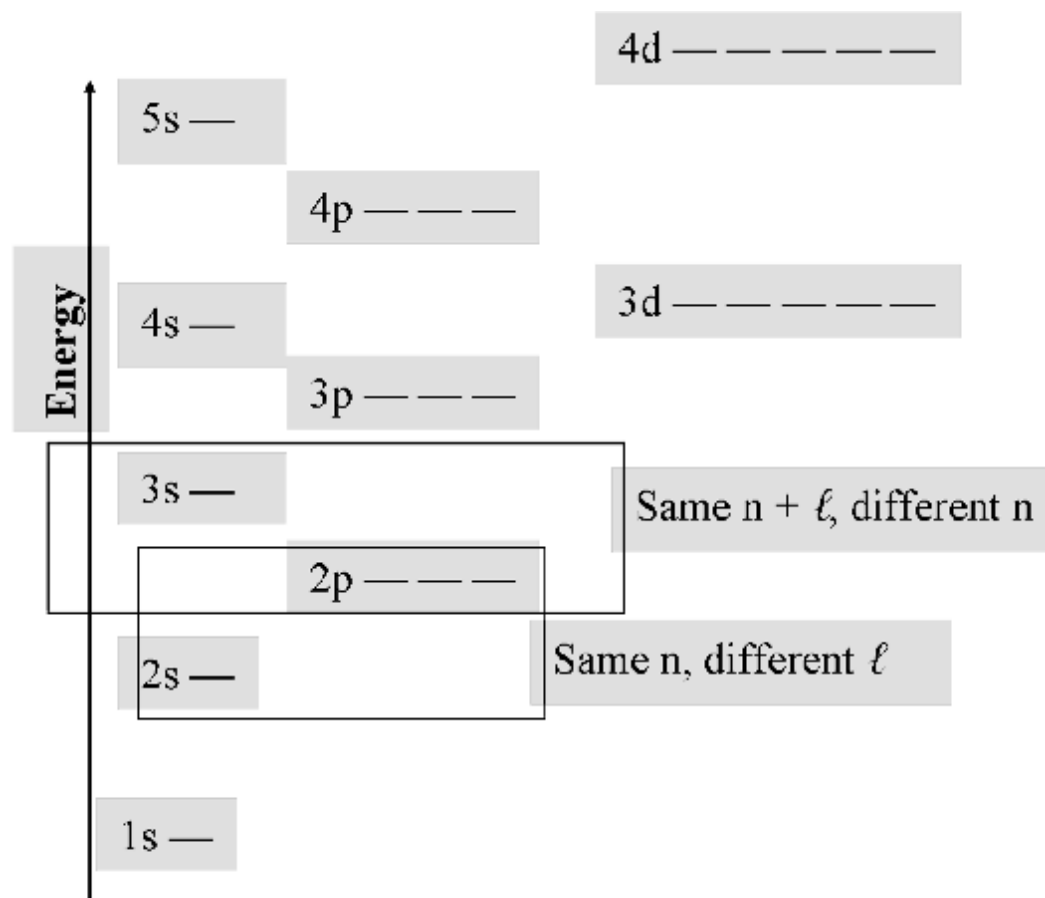
$$3d: (n+\ell) = 3+2 = 5$$

$$4s: (n+\ell) = 4+0 = 4$$



orbitals	n	ℓ	$n+\ell$
1s	1	0	1
2s	2	0	2
2p	2	1	3
3s	3	0	3
3p	3	1	4
3d	3	2	5
4s	4	0	4
4p	4	1	5
4d	4	2	6
4f	4	3	7
5s	5	0	5

n The following diagram is helpful in determining the order of filling orbitals (their relative energy)

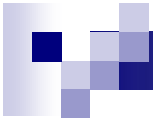


1s-2s-2p-3s-3p-4s-3d-4p-5s-4d-5p-6s-4f-5d-6p



The Hund's rule

- n The most stable arrangement of electrons is that with the maximum number of *unpaired electrons*, all with the same spin direction
- n When electrons are assigned to p, d, or f orbitals, each electron is assigned a different orbital of the subshell
- n This proceeds until the subshell is *half full*, after which *pairs of electrons* must be assigned a common orbital



p_x p_y p_z

#	#	#
---	---	---

$+1/2 + 1/2 + 1/2$

$S_{spin} = 3/2$

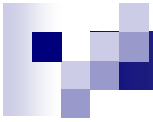
p_x p_y p_z

\$	\$	\$
----	----	----

$-1/2 - 1/2 - 1/2$

$S_{spin} = 3/2$

possible



p_x	p_y	p_z
\$	#	\$

$$-1/2 + 1/2 - 1/2$$

$$\Sigma s_{\text{pin}} = 1/2$$

p_x	p_y	p_z
E	#	

$$-1/2 + 1/2 + 1/2$$

$$S_{\text{spin}} = 1/2$$

impossible



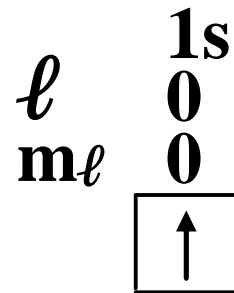
Electron configurations of the main group elements

n The order of assignment electrons to
orbitals:

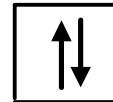
**1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d
6p**

