Inorganic Pharmaceutical Chemistry

Reference text:-

1- Inorganic Medicinal and Pharmaceutical Chemistry by Block ,Roche Soine and Wilson

2- Textbook of Organic Medicinal and pharmaceutical Chemistry by Wilson and Gisvold

Course Coverage

Atomic and Molecular Structure

1-Structure of the Atom

2-Atomic Number, Mass Number, & Isotopes

3-Classification of the Elements

4- Quantum Mechanics, Quantum Numbers

5- Electronic Configuration

6-Shielding

7-Atomic Radius, Ionic Radius, Ionization Energy, Electron Affinity, Electronegativity

8-Chemical bond

Course Coverage

Complexes

1- Orbital hybridization

2-Types of hybridization

3- Basic theory

- Valence bond theory

4- Rules for Naming Coordination Complexes

5- Ligand

Quiz 1/

Write chemical symbol for first ***10*** elements in proper locationon blank periodic table

Atomic Structure

Structure of the Atom

Composed of:

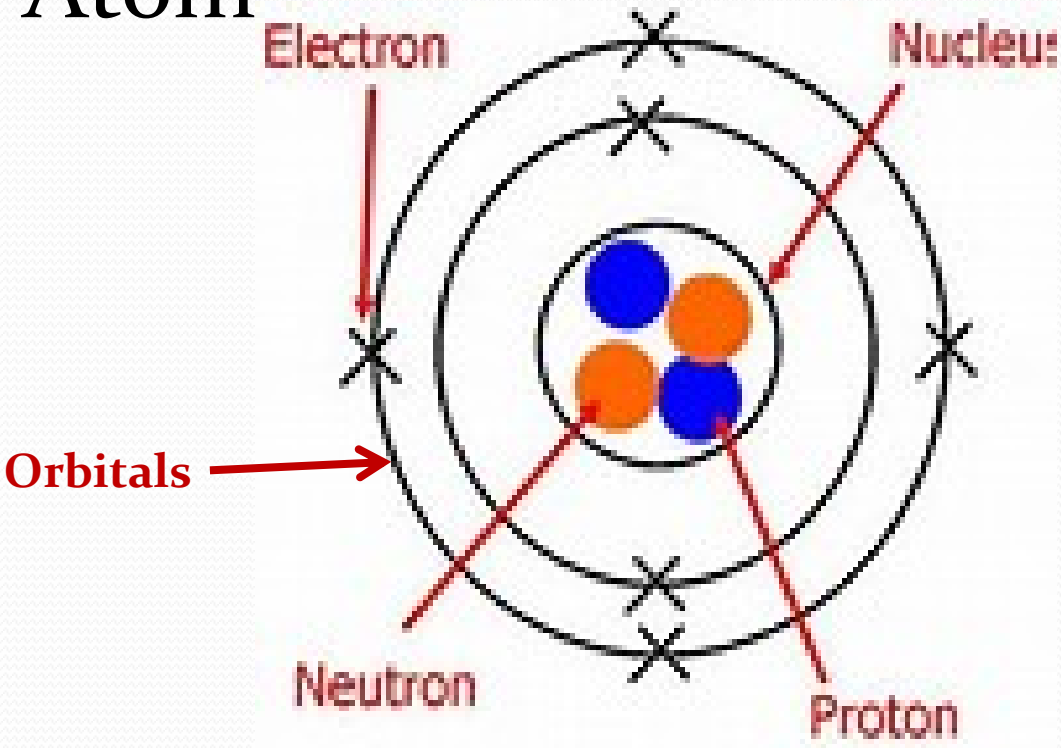
1- Nucleus

protons

Neutrons

2- Orbitals

electrons



protons

found in nucleus

relative charge of +1 , relative mass of 1.0073 amu

neutrons

found in nucleus

neutral charge , relative mass of 1.0087 amu

electrons

found in electron cloud

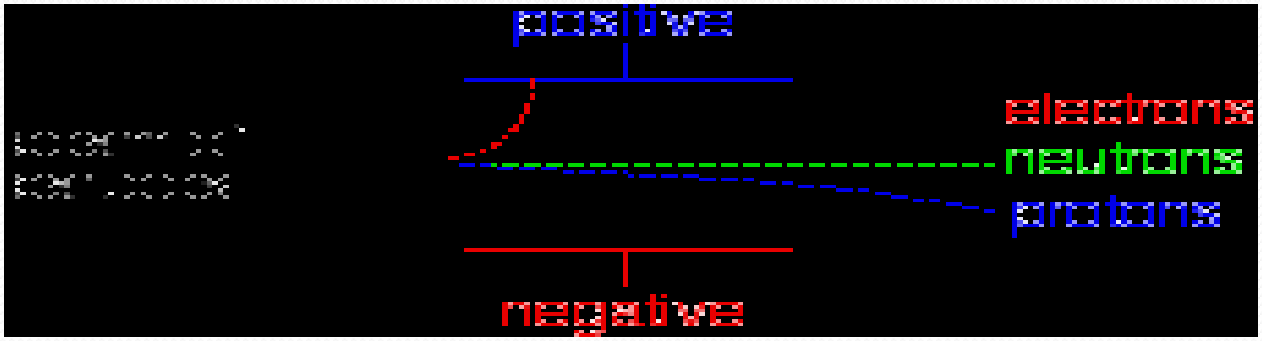
relative charge of -1 , relative mass of 0.00055 amu

Protons are positively charged and so would be deflected on a curving path towards the negative plate.

Electrons are negatively charged and so would be deflected on a curving path towards the positive plate.

Neutrons don't have a charge, and so would continue on in a straight line.

If beams of the three sorts of particles, all with the same speed, are passed between two electrically charged plates:



The nucleus

The nucleus is at the centre of the atom and contains the protons and neutrons. Protons and neutrons are collectively known as ***nucleons.***

Virtually all the mass of the atom is concentrated in the nucleus, because the electrons weigh so little.

Working out the numbers of protons and neutrons

No of protons = ATOMIC NUMBER of the atom

The atomic number is also given the more descriptive name of ***proton number.***

No of protons + no of neutrons = MASS NUMBER of the atom

The mass number is also called the ***nucleon number.***
This information can be given simply in the form:

Mass number 19

$^{19}_{9}F$

Atomic number 9

Atomic Number, Mass Number, & Isotopes

Atomic number, Z

the number of protons in the nucleus

the number of electrons in a neutral atom

