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CHEMISTRY

Course 1

Chemistry → the science of matter
→ the center of science
→ a science at three levels
- symbolic level (chemical symbols, mathematical eqs)
- macroscopic level (large, visible objects)
- microscopic level (change of atoms & molecules)

$$\underbrace{Mg_{(s)} + \tfrac{1}{2} O_{2(g)}}_{\text{reactants}} \xrightarrow{\text{heat}} \underbrace{MgO_{(s)}}_{\text{products}} \quad \text{(magnesium oxide)}$$

"gives" — cond. for reaction (heat, catalyst)

OUTLINE

→ periodic system of the elements
→ atomic structure
→ chemical bonds
→ thermodynamics
→ gases, liquids, solids

MATERIALS CHEMISTRY

→ studies the rel between the structure/morphology and the properties of materials

Materials science <=> Materials Engineering

Structure <=> Morphology (shape, size)
⇓
Properties

What is matter? → substance
→ physical properties
→ chemical properties
→ energy

Chemical species
- atoms
- ions
- molecules

Chemical compound

THE ENERGY

1) Kinetic energy, E_k
   - m – mass, kg
   - v – velocity, m/s

$$\boxed{E_k = \frac{1}{2} m \cdot v^2}$$

2) Potential energy, E_p

$$\boxed{E_p = m \cdot g \cdot h}$$

The Coulomb potential energy

$$E_p = \frac{q_1 \cdot q_2}{4\pi \varepsilon_0 \cdot r}$$

q_1, q_2 – the charges
r – the distance between q_1, q_2
ε_0 – the vacuum permittivity $(8.854 \cdot 10^{-12} J^{-1} \cdot C^2 \cdot m^{-1})$
e – $1,6 \cdot 10^{-19}$ C – fundamental charge

Electromagnetic energy: → the energy of the electromagnetic field

→ radiowaves
→ lightwaves
→ X-rays

Chemical species: atoms, ions, molecules

→ atom: O
→ Ion: O^{2-}; SO_4^{2-}; CO_3^{2-}; Na^+
→ molecules: O_2; O_3 (ozone); P_4; S_8; CH_4; CO_2

Na_2SO_4; $CaCO_3$

~~SO_4Na_2~~

CH_4; CH_2Cl_2

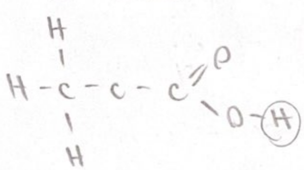
N_2H_4 – hydrazine

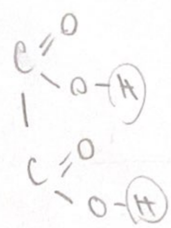
Stoechiometry – the ratio ⇒ N : H = 2 : 4 = 1 : 2

ex: NH_2OH ⇒ 1 : 3 : 1 ⇒ N : H : O

↳ hydroxylamine

CH_3-COOH monoprotic acid





oxalic acid

The nomenclator of compounds:

a) Names of cations

Na^+ = Sodium cation (ion)
Cu^+ = copper (I) ion
Cu^{2+} = copper (II) ion
Fe^{2+} = iron (II) ion ferrous ion
Fe^{3+} = iron (III) ion ferric ion

b) Names of anions

c) Names of ionic compounds

$CuSO_4 \cdot 5H_2O$ – copper (II) sulphate pentahydrate
$CrCl_3 \cdot 6H_2O$ – chromium (III) chloride hexahydrate

Common anions and their parent acid:

Anion	Parent acid	Chemical formula	Ex:
floride ion, F^-	hydrofloric acid OR hydrogen floride	HF	NaF, CaF_2
chloride ion, Cl^-	hydrochloric acid OR hydrogen chloride	HCl	KCl, $MgCl_2$, $FeCl_3$, $FeCl_2$
bromide ion, Br^-	hydrobromic acid OR hydrogen bromide	HBr	
iodide ion, I^-	hydroiodic acid OR hydrogen iodide	HI	

Anion	Parent acid	Chemical formula	* Examples
oxide ion, O^{2-}	water	H_2O	
hydroxide ion, OH^-	— ǁ —		
peroxide ion, O_2^{2-}	hydrogen peroxide	H_2O_2	
sulfide ion, S^{2-} (ph)	hydrogen sulphide hydrosulphoric acid	H_2S	
hydrogen sulphide			
sulfite ion, SO_3^{2-}	sulphurous acid	H_2SO_3	
hydrogen sulfite ion HSO_3^-			
sulfate ion, SO_4^{2-} hydrogen sulfate ion HSO_4^-	sulfuric acid	H_2SO_4	

$$H_2S \rightleftharpoons HS^- + H^+$$
$$HS^- \rightleftharpoons S^{2-} + H^+$$

hydrochlorite ion ClO^-	hypochlorous c	$HClO$	
chlorite ion, ClO_2^-	chlorous acid	$HClO_2$	
chlorate ion, ClO_3^-	chloric acid	$HClO_3$	
perchlorate ion, ClO_4^-	perchloric acid	$HClO_4$	
cyanide ion, CN^-	hydrogen cyanide hydrocyanic acid	HCN	

$Fe_4[Fe(CN)_6]_3 \cdot xH_2O$ iron (III) hexacyanoferrate (II) "Prussian blue"

thiocyanide ion, SCN^-	thiocyanic acid	$HSCN$	
hydrogen carbonate ion, HCO_3^- (bicarbonate ion) $NaHCO_3$	carbonic acid	H_2CO_3	