- The first two electrons must be assigned to the 1s orbital – *H, He*

H 1s¹




He 1s²



- The third electron must use the $n = 2$ shell
- According to the order of assignment , that electron must be assigned to the 2s orbital - *Li*

	1s	2s	2p	
l	0	0	1	
m_l	0	0	+1 0 -1	
Li	$\boxed{\uparrow\downarrow}$	$\boxed{\uparrow}$	$\boxed{} \boxed{} \boxed{}$	$1s^2 2s^1$

	1s	2s	2p	
l	0	0	1	
m_l	0	0	+1 0 -1	
Li	$\uparrow\downarrow$	\uparrow	$\square \square \square$	$1s^2 2s^1$
Be	$\uparrow\downarrow$	$\uparrow\downarrow$	$\square \square \square$	$1s^2 2s^2$

- 
- n The position of an atom in the periodic table tells you its configuration immediately
 - n All the elements of Group 1A (H, Li, Na, K, Rb, Cs, Fr) have one electron assigned to an s orbital of the nth shell, where n is the number of the period in which the element is found



	1s	2s	2p
Li $1s^2 2s^1$	$\boxed{\uparrow\downarrow}$	$\boxed{\uparrow}$	$\boxed{}\boxed{}\boxed{}$
Be $1s^2 2s^2$	$\boxed{\uparrow\downarrow}$	$\boxed{\uparrow\downarrow}$	$\boxed{}\boxed{}\boxed{}$

n The configuration of Be $1s^2 2s^2$

n All elements of Group 2A (Be, Mg, Ca, Sr, Ba, Ra) have electron configurations:

preceding rare gas + ns^2 ,

where n is the period in which the element is found in the periodic table



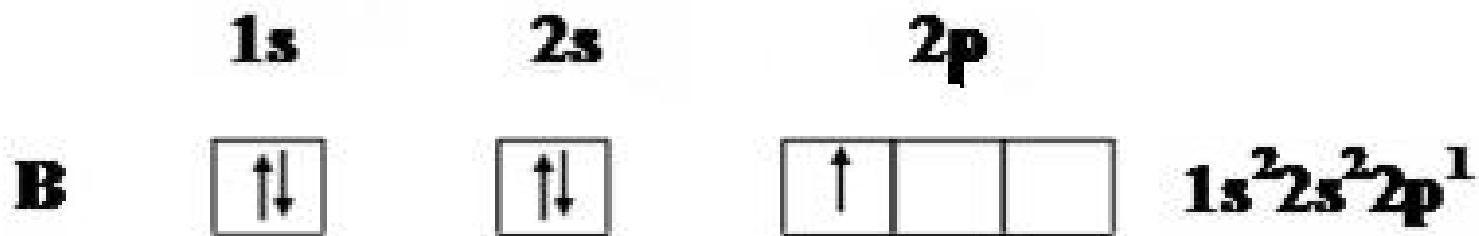
ПЕРИОДИЧЕСКАЯ СИСТЕМА ХИМИЧЕСКИХ ЭЛЕМЕНТОВ Д. И. МЕНДЕЛЕЕВА

Свойства атомов химических элементов, а также состав и свойства их соединений находятся в периодической зависимости от заряда атомных ядер