the integer on the periodic table for each element

Mass Number, A

integer representing the ***approximate*** mass of an atom

equal to the sum of the number of protons and neutrons in the nucleus

Isotopes

atoms of the same element which differ in the number of neutrons in the nucleus

designated by mass number

Isotopes vs. Allotropes

Isotopes - atoms of the same element with different numbers of neutrons

- different compounds with the same formula

Allotropes - different forms of an element

Carbon exhibits both

Isotopes: C-12 C-13 C-14

Allotropes: graphite, diamond, and fullerenes

Isotopes :- The number of neutrons in an atom can vary within small limits. For example, there are three kinds of carbon atom 12C, 13C and 14C. They all have the same number of protons, but the number of neutrons varies

	Protons	neutrons	mass number
carbon-12	6	6	12
carbon-13	6	7	13
carbon-14	6	8	14

These different atoms of carbon are called ***isotopes***. The fact that they have varying numbers of neutrons makes no difference whatsoever to the chemical reactions of the carbon.

Isotopes are atoms which have the same atomic number but different mass numbers. They have the same number of protons but different numbers of neutrons

The electrons

Working out the number of electrons

Atoms are electrically neutral, and the positiveness of the protons is balanced by the negativeness of the electrons. It follows that in a neutral atom:

no of electrons = no of protons

So, if an oxygen atom (atomic number = 8) has 8 protons, it must also have 8 electrons; if a chlorine atom (atomic number = 17) has 17 protons, it must also have 17 electrons

In Summary…

For any element:

Number of Protons = Atomic Number

Number of Electrons = Number of Protons = Atomic Number

For krypton: Number of Neutrons = Mass Number - Atomic Number

Number of Protons = Atomic Number = 36

Number of Electrons = Number of Protons = Atomic Number = 36

Number of Neutrons = Mass Number - Atomic Number = 84 - 36 = 48

The Origin of the Elements

Nucleosynthesis of light elements

Nucleosynthesis of heavy elements

Hydrogen Burning

Hydrogen Burning (fusion)

$4\ {}^{1}H \rightarrow {}^{4}He + 2\ \text{positrons} + 2\ \text{neutrinos}$

$+ \ 2.5 \times 10^{6}\ \text{MJ/mol}$

after about 1/10 of hydrogen consumed, changes to helium burning

Classification of the Elements

Metals

- Lustrous, malleable, ductile, electrically conducting solids at room temperature