CH_3-COOH

$M_{CH_3-COOH} = A_C + 3 \cdot A_H + A_C + 2A_O + A_H = 60$ g/mol

- titanium dioxide: TiO_2
- silicon tetrachloride: $SiCl_4$
- barium nitrate: $Ba(NO_3)_2$
- xenon tetrafluoride: XeF_4

Course 2

Periodic Table / Periodic trends

Atomic Theory / Atomic Structure

1986: Ellie Wiesel - Nobel Price (Peace)
1974: Emil Palade - Nobel Price (Medicine)
2009: Herta Müller - Nobel Price (Literature)
2014: Stefan Hell — Nobel Price (Chemistry)

integer

$^{23}_{11}Na$

Mass number (A)

Atomic masses = (for Carbon)

$A_C = 12.012$ u.a.m (units of atomic masses)

$A_{Cr} = 51.8$ a m u

$\boxed{Mass = p^+ + n^0}$ ~~= 33 + 42 = 75~~

Nuclide	p^+	n^0	e^-	Mass #
Arsenic	33	42	33	75
Phosphorus — 31	15	16	15	31

The periodicity of atomic properties

Atomic Radius - raza atomica - half of the distance between the centers of neighbouring atoms

→ metal - solid sample
(metallic radius)
copper (solid) — the distance between 2 atoms → 256 pm (picometer)
$r_a = 128$ pm
atomic radius

→ non-metal (metalloid)
(covalent radius of the element)
Cl_2 molecule — the distance between the nuclei is 198 pm
chlorine
$r_a = 99$ pm

→ nobel gas = we will consider the sample of the solidified gas

Ionic radius - the distance between the centers of neighbouring ions in an ionic solid

MgO ; Mg^{2+} ~ 86 pm, O^{2-} 126 pm

86 pm + 126 pm = 212 pm
(bond length in MgO)

Ionization Energy, i (eV) - the energy needed to remove an electron from an atom in the gas phase

$X(g) \rightarrow X^+(g) + e^-(g)$

$i = E(X^+) - E(X)$

(eV) or $kJ \cdot mol^{-1}$

The first ionization energy, i_1 - the energy needed to remove ..

ex: $Cu(g) \rightarrow Cu^+(g) + e^-(g)$
monovalent

$i_1 = 7.73\ eV = 746\ kJ \cdot mol^{-1}$

The second ionization energy, i_2

$Cu^+(g) \rightarrow Cu^{2+}(g) + e^-(g)$

$i_2 = 20.29\ eV = 1958\ kJ \cdot mol^{-1}$

Electron affinity, E_{ea}
released when an electron is added to a gas - phase atom

$X(g) + e^-(g) \rightarrow X^-(g)$

$E_{ea}(X) = E(X) - E(X^-)$

ex: $Cl(g) + e^-(g) \rightarrow Cl^-(g)$

$E_{ea} = 3.62\ eV = 349\ kJ/mol^{-1}$

Electronegativity - a measure of the ability of an atom in a chemical compound to attract electrons

$$\chi_A = \frac{i_A + E_a}{2}$$

Applications

1) Arrange the elements in each set in order of decreasing atomic radius

a) Sulphur, chlorine, silicon
b) Cobalt, titanium, chromium
c) zinc, mercury, cadmium
d) antimony, bismuth, phosphorus

a) Si > S > Cl (pm)
Å

b) Ti > Cr > Co
c) Hg > Cd > Zn
d) Bi > Sb > P

2) Ionic radius : Place the following ions in order of increasing ionic radius

S^{2-} ; Cl^- ; P^{3-} $S^{2-} < Cl^- < P^{3-}$

$P^{3-} > Cl^- > S^{2-}$
sulphur

3) which sub. has the smaller ionization energy

a) Ca or Mg Ca
b) Mg or Na Na
c) Al or Na Na

4) the mollecular formula for a compound
Phosphorus and oxygen react to form two different phosphorus oxides.
The mass percentage of phosphorus in one of these oxides is 43.64%, in the other is 56.34%

a) write the empirical formula
b) The molar mass of the former oxide is 283.33 $g \cdot mol^{-1}$ and that of the latter is 219.88 $g \cdot mol^{-1}$, det the molecular formula and name of each oxide.

a) I P : $\frac{43.64\ g}{31\ g/mol} = 1.4$ moles

O : $\frac{56.36\ g}{16\ g/mol} = 3.5$ moles

P : O = 1.4 : 3.5 = 1 : 2.5 =
= 10 : 25 = 2 : 5

$P_2O_5 \rightarrow$ diphosphorus pentoxide

II P : 1.82 moles

O : 2.73 moles

P : O = 1 : 1.5 = 2 : 3
$P_2O_3 \rightarrow$ diphosphorus trioxide

b) $M_{P_2O_5} = 142\ g \cdot mol^{-1}$ 283.33 $\Rightarrow P_4O_{10}$ phosphorus (V) oxide
$M_{P_2O_3} = 110\ g \cdot mol^{-1}$ 219.88 $\Rightarrow P_4O_6$ phosphorus (III) oxide

Course 3

Dalton → the indivisible unit of an element is the atom

Faraday → electrolysis law

Thomson → the "plum pudding" model

Rutherford → an atom consists of a nucleus many times smaller than the atom itself, e^- - s occupy the remaining space

Q: How are the electrons distributed in this space?