I A												VIII A							
1												18							
1	1,00794 1 H ВОДОРОД -1 1											4,00260 2 He ГЕЛИЙ							
2	6,941 3 Li ЛИТИЙ 1	II A												10 Ne НЕОН					
		2												9 F ФТОР -1					
3	22,9898 11 Na НАТРИЙ 1	12 Mg МАГНИЙ 2												18 Ar АРГОН					
														17 Cl ХЛОР -1 3 5 7					
4	39,0983 19 K КАЛИЙ 1	40,078 20 Ca КАЛЬЦИЙ 2		III B	IV B	V B	VI B	VII B	VIII B		I B	II B	13 Al АЛЮМИНИЙ 3	14 Si КРЕМНИЙ -4 2 4	15 P ФОСФОР -3 3 5	16 S СЕРА -2 4 6	17 Cl ХЛОР -1 3 5 7	18 Ar АРГОН	
				3	4	5	6	7	8	9	10	11	12	3	4	5	6	7	8
5	85,4678 37 Rb РУБИДИЙ 1	87,62 38 Sr СТРОНЦИЙ 2		44,9559 21 Sc СКАНДИЙ 3	47,867 22 Ti ТИТАН 2 3 4	50,9415 23 V ВАНАДИЙ 2 3 4 5	51,9961 24 Cr ХРОМ 2 3 4 6	54,9380 25 Mn МАРГАНЕЦ 2 3 4 6 7	55,845 26 Fe ЖЕЛЕЗО 2 3 6	58,9332 27 Co КОБАЛЬТ 2 3	58,6934 28 Ni НИКЕЛЬ 2 3	63,546 29 Cu МЕДЬ 1 2 3	65,38 30 Zn ЦИНК 2	69,723 31 Ga ГАЛЛИЙ 3	72,64 32 Ge ГЕРМАНИЙ 2 4	74,9216 33 As МЫШЬЯК -3 3 5	78,96 34 Se СЕЛЕН -2 4 6	79,904 35 Br БРОМ -1 1 3 5 7	83,798 36 Kr КРИПТОН 2 4
6	132,905 55 Cs ЦЕЗИЙ 1	137,327 56 Ba БАРИЙ 2		88,9058 39 Y ИТТРИЙ 3	91,224 40 Zr ЦИРКОНИЙ 3 4	92,9064 41 Nb НИОБИЙ 2 3 4 5	95,96 42 Mo МОЛИБДЕН 2 3 4 6	[98] 43 Tc ТЕХНЕЦИЙ 2 4 6 7	101,07 44 Ru РУТЕНИЙ 2 3 4 6 7 8	102,905 45 Rh РОДИЙ 2 3 4 6	106,42 46 Pd ПАЛЛАДИЙ 2 4	107,868 47 Ag СЕРЕБРО 1 2 3	112,411 48 Cd КАДМИЙ 2	114,818 49 In ИНДИЙ 3	118,710 50 Sn ОЛОВО 2 4	121,760 51 Sb СУРЬМА -3 3 5	127,60 52 Te ТЕЛЛУР -2 4 6	126,904 53 I ИОД -1 1 3 5 7	131,293 54 Xe КСЕНОН 2 4 6 8
				3	3 4	2 3 4 5	2 3 4 6	2 3 4 6 7	2 3 4 5 6 7 8	2 3 4 5 6	2 4 5 6	1 2 3	2	3	2 4	-3 3 5	-2 4 6	-1 1 3 5 7	2 4 6 8
7	[223] 87 Fr ФРАНЦИЙ 1	[226] 88 Ra РАДИЙ 2		174,967 71 Lu ЛЮТЕЦИЙ 3	178,49 72 Hf ГАФНИЙ 3 4	180,948 73 Ta ТАНТАЛ 2 3 4 5	183,84 74 W ВОЛЬФРАМ 2 3 4 6	186,207 75 Re РЕНИЙ 2 3 4 6 7	190,23 76 Os ОСМИЙ 2 3 4 5 6 8	192,217 77 Ir ИРИДИЙ 2 3 4 5 6	195,084 78 Pt ПЛАТИНА 2 4 5 6	196,967 79 Au ЗОЛОТО 1 3	200,59 80 Hg РУТУТЬ 1 2	204,383 81 Tl ТАЛЛИЙ 1 3	207,2 82 Pb СВИНЕЦ 2 4	208,980 83 Bi ВИСМУТ -3 3 5	[209] 84 Po ПОЛОНИЙ -2 2 4 6	[210] 85 At АСТАТ -1 1 5	[222] 86 Rn РАДОН 2 4 6
				3	3 4	2 3 4 5	2 3 4 6	2 3 4 6 7	2 3 4 5 6 8	2 3 4 5 6	2 4 5 6	1 3	1 2	1 3	2 4	-3 3 5	-2 2 4 6	-1 1 5	2 4 6
				[262] 103 Lr ЛОУРЕНСИЙ 3	[267] 104 Rf РЕЗЕРФОРДИЙ 4	[270] 105 Db ДУБНИЙ 5	[271] 106 Sg СИБОРГИЙ 6	[274] 107 Bh БОРИЙ 7	[277] 108 Hs ХАССИЙ 8	[278] 109 Mt МЕЙТНЕРИЙ	[281] 110 Ds ДАРМШТАДИЙ	[281] 111 Rg РЕНТГЕНИЙ	[285] 112 Cn КОПЕРНИЙ	[286] 113 Uut	[289] 114 Uuq	[289] 115 Uup	[293] 116 Uuh	[294] 117 Uus	[294] 118 Uuo

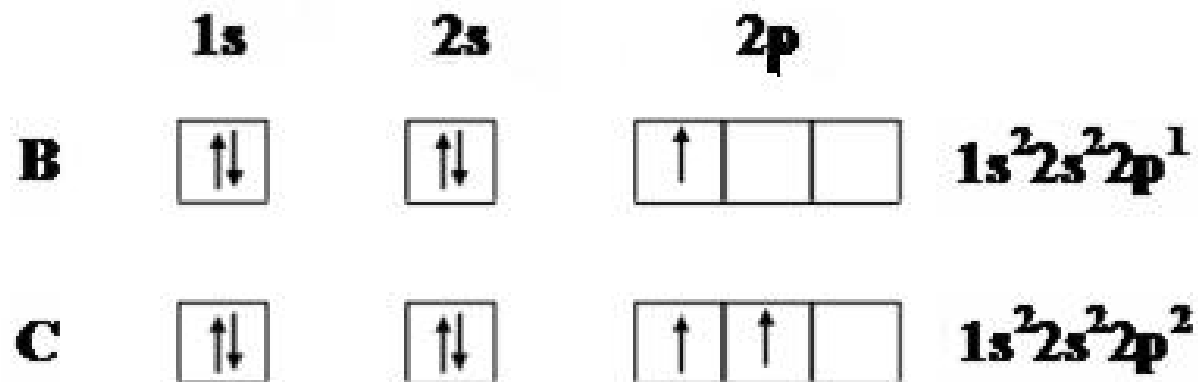
* ЛАНТАНОИДЫ	138,905 57 La ЛАНТАН 3	140,116 58 Ce ЦЕРИЙ 3 4	140,908 59 Pr ПРАЗЕДИМ 2 3 4	144,242 60 Nd НЕОДИМ 2 3 4	[145] 61 Pm ПРОМЕТИЙ 3	150,36 62 Sm САМАРИЙ 2 3	151,964 63 Eu ЕВРОПИЙ 2 3	157,25 64 Gd ГАДОЛИНИЙ 3	158,925 65 Tb ТЕРБИЙ 3 4	162,500 66 Dy ДИСПРОЗИЙ 3 4	164,930 67 Ho ГОЛЬМИЙ 3	167,259 68 Er ЭРБИЙ 3	168,934 69 Tm ТУЛИЙ 2 3	173,054 70 Yb ИТТЕРБИЙ 2 3
** АКТИНОИДЫ	[227] 89 Ac АКТИНИЙ 3	232,038 90 Th ТОРИЙ 2 3 4	231,036 91 Pa ПРОТАКТИНИЙ 3 4 5	238,029 92 U УРАН 3 4 5 6	[237] 93 Np НЕПТУНИЙ 3 4 5 6 7	[244] 94 Pu ПЛУТОНИЙ 3 4 5 6 7	[243] 95 Am АМЕРИЦИЙ 2 3 4 5 6	[247] 96 Cm КЮРИЙ 2 3 4 6	[247] 97 Bk БЕРКЛИЙ 2 3 4	[251] 98 Cf КАЛИФОРНИЙ 2 3 4	[252] 99 Es ЭЙНШТЕЙНИЙ 2 3	[257] 100 Fm ФЕРМИЙ 2 3	[258] 101 Md МЕНДЕЛЕВИЙ 1 2 3	[259] 102 No НОБЕЛИЙ 2 3