Nonmetals

- Often gases, liquids, or solids that do not conduct electricity appreciably

Metalloids

- Elements, alloys or compounds that possess some of the characteristics of metals and some of nonmetals

Classification of the Elements

- Metallic elements combine with nonmetallic elements to give compounds that are typically hard, non-volatile solids
- When combined with each other, the nonmetals often form volatile molecular compounds
- When metals combine (or simply mix together) they produce alloys that have most of the physical characteristics of metals

Development of Periodic Table

Dmitri Mendeleev - Russian

1869 - Periodic Law - allowed him to predict properties of unknown elements

Mendeleev's periodic table

Row	Group I — R_2O	Group II — RO	Group III — R_2O_3	Group IV RH_4 RO_2	Group V RH_3 R_2O_5	Group VI RH_2 RO_3	Group VII RH R_2O_7	Group VIII — RO_4
1	H = 1							
2	Li = 7	Be = 9.4	B = 11	C = 12	N = 14	O = 16	F = 19	
3	Na = 23	Mg = 24	Al = 27.3	Si = 28	P = 31	S = 32	Cl = 35.5	
4	K = 39	Ca = 40	___ = 44	Ti = 48	V = 51	Cr = 52	Mn = 55	Fe = 56, Co = 59, Ni = 59, Cu = 63
5	(Cu = 63)	Zn = 65	___ = 68	___ = 72	As = 75	Se = 78	Br = 80	
6	Rb = 83	Sr = 87	?Yt = 88	Zr = 90	Nb = 94	Mo = 96	___ = 100	Ru = 104, Rh = 104, Pd = 106, Ag = 108
7	(Ag = 108)	Cd = 112	In = 113	Sn = 118	Sb = 122	Te = 125	I = 127	
8	Cs = 133	Ba = 137	?Di = 138	?Ce = 140				
9								
10			?Er = 178	?La = 180	Ta = 182	W = 184		Os = 195, Ir = 197, Pt = 198, Au = 199
11	(Au = 199)	Hg = 200	Tl = 204	Pb = 207	Bi = 208			
12				Th = 231		U = 240		

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Missing elements: 44, 68, 72, & 100 amu

Predicted properties of ekasilicon

Property	Predicted properties of Ekasilicon	Observed properties of Germanium (Ge)
Atomic weight	72	72.6
Color of element	Gray	Gray
Density of element (g/mL)	5.5	5.36
Formula of oxide	EsO_2	GeO_2
Density of oxide (g/mL)	4.7	4.228
Formula of chloride	$EsCl_4$	$GeCl_4$
Density of chloride	1.9	1.884
Boiling point of chloride (°C)	< 100	84

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Periodic Table of the Elements

	I A	II A	III B	IV B	V B	VI B	VII B		VIII B		I B	II B	III A	IV A	V A	VI A	VII A	VIII A
	1																1	2
1	H																H	He
	1.008																1.008	4.0026
	3	4											5	6	7	8	9	10
2	Li	Be											B	C	N	O	F	Ne
	6.939	9.0122											10.811	12.011	14.007	15.999	18.998	20.183
	11	12											13	14	15	16	17	18
3	Na	Mg											Al	Si	P	S	Cl	Ar
	22.99	24.312											26.982	28.086	30.974	32.064	35.453	39.948
	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	39.102	40.08	44.956	47.89	50.942	51.996	54.938	55.847	58.932	58.71	63.54	65.37	69.72	72.59	74.922	78.96	79.909	83.8
	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
	85.468	87.62	88.906	91.224	92.906	95.94	* 98	101.07	102.91	106.42	107.9	112.41	114.82	118.71	121.75	127.61	126.9	131.29
	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
6	Cs	Ba	**La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	132.91	137.33	138.91	178.49	180.95	183.85	186.21	190.2	192.22	195.08	196.97	200.29	204.38	207.2	208.98	* 209	* 210	* 222
	87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116		118
7	Fr	Ra	***Ac	Rf	Ha	Sg	Ns	Hs	Mt	Uun	Uuu	Uub	Uut	Uuq	Uup	Uuh		Uuo
	* 223	226.03	227.03	* 261	* 262	* 263	* 262	* 265	* 268	* 269	* 272	* 277	*284	*285	*288	*292		*294