A = The wave nature of light

wave (λ) { ↳ wavelength ↳ frequency   Å pm

$5.55 \cdot 10^{-7}\, m = 555\, nm$

$\lambda_{max} \approx \frac{1}{T} \rightarrow T \cdot \lambda_{max} = constant = 2.9\, mm \cdot K$

$\boxed{E = n \cdot h \cdot \nu}$; n - quantum numbers
$n = 1, 2, 3, \ldots$

h - Planck's constant $= 6.63 \cdot 10^{-34}\, J \cdot s$

$h\nu, 2h\nu, 3h\nu$

1) Energy level postulate

$E = -\frac{R_H}{n^2}$; R_H - Rydberg constant $= 2.179 \cdot 10^{-18}\, J$

2) Transitions between energy levels

- an e^- in a higher energy level (initial) undergoes a transition to a lower energy level (final)

$\boxed{\Delta E = E_{fin} - E_{init} \;\Big|\; E_f = -\frac{R_H}{n_{fin}^2} \;\Big|\; E_i = -\frac{R_H}{n_{init}^2}}$

n_i - the principal quantum number of the initial energy level
n_f - the principal quantum number of the final energy level

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

e.g.: $n_i = 4$ to $n_f = 2$
$\Delta E = -2.179 \cdot 10^{-18}\, J \left(\frac{1}{2^2} - \frac{1}{4^2}\right) = -4.086 \cdot 10^{-19}\, J$

The negative sign means that energy is lost by the atom in the form of photon

$h\nu = -\Delta E$

$h\nu = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$ c - speed of light

$\nu = \frac{c}{\lambda} \rightarrow \frac{1}{\lambda} = \underbrace{\frac{R_H}{h \cdot c}}_{1.097 \cdot 10^7\, m^{-1}}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$n = 1$ → the ground state of the atom

$E = 0 \Rightarrow n \rightarrow \infty$ → ionization

/ ionization energy - minimum /

Quantum numbers

1) Principal quantum number

$n = 1, 2, 3 \ldots$

→ is related to the size and energy of the orbital

Letter	K	L	M	N	(the shell)
n	1	2	3	4	

2) The second quantum number – the angular momentum q. n, l,
– the shape of atomic orbitals

value of e =	0	1	2	3	4
letter =	s	p	d	f	(g)

3) The magnetic quantum number, me : – integral values between e and –e (including 0)
– is related to the orientation

4) The electron spin quantum member
– presents only two values $-\frac{1}{2}$ and $+\frac{1}{2}$

$+\frac{1}{2}$ e^- $-\frac{1}{2}$ e^-

W. Pauli postulate =
– in a given atom no 2 electrons can have the same set of four quantum numbers (n, l, me, ms)

Pauli exclusion principle: An orbital can hold at most 2 electrons, and then only if the electrons have opposite spins (ms)

Electron configuration

1) The number of principal quantum number (shell), n
2) The letter that designated the orbital type (the subshell)
3) A superscript number that designated the number of the electrons in that particular subshe

	atomic nb		
H	Z=1	$1s^1$	$\boxed{\uparrow}$
He	Z=2	$1s^2$	$\boxed{\uparrow\downarrow}$
Li	Z=3	$1s^2 2s^1$	
Be	Z=4	$1s^2 2s^2$	
B	Z=5	$1s^2 2s^2 2p^1$	valence electron
Na	Z=11	$\underbrace{1s^2 2s^2 2p^6}_{\text{core electrons}} 3s^1$	valence electron
		$[Ne]\, 3s^1$	
Ca	Z=20	$[Ar]\, 4s^2$	2 valence e^-
Ca^{2+}		$[Ar]\, 4s^0$	
Sc	Z=21	$[Ar]\, 3d^1 4s^2$	
! Cr	Z=24	$\cancel{[Ar]\, 3d^4 4s^2}$	
		$[Ar]\, 3d^5 4s^1$	

! Co $Z=29$ $[Ar]\ \cancel{3d^9\ 4s^2}$

$[Ar]\ 3d^{10}\ 4s^1$

d^5 d^{10}

1) The maximum intensity of solar radiation occurs at 490 mm. What is the temp of the surface of the ... constant $2.9 \cdot 10^{-3}$ m·k

$$\lambda max = \frac{1}{T} \rightarrow T \cdot \lambda max = 2.9 \cdot 10^{-3}$$

$$T = \frac{2,9 \cdot 10^{-3}}{490\ mm} = \cancel{0,005 \cdot 10^{-3}}\ 5918.36\ K$$

2) What is the wavelength of light emitted when the electron in a hydrogen atom undergoes a transition from energy level n=4 to level n=2

$$\Delta E = -2.179 \cdot 10^{-18}\left(\frac{1}{2^2} - \frac{1}{4^2}\right) = -4.086 \cdot 10^{-19}\ J$$

$$\left.\begin{aligned} h\nu &= -\Delta E \\ \nu &= \frac{c}{\lambda} \end{aligned}\right\} \quad \frac{c}{\lambda} \cdot h = -\Delta E \rightarrow \lambda = \frac{c \cdot h}{-\Delta E} = \cancel{300.000.000}$$

$$= \frac{1,097 \cdot 10^{7}}{+4,086 \cdot 10^{-19}} = +0,26 \cdot 10^{26}.$$

$$E_i = -\frac{RH}{4^2} = -\frac{RH}{16}$$

$$E_f = -\frac{RH}{2^2} = -\frac{RH}{4}$$

$$\Delta E = E_f - E_i = -RH\left(\frac{1}{4^2} - \frac{1}{2^2}\right) = \frac{3RH}{16} = h\nu = \frac{hc}{\lambda}$$

$$\lambda = \frac{16 \cdot h \cdot c}{3\,RH} = 486 \cdot 10^{-9} m = 486\ nm$$

↳ blue-green

3) Calculate the energy release when an electron is brought from infinity to a dist. of 53 pm from a proton