- n Boron (Group 3A) is the first element in the p block of elements on the right side of the periodic table
- n The fifth electron must be assigned to a 2p orbital (since the 1s and 2s orbitals are filled in a boron atom)



n Carbon (**Group 4A**) is the second element in the p block, so there is a second electron assigned to the 2p orbitals

n The configuration of ${}_6\text{C}$: **$1s^2 2s^2 2p^2$**



	1s	2s	2p	
B	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \square \square	$1s^2 2s^2 2p^1$
C	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \uparrow \square	$1s^2 2s^2 2p^2$
N	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \uparrow \uparrow	$1s^2 2s^2 2p^3$
O	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ \uparrow \uparrow	$1s^2 2s^2 2p^4$
F	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow	$1s^2 2s^2 2p^5$
Ne	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	$1s^2 2s^2 2p^6$

All the elements
from Group 3A
through Group 8A
are characterized
by electrons
assigned to
p-orbitals

These elements are called the *p-block* elements,
all have the general configuration
preceding rare gas + ns²np^x
where **x** = group number

I A												VIII A																							
1												18																							
1,00794 H ВОДОРОД 1 1												4,00260 2 He ГЕЛИЙ																							
II A												III A																							
2												13																							
6,941 Li ЛИТИЙ 1 1		9,01218 4 Be БЕРИЛЛИЙ 2 2												10,811 5 B БОР -3 3		12,0107 6 C УГЛЕРОД -4 2 4		14,0067 7 N АЗОТ -3 2 3 4 5		15,9994 8 O КИСЛОРОД -2 -1 2		18,9984 9 F ФТОР -1		20,1797 10 Ne НЕОН											
22,9898 Na НАТРИЙ 1 1		24,3050 12 Mg МАГНИЙ 2 2		III B		IV B		V B		VI B		VII B		VIII B		I B		II B		26,9815 13 Al АЛЮМИНИЙ 3 3		28,0855 14 Si КРЕМНИЙ -4 2 4		30,9738 15 P ФОСФОР -3 3 5		32,065 16 S СЕРА -2 4 6		35,453 17 Cl ХЛОР -1 1 3 5 7		39,948 18 Ar АРГОН					
39,0983 19 K КАЛИЙ 1 1		40,078 20 Ca КАЛЬЦИЙ 2 2		3		4		5		6		7		8		9		10		11		12		69,723 31 Ga ГАЛЛИЙ 3 3		72,64 32 Ge ГЕРМАНИЙ 2 4		74,9216 33 As МЬШЬЯК -3 3 5		78,96 34 Se СЕЛЕН -2 4 6		79,904 35 Br БРОМ -1 1 3 5 7		83,798 36 Kr КРИПТОН 2 4	
				44,9559 21 Sc СКАНДИЙ 3 3		47,867 22 Ti ТИТАН 2 3 4		50,9415 23 V ВАНАДИЙ 2 3 4 5		51,9961 24 Cr ХРОМ 2 3 4 6		54,9380 25 Mn МАРГАНЕЦ 2 3 4 6 7		55,845 26 Fe ЖЕЛЕЗО 2 3 6		58,9332 27 Co КОБАЛЬТ 2 3		58,6934 28 Ni НИКЕЛЬ 2 3		63,546 29 Cu МЕДЬ 1 2 3		65,38 30 Zn ЦИНК 2 2													

n The periodic table indicates that the next element is potassium $_{11}\text{Na } 1s^2 2s^2 2p^2 3s^1$

n The 3s and 3p subshells are filled at argon - $_{18}\text{Ar}$



Electron configurations of the transition elements

n **Potassium** $_{19}\text{K}$ is the first element of the fourth period, so potassium has the electron configuration of the element preceding it in the table (Ar) plus a final electron assigned to the 4s orbital:



n **Calcium** $_{20}\text{Ca}$ $[\text{Ar}] 4s^2$

3d- orbitals are free in K and Ca



n After 4s orbital , the 3d orbitals are filled

$$3d: (n+l) = 3+2 = 5$$





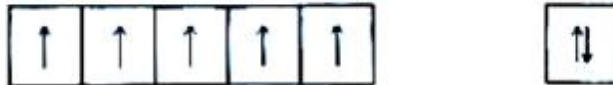
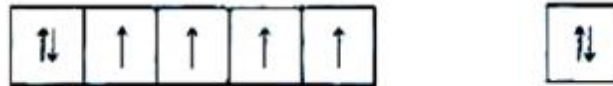