Based on symbols used by ACS — S.M.Condren 2007

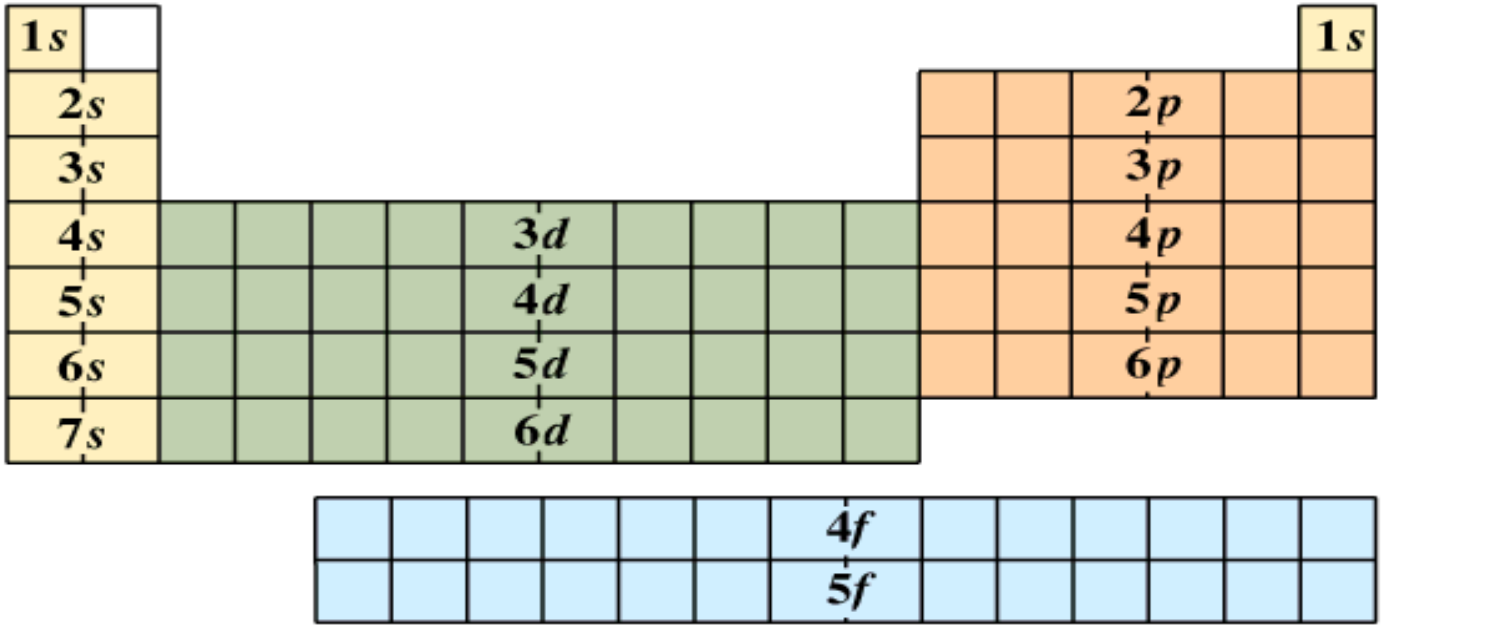
	58	59	60	61	62	63	64	65	66	67	68	69	70	71
	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
	140.12	140.91	144.24	* 145	150.36	151.96	157.25	158.93	162.51	164.93	167.26	168.93	173.04	174.97
	90	91	92	93	94	95	96	97	98	99	100	101	102	103
	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
	232.04	231.04	238.03	237.05	* 244	* 243	* 247	* 247	* 251	* 252	* 257	* 258	* 259	* 260

* Designates that all isotopes are radioactive

**Lanthanum Series

*** Actinium Series

Electron configuration and the periodic table



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Quantum Numbers

n => principal quantum number, quantized energy levels, which energy level

n = 1, 2, 3, 4, 5, 6, 7, etc.