13.6 eV

$$E_p = \frac{q_1 \cdot q_2}{4\pi \cdot \varepsilon_0 \cdot r} = \frac{(-e) \cdot (+e)}{4\pi \cdot 8.8519 \cdot 10^{-12} \cdot C^2 \cdot J^{-1} \cdot m^{-1} \ (53 \cdot 10^{-12} m)} = -27 eV$$

$E = E_k + E_p$

1) ⓐ Boron-11

5 protons ; 6 neutrons ; 5 electrons

ⓑ ^{10}B

5 protons, 5 neutrons, 5 electrons

ⓒ Phosphorus-31

15 protons, 16 neutrons, 15 electrons

ⓓ ^{238}U

92 protons ; 146 neutrons ; 92 e^-

2) ⓐ Ethanol, C_2H_5OH

$M_{C_2H_5OH} = 2 \cdot A_C + 6 \cdot A_H + 1 \cdot A_O = 2 \cdot 12 + 6 \cdot 1 + 1 \cdot 16 = 24 + 6 + 16 = 46$ g/mol

ⓑ Sodium carbonate decahydrate

$M_{Na_2CO_3 \cdot 10H_2O} = 2 \cdot A_{Na} + A_C + 3 \cdot O + 10 \cdot 2 \cdot A_H + 10 \cdot A_O$

$= 2 \cdot 23 + 1 \cdot 12 + 3 \cdot 16 + 10 \cdot 2 \cdot 1 + 10 \cdot 16 = 286$ g/mol

ⓒ Copper sulphate pentahydrate

$M_{CuSO_4 \cdot 5H_2O} = A_{Cu} + A_S + 10 A_H + 9 \cdot A_O = 249,68$ g/mol ≈ 250 g/mol

ⓓ Hydrogen peroxide

$M_{H_2O_2} = 2 \cdot A_H + 2 \cdot A_O = 34$ g/mol

3) isoelectronic with Br^+ are: Se ; As^-

isoelectronic = same nb. of electrons

Br^+: $34 e^-$

$Se^{2+} = 32 e^-$

$Se = 34 e^-$ ✓

$As^- = 34 e^-$ ✓

$Kr = 36 e^-$

$Ga^{3+} = 28 e^-$

$Cl^- = 18 e^-$

4) ⓐ [Ar] $3d^2$, $4s^2$

ⓑ [Ar] $3d^5$, $4s^1$

ⓒ [Kr] $4d^{10}$, $5s^2$, $5p^3$

ⓓ [Ar] $3d^{10}$, $4s^2$, $4p^1$

Co $Z=29$ $[Ar]\ 3d^9\ 4s^2$

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$Cl^- = 18 e^-$

4) ⓐ $[Ar]\ 3d^2, 4s^2$
ⓑ $[Ar]\ 3d^5, 4s^1$
ⓒ $[Kr]\ 4d^{10}, 5s^2, 5p^3$
ⓓ $[Ar]\ 3d^{10}, 4s^2, 4p^1$

Course 4

Chemical bonds : → ionic, covalent; metallic

$Na^+ + Cl^-$ $N_2 + H_2$ $Cu + Cu$

Ionic bond : → the ions that elements form → the octet of electrons

Na   Cl

Metal atom   Non-metal

ns^2np^6

Na $[Ne]3s^1 \longrightarrow Na^+[Ne]$

1) $H \rightarrow H^+$ proton / hidrides - H^-

2) Li $[He]2s^1 \rightarrow Li^+[He]$ helium like dublet   7. correction

3) Be $[He]2s^2 \rightarrow Be^{2+}[He]$

Al $[Ne]3s^2 3p^1 \rightarrow Al^{3+}[Ne]$

Ga $[Ar]3d^{10}4s^2 4p^1$

Ga^{3+} $[Ar]3d^{10}$

SnO - tin (II) oxide

SnO_2 - tin (IV) oxide

d-block   ns - electrons

(n-1)d - electrons

Fe $[Ar]3d^6 4s^2$

Fe^{2+} $[Ar]3d^6$ electron configuration

Fe^{3+} $[Ar]3d^5$ ★   of Fe (ion)

O^{2-} nitrite ion

N $[He]2s^2 2p^3$ N^{3-} $[Ne]$

Cl $[Ne]3s^2 3p^5$ Cl^- $[Ar]$

chlorine ion

Lewis symbols:

$Na\cdot + \cdot\ddot{\underset{\times\times}{Cl}}\,\dot{\times} \rightarrow [Na]^+[\,\ddot{\underset{\times\times}{Cl}}\,]^-$

electron transfer from sodium to chlorine

→ the energetics of ionic bond formation

$H\cdot$; $H=$, $\cdot\ddot{\underset{\cdot\cdot}{O}}\cdot$; $\cdot\ddot{N}\cdot$ → $2s^2$

$2p^3$

$2p_x^1 2p_y^1 2p_z^1$

Na^+ $[\ddot{\underset{\times\times}{Cl}}]^-$

1) → sublimation of sodium

→ dissociation of chlorine

2) Sodium atoms release electrons → these electrons are attached to chlorine atoms
3) the resulting cations and anions clump together a crystal pattern (structure)