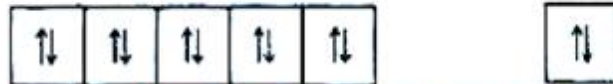
$$4s: (n+l) = 4+0 = 4$$

n **Scandium** $_{21}\text{Sc}$ has the configuration
[Ar] 4s²3d¹

n **Titanium** $_{22}\text{Ti}$ follows with *[Ar] 4s²3d²*

n **and vanadium** $_{23}\text{V}$ with *[Ar] 4s²3d³*

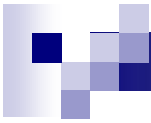
Orbital Box Diagrams for the Transition Elements Sc - Zn

Sc	[Ar] $3d^14s^2$	
Ti	[Ar] $3d^24s^2$	
V	[Ar] $3d^34s^2$	
Cr*	[Ar] $3d^54s^1$	
Mn	[Ar] $3d^54s^2$	
Fe	[Ar] $3d^64s^2$	
Co	[Ar] $3d^74s^2$	
Ni	[Ar] $3d^84s^2$	
Cu*	[Ar] $3d^{10}4s^1$	
Zn	[Ar] $3d^{10}4s^2$	

• **Chromium $_{24}\text{Cr}$** has an anomaly in the order of orbital assignment

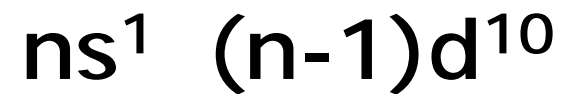
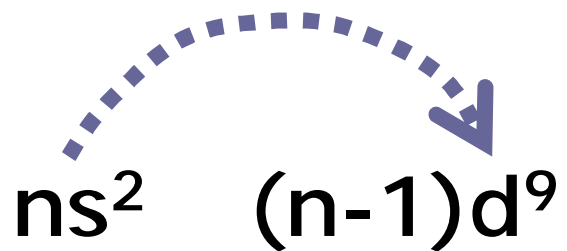
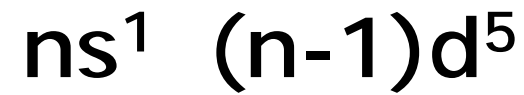
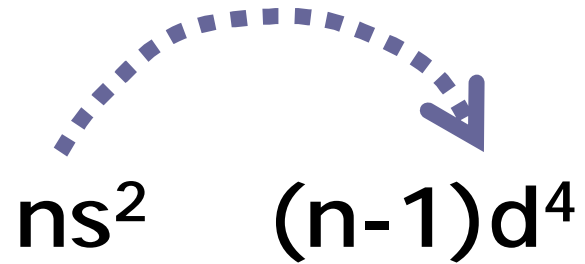
• $_{24}\text{Cr}$ has one electron assigned to each of the six available 4s and 3d orbitals

• The minimization of electron-electron repulsions



Excited state of the atom

Stable state of the atom





	Excited state of the atom	Stable state of the atom
Cr	$4s^2 3d^4$	$4s^1 3d^5$
Mo	$5s^2 4d^4$	$5s^1 4d^5$
Cu	$4s^2 3d^9$	$4s^1 3d^{10}$
Ag	$5s^2 4d^9$	$5s^1 4d^{10}$
Au	$6s^2 5d^9$	$6s^1 5d^{10}$