Quantum Numbers

l => secondary quantum number, quantized orbital angular momentum, which sublevel or type of orbital

s type orbital l = 0

p type orbital l = 1

d type orbital l = 2

f type orbital l = 3

g type orbital l = 4

Quantum Numbers

m => magnetic quantum number, quantized orientation of angular momentum, which orbital within sublevel

s type orbital m = 0

p type orbital m = +1, 0 or -1

one value for each of the three p orbitals

d type orbital m = +2, +1, 0, -1 or -2

one value for each of the five d orbitals

f type orbital m = +3, +2, +1, 0, -1, -2 or -3

one value for each of the seven f orbitals

Hydrogenic Energy Levels

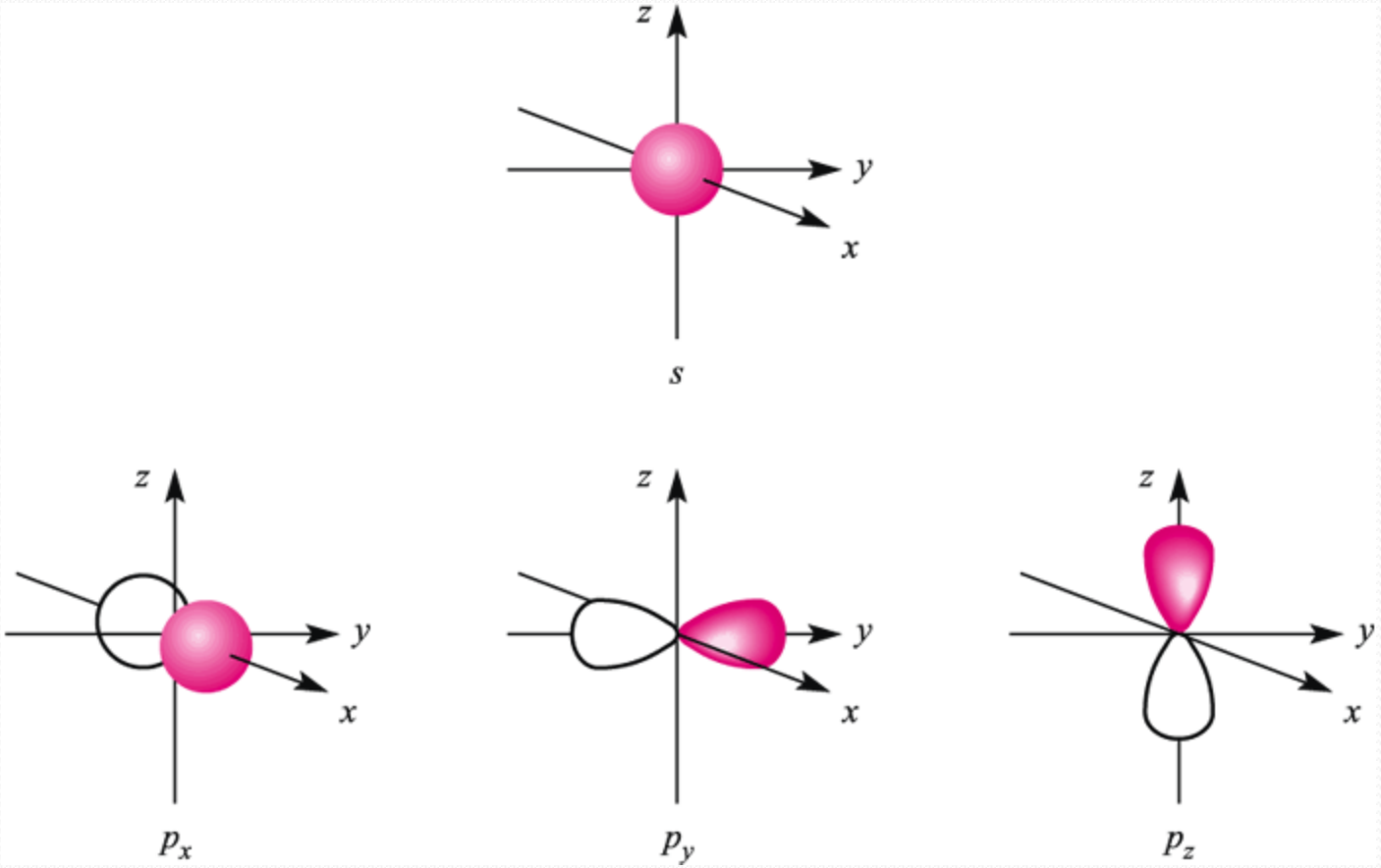
$$E = -\frac{hcZ^2R}{n^2}$$

where n = 1, 2, 3, • • •

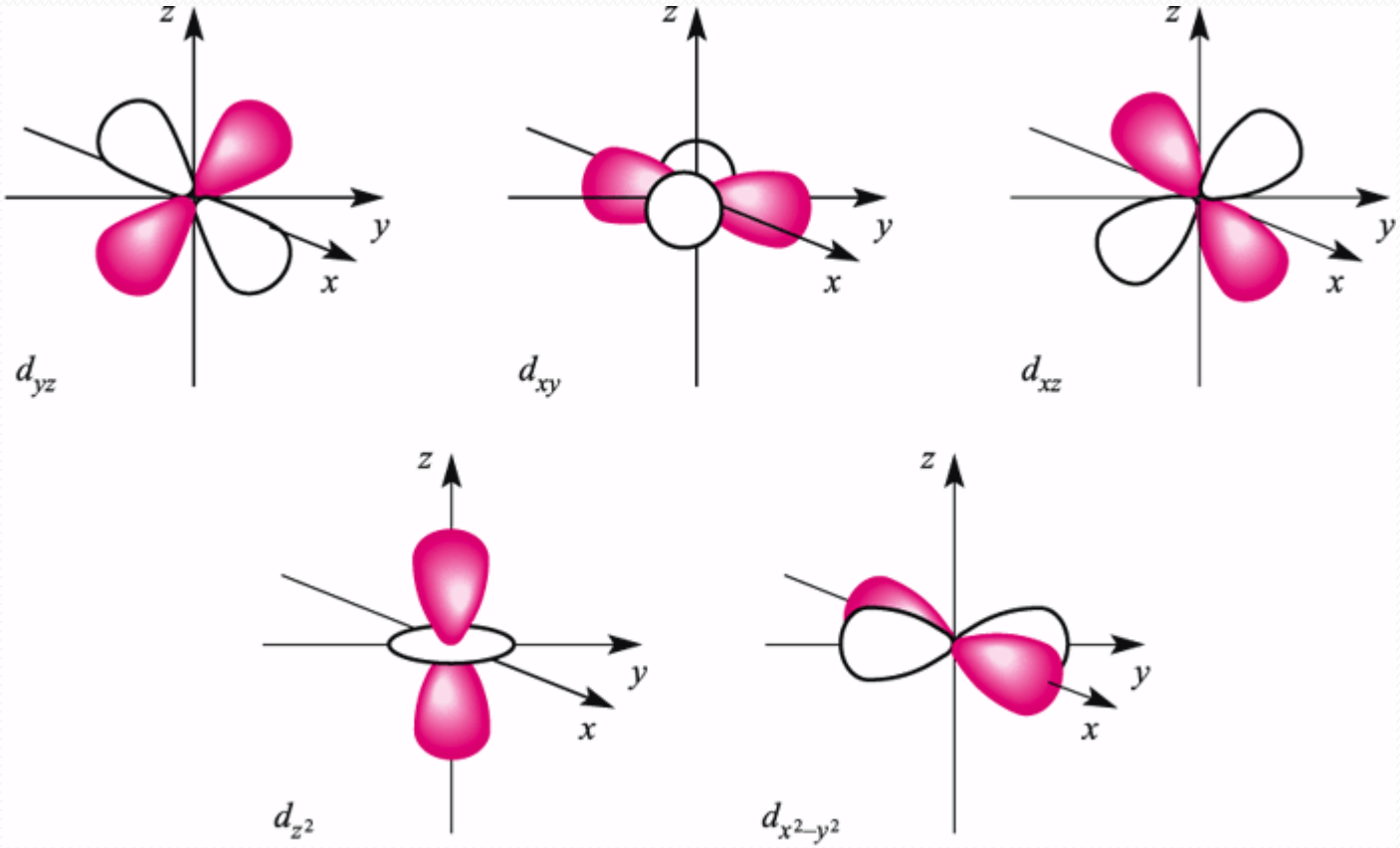
R = Rydberg constant

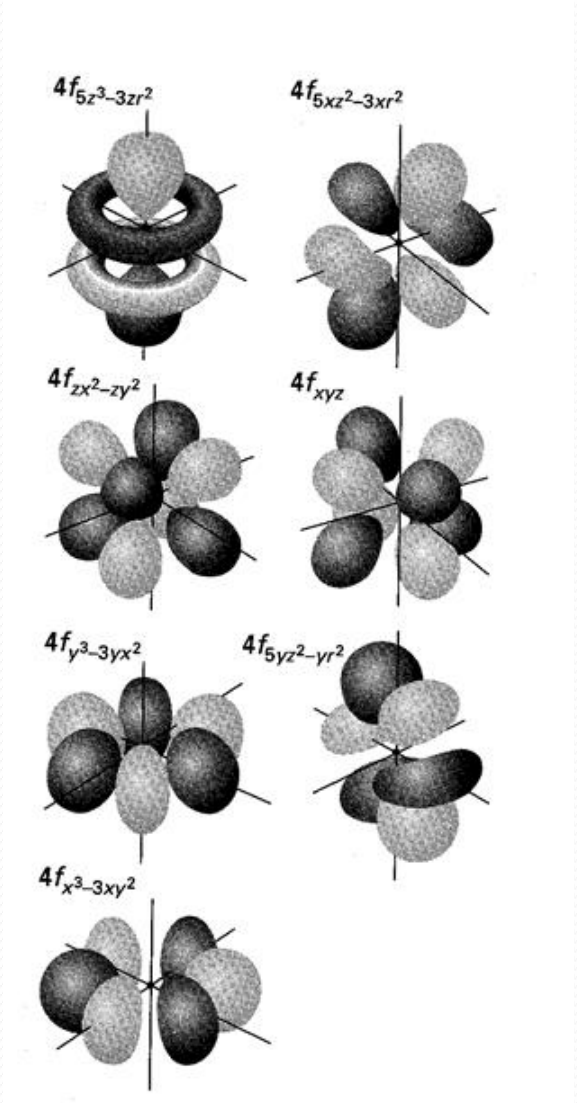
$$R = \frac{m_c e^4}{8h^3 c\varepsilon_o^{\,2}} = 13.6 \text{ eV}$$

s- and p-orbitals



d-orbitals



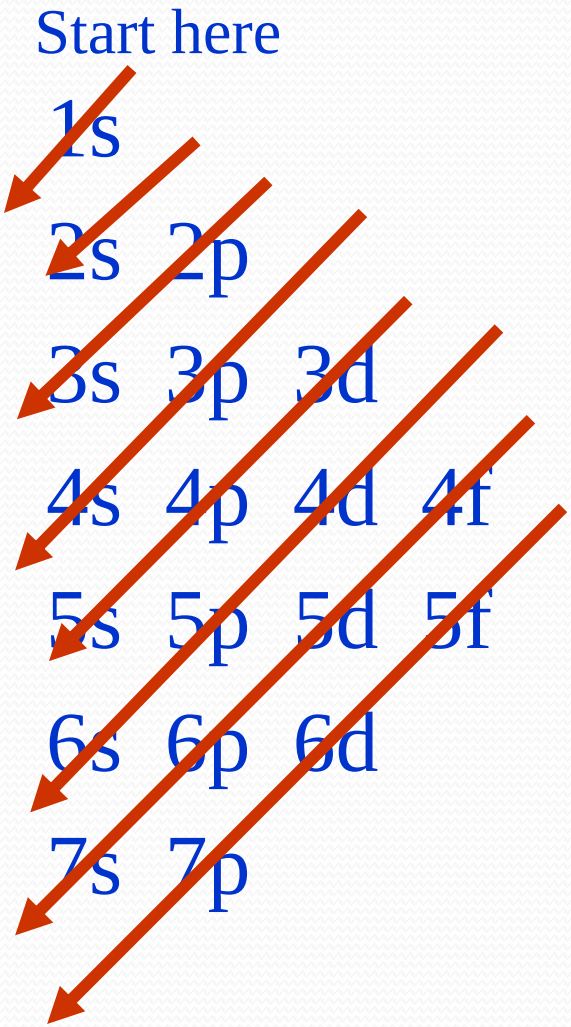

$4f_{5z^3-3zr^2}$
$4f_{5xz^2-3xr^2}$
$4f_{zx^2-zy^2}$
$4f_{xyz}$
$4f_{y^3-3yx^2}$
$4f_{5yz^2-yr^2}$
$4f_{x^3-3xy^2}$

f-orbitals

Many Electron Atoms

- Electronic Configuration
- Pauli exclusion principle
  - No more than 2 electrons can occupy a single orbital
  - No two electrons can have the exact same four quantum numbers

Electron Filling Order Diagram



Pauli Exclusion Principle

The Pauli exclusion principle states no two electrons (or other fermions) can have the identical quantum mechanical state in the same atom

Aufbau Principle

Fill from the bottom up

Hund's Rule

If multiple orbitals have the same energy, one electron goes into each of them before they start to double up.