1) $Na(s) \xrightarrow{\Delta H_{sub}} Na(g)$

solid → gas

H_{sub} = heat of sublimation = the heat required to change a molecule/substance from solid state to gaseous state

2) (STP) - standard temperature and pressure

$Na(g) \rightarrow Na^+(g) + e^-(g)$

$\frac{1}{2}Cl_2(g) \rightarrow Cl(g)$

dissociation = from molecular state to atomic state

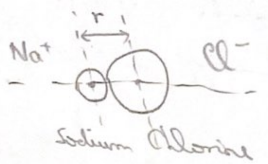
$Cl(g) + e^-(g) \rightarrow Cl^-$ energy is released

$Na^+(g) + Cl^-(g) \rightarrow NaCl(s)$

$-788\ kJ/mol$ <u>Lattice energy</u>

$$\boxed{E_p = \frac{(z_1 \cdot e) \cdot (z_2 \cdot e)}{4 \cdot \pi \cdot \varepsilon_0 \cdot r}}$$

; e - fundamental charge
$z_{1,2}$ - the charge number of the 2 ions
r - the distance between the centers of the ions
ε_0 - the vacuum permitivity

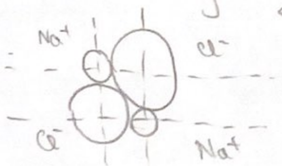


Na^+ $r_{Na^+} = 116\ pm$ (ionic radius)

Cl^- $r_{Cl^-} = 167\ pm$

$$E_p = E = U = -\frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot (r_{Na^+} + r_{Cl^-})} \quad ; \quad \frac{1}{4\pi\varepsilon_0} = k = 9 \cdot 10^9\ N \cdot m^2 \cdot C^{-2}$$

neg. charge <u>Coulomb constant</u>



$$E_p = -4k \cdot \frac{e^2}{r} + 2 \cdot r \cdot \frac{e^2}{r\sqrt{2}} = -2.59\, k \cdot \frac{e^2}{r}$$

atracție respingere

$$E_p = U = k\left[-6 \cdot \frac{e^2}{r} + 12 \cdot \frac{e^2}{r\sqrt{2}} - 8 \cdot \frac{e^2}{r\sqrt{3}} + 6 \cdot \frac{e^2}{r\sqrt{4}} - 12 \frac{e^2}{r\sqrt{5}} \ldots\right] = -A \cdot k \cdot \frac{e^2}{r}$$

M, A = const. of Madelung.

$$A = \frac{6}{1} + \frac{12}{\sqrt{2}} - \frac{8}{\sqrt{3}} + \frac{6}{\sqrt{4}} + \ldots$$

cubic crystalline structure (NaCl)

$$E_p = -N_A \cdot A \cdot k \cdot \frac{e^2}{r}$$

(M)

for a gram molecule

Avogadro number

anion charge cation charge

For a polyatomic compound: $E_p = -k \cdot N_A \cdot A \frac{e^2 \cdot z_a \cdot z_c}{r}$

Applications:

1) NaCl   KCl

$Na^+ \rightarrow r_{Na^+} = 116$ pm

$K^+ \rightarrow r_{K^+} = 152$ pm

$Cl^- \rightarrow r_{Cl^-} = 167$ pm

2) KCl   CaO

$Ca^{2+} \rightarrow r_{Ca^{2+}} = 114$ pm

$O^{2-} \rightarrow r_{O^{2-}} = 126$ pm

↳ 4. . . . . .

The coordination number (N.C.) = the number of bonds formed by metal ions to other ions (ligands)

NaCl	Na^+ N.C. – 6 Cl^- N.C. – 6	
CsCl	Cs^+ N.C. – 8 Cl^- N.C. – 8	
ZnS	Zn^{2+} N.C. – 4 S^{2-} N.C. – 4	
CaF_2	Ca^{2+} N.C. – 8 F^- N.C. – 4	

Covalent bond

- diamond / graphite
- paramagnetism of O_2

→ atoms go as far as possible to complete their octets

Lewis structures

H· + ·H → H:H   H – H

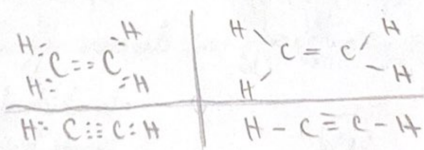
H – F   H – O – H   :NH_3 CH_4

:Ö = Ö: :N ≡ N: :C = C: –C ≡ C–

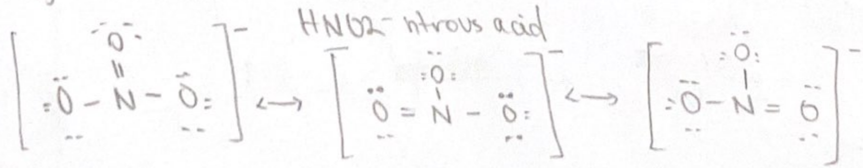
O = C = O   O = S = O   H – C ≡ N

H_2, F_2, O_2, N_2 single
CH_2O, C_2H_4 double
CO, CN^- triple
} bonds

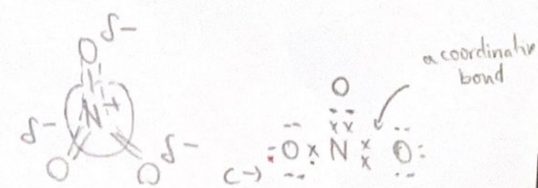
- ethylene : C_2H_4 ⇒
- acetylene : C_2H_2 →