The Periodic Table

Atomic Properties and Periodic Trends



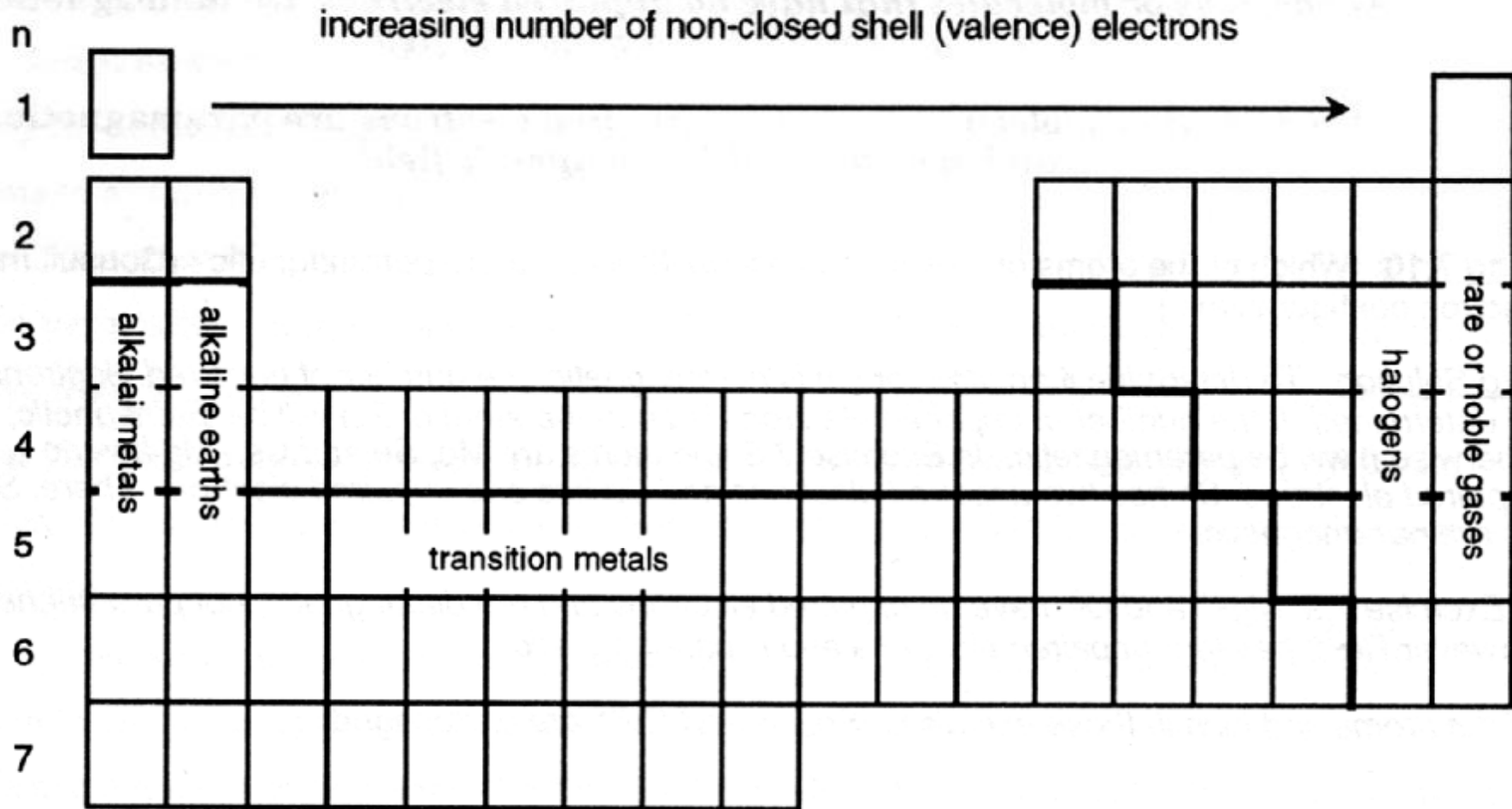
- n Elements with **similar chemical properties** are arranged vertically in columns
- n **The electron configuration** of the non-closed shell (highest-energy) electrons **is the same** in each column

	I A		
	1		
1	1,00794 1 H ВОДОРОД -1 1		II A 2
2	6,941 3 Li ЛИТИЙ 1	9,01218 4 Be БЕРИЛЛИЙ 2	
3	22,9898 11 Na НАТРИЙ 1	24,3050 12 Mg МАГНИЙ 2	
4	39,0983 19 K КАЛИЙ 1	40,078 20 Ca КАЛЬЦИЙ 2	
5	85,4678 37 Rb РУБИДИЙ 1	87,62 38 Sr СТРОНЦИЙ 2	
6	132,905 55 Cs ЦЕЗИЙ 1	137,327 56 Ba БАРИЙ 2	
7	[223] 87 Fr ФРАНЦИЙ 1	[226] 88 Ra РАДИЙ 2	

- n Sodium, lithium, potassium and the other alkali metals all share the ns^1 electron configuration above the closed shell configuration
- n These electrons are the highest in energy and the furthest away from the nucleus and are the electrons that participate in the formation of bonds with other atoms
- n These electrons are called **valence electrons**



n The similar electron configuration is the reason of similar chemical properties



- The number of valence electrons increases in each row

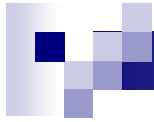


- n Moving from left to right across a row in the periodic table, n remains constant, but Z increases
- n The valence electrons feel a stronger attraction to the nucleus




Atomic size

- n Atomic size is determined by the volume occupied by the electrons, which in turn is determined by the sizes of the orbitals
- n A measure of atomic size is **the atomic radius** which is defined as one half the distance between the nuclei in a substance containing identical atoms




n For the main group elements, atomic radii increase going down a group in the periodic table and decrease going across a period



n Moving left to right in a row (n is constant, increasing number of valence electrons):

**Orbitals become smaller
and more stable**



n As we move down a column in the periodic table, both Z and n increase

n Moving down a group (increasing n , same number of valence electrons):