NO_3^- – nitrate ion HNO_3 – nitric acid
HNO_2 – nitrous acid



N – O → 140 pm
N = O → 120 pm
} ↓ 124 pm



Course 5

Substances	Conduct electricity YES / NO	Measurements Solubility YES / NO	Conduct el. in solution YES / NO
Al-Li	✓	X	
Cu	✓	X	
Al	✓	X	
Graphite, C	✓	X	
$CuSO_4$	X	✓	✓
NaCl	X	✓	✓
$-(CH_2)_n-$ polietilen	X	X	
SO_2	X	X	
$C_{12}H_{22}O_{11}$	X	✓	X
ethanol	X	✓	X
H_2O (pure)	X	✓	X

Solubility
- YES → Conduct electricity
  - YES → $CuSO_4$, NaCl — salt, ionic bond
  - NO → ethanol, $C_{12}H_{22}O_{11}$
- NO → Conduct electricity
  - YES → AlLi, Cu, Al — metals / metallic bond
  - NO → SiO_2, $-(CH_2)_n-$ — ceramic polimer, covalent bond

Chemical bonds
- pure (non-polar) covalent
- polar covalent
- ionic

• in which of the following compound do the bonds have greater covalent character

a) NaBr or $MgBr_2$ b) CaO or CaS

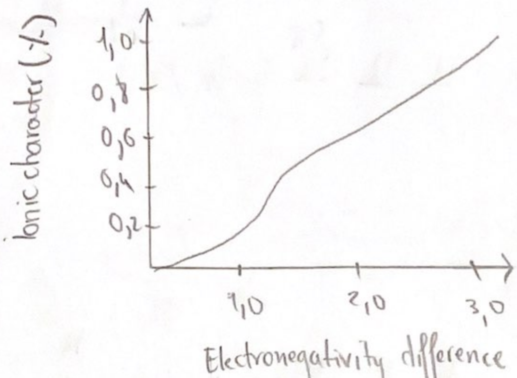
X – the average of the ionization energy and electron affinity of the element

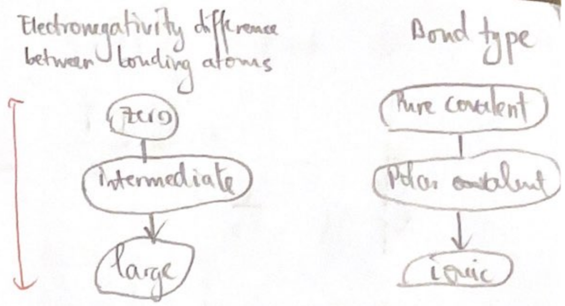
$X = (I + Ea)/2$

• in which of the following compounds do the bonds have greater ionic character?

• P_4O_{10} I (≈40%) — PCl_5 II (20%)

CO_2 $\Delta X = 1$ ≈ 20% — NO_2 $\Delta X = 0.5$ 6%





covalent character decreases;
ionic character increases;

ΔX:	0,5	1,0	1,5	1,8	2,0	2,5	3,0	3,2
% ionic character:	6	22	43	55	63	79	89	92

Hybridization:

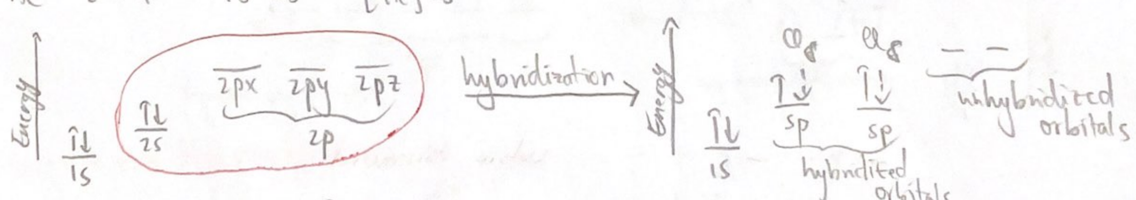
Important issues: → covalent bonds

1) Hybrid orbitals do not exist in isolated atoms.
2) — " — have shapes and orientation.
3) The number of hybrid orbitals is equal to the nb of atomic orbitals that combine to produce the chemical compound.
4) the hybrid orbitals are equivalent in shape and energy.
5) The type of hybrid orbitals in a bonding atom depend on its electron-pair-geometry
6) Hybrid orbitals will form σ bonds
Unhybridized orbitals will form π-bonds.