Orbitals become larger and less stable

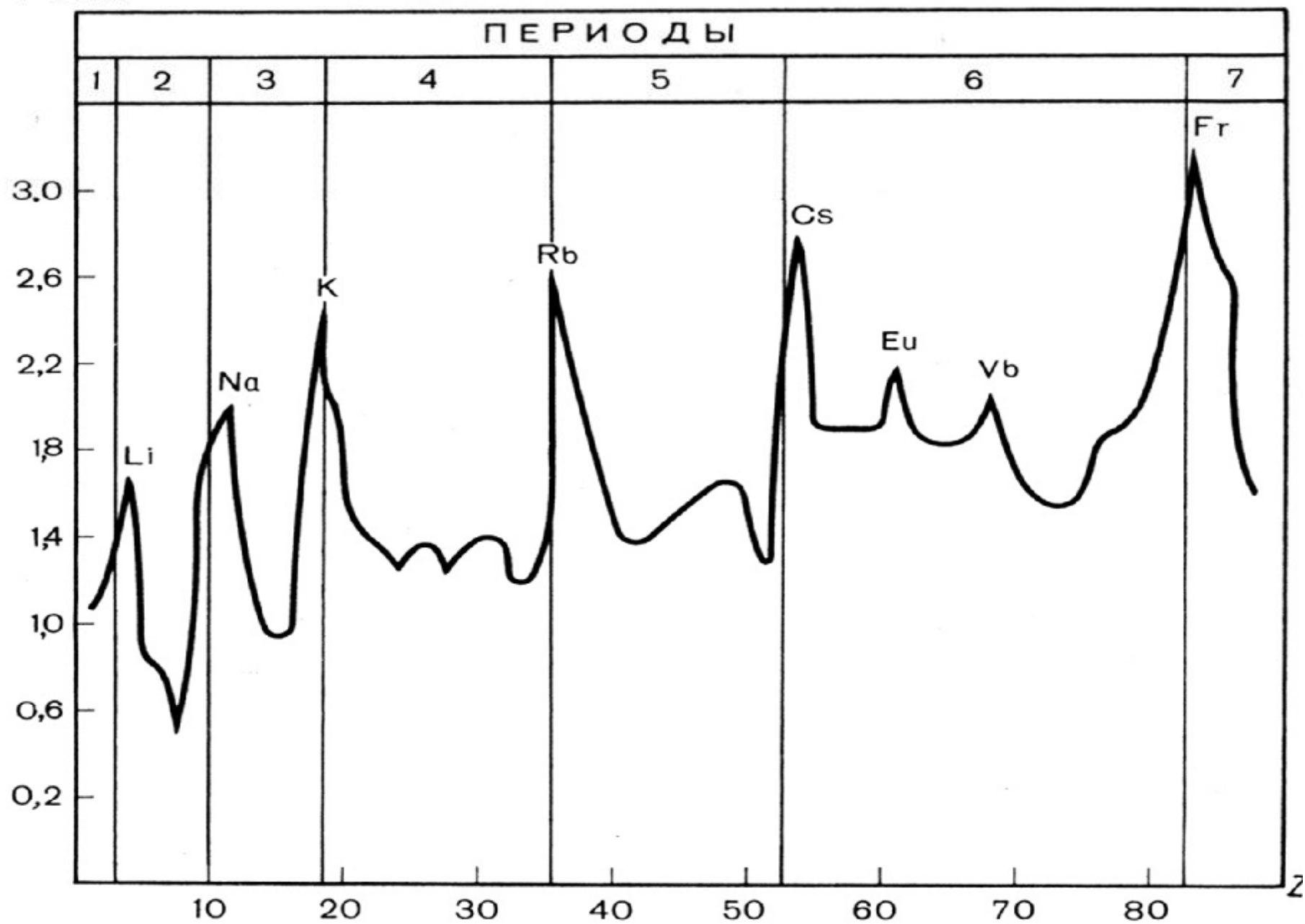


n The atomic radius changes as predicted by the trends in orbital size:

Moving down a group, atoms become larger

Moving left to right in a row, atoms become smaller

г · 10 нм





Ionization energy

- n The ionization energy of an atom is the energy required to remove electron from an atom or ion in the gas phase:



- n The process is endothermic



n Each atom can have a series of ionization energies, since more than one electron can be removed (except for H)

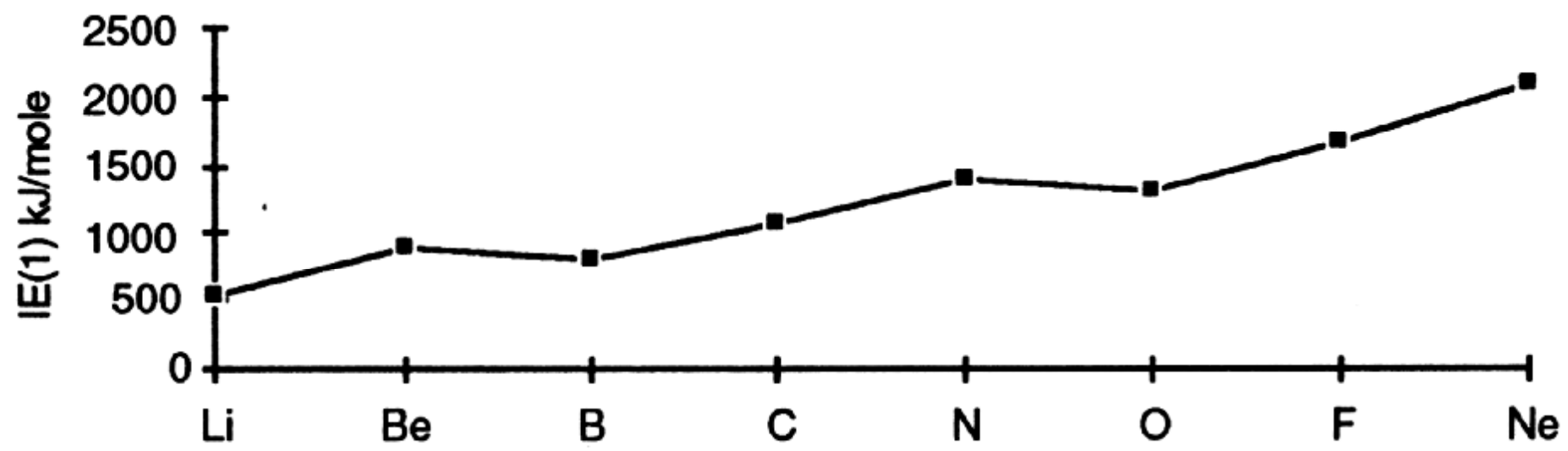
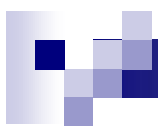
n For example, the first three ionization energies of Mg are:

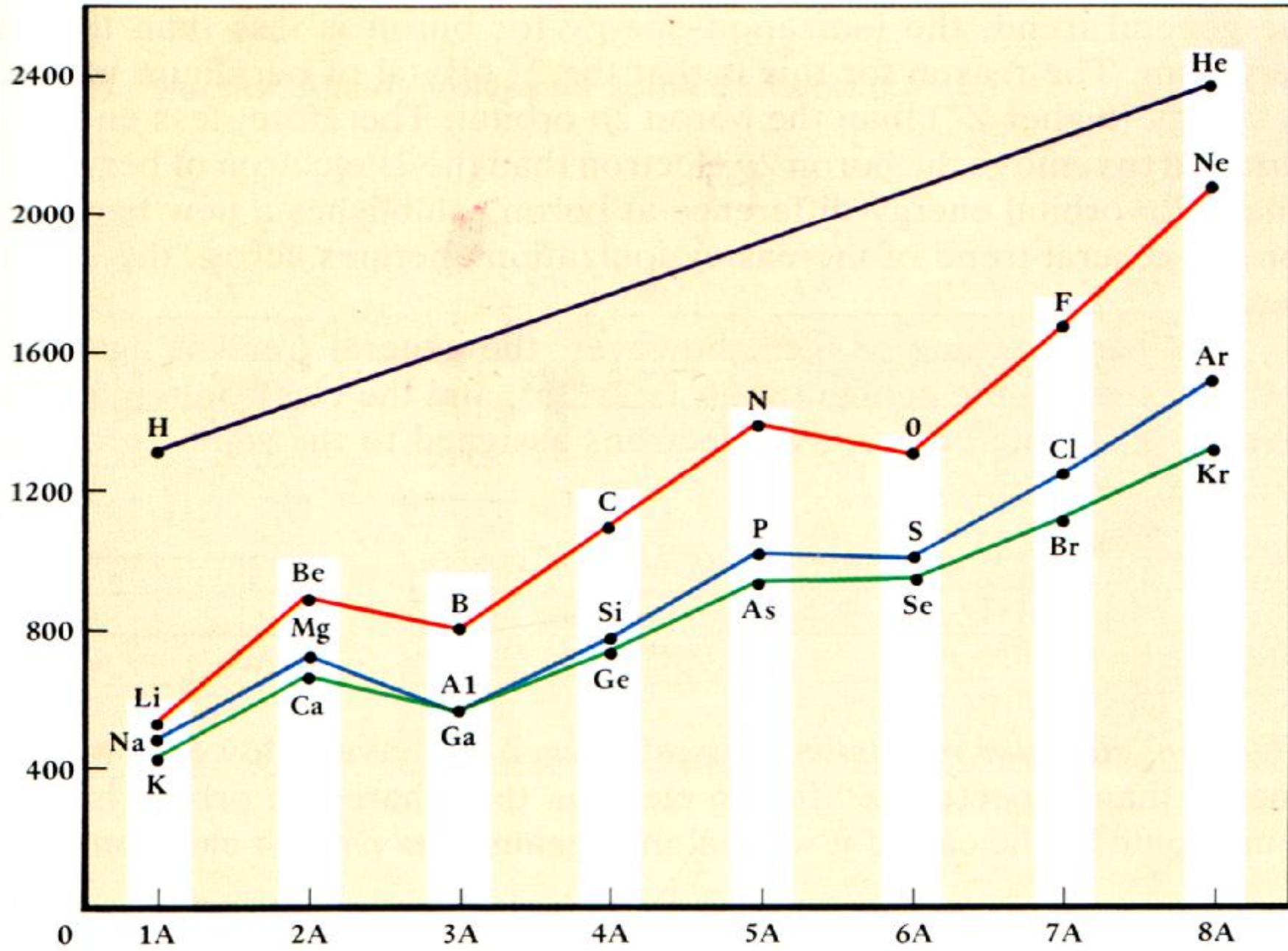
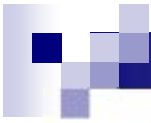




n The first ionization energy:

- *increases from left to right across a row*
- *decreases from top to bottom down a column*







n The reason for this trend is the same as for the trends observed in atomic radius:

they reflect the increasing stability from left to right and decreasing stability going down a column of atomic orbitals



Electron affinity

- n A measure of the electron affinity of an element is the energy involved when an electron is brought from an infinite distance away up to an atom and absorbed by it to form an ion



$\Delta E = \text{electron affinity (EA)}$

- n The process is exothermic



n The electron affinity:

- *increases from left to right across a row*
- *decreases from top to bottom down a column*