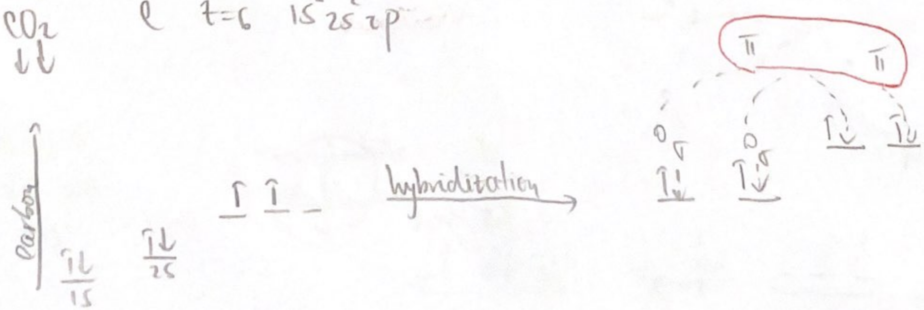
Sp Hybridization

$BeCl_2$ - berillium chloride

Be $Z=4$ $1s^2 2s^2$ $[He]2s^2$

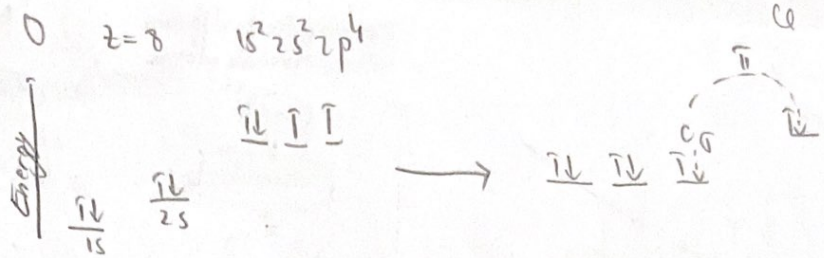


CO_2 C $Z=6$ $1s^2 2s^2 2p^2$



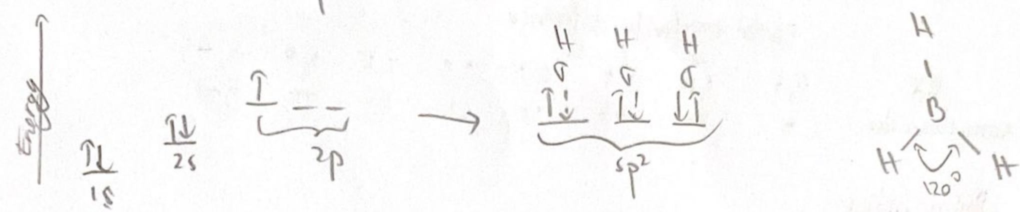
O=C=O

O $z=8$ $1s^2 2s^2 2p^4$



BH_3 - borane molecule

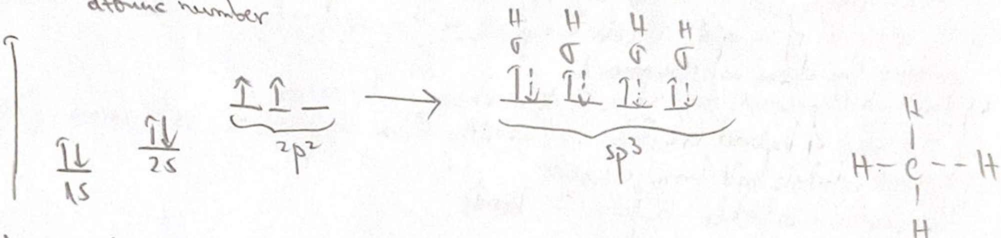
B $z=5$ $1s^2 2s^2 2p^1$



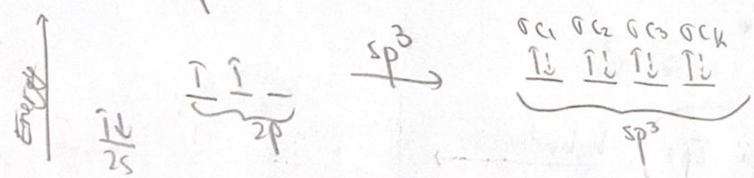
CH_4 - methan molecule

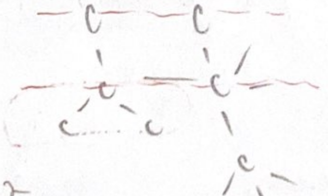
C $z=6$ $1s^2 2s^2 2p^2$

↓ atomic number



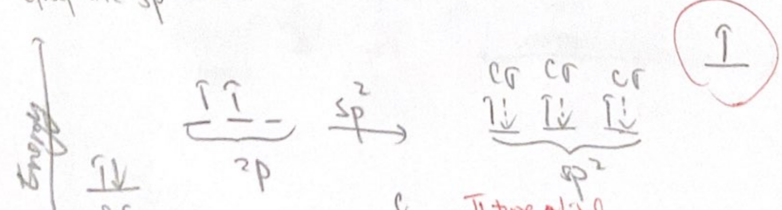
Diamond sp^3

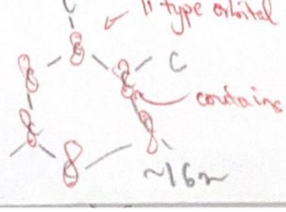




cubic diamond x tal structure

Graphite sp^2



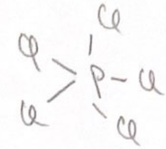


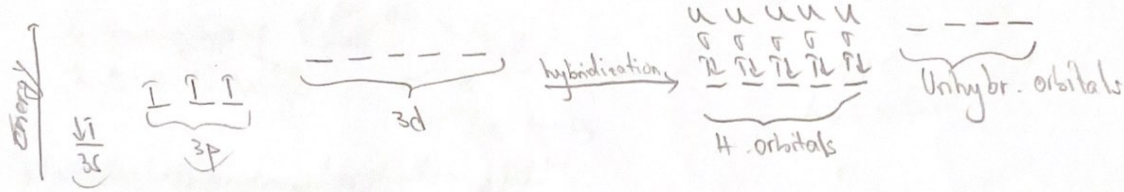
Course 6

Chemical bounds

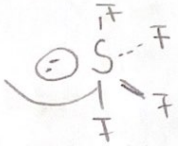
PCl_5 [Ne] $3s^2 3p^3$

$Z = 15$



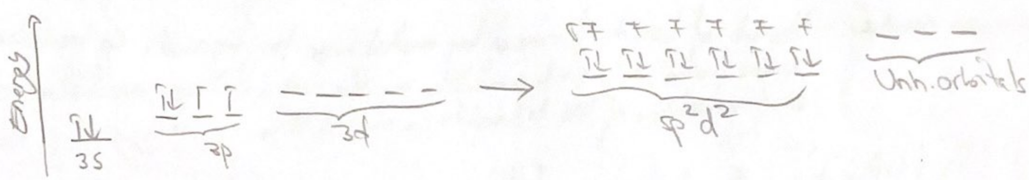


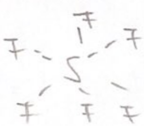
SF_4 – sulphur tetrafluorine



SF_6

S $Z = 16$ [Ne] $3s^2 3p^4$

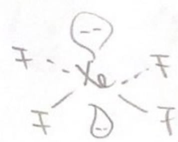




$IF_5 \Longrightarrow$

square pyramid

$XeF_4 \Longrightarrow$

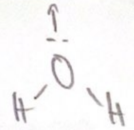


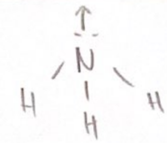
square planar

Negative ions that can form are:

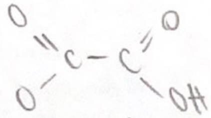
NH_2OH
CH_2NH_2
NO^+

monodentate
polydentate – di, tri, tetra, hexa

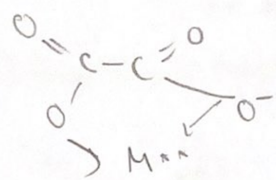




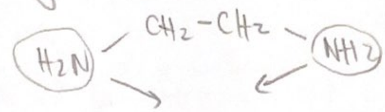
oxalate (ox)



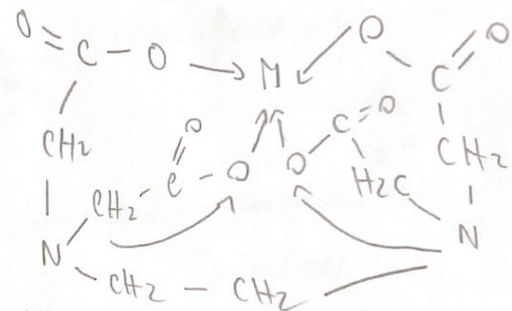
oxalic acid



ethylenediamimine



EDTA – ethylenediamminatetracetate

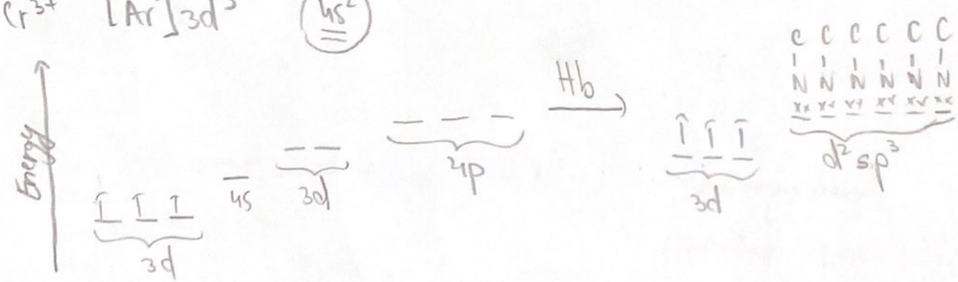


Coordination number – the nb. of bonds formed by metal ions to ligands in complex ions
varies from 2 to 8 depending on the size, charge, and electron configuration of the transition metal ion

$3\,K^+\ \underbrace{[Cr(CN)_6]^{3-}}\ 3d^5\ 4s^1$ $\qquad CN^-$

$Cr \quad Z=24 \quad [Ar]\ \underbrace{4s^1\,3d^5}$

$Cr^{3+} \quad [Ar]\,3d^3 \quad 4s^2$



$CuSO_4 \cdot 5H_2O$

I $ZnC_2O_4 \cdot 2H_2O \xrightarrow{T<200^\circ C} ZnC_2O_4$ anh. $+ 2H_2O$

II $ZnC_2O_4 \xrightarrow{T>200^\circ C} ZnO + CO\uparrow + CO_2\uparrow$

Course 7

B_2H_6 - diborane

B $1s^2 2s^2 2p^1$ $3e^- \times 2 \to 6e^-$

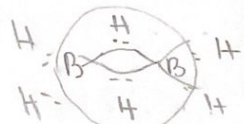
H $1s^1$ $1e^- \times 6 \to 6e^-$

4 terminal H-B bond $8e^-$

2 B-H-B bridge $4e^-$

$2e^-/B-H-B$

- electron deficient compound



$\sigma_{1s}^2 \sigma_{1s}^{*0}$

Molecular orbital theory (MO)

↳ model for describing the energies of electrons in a molecule and the probable location of these electrons

O: $1s^2 2s^2 p^4$

N: $1s^2 2s^2 p^3$

Course 8 - DISCORD

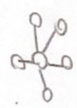
Course 9

Ne $-246°C$: 1 atm

1.77 kj/mol < 0.23 kj/mol ; 1.54 kj/mol

$\frac{1.54 \text{ kj/mol}}{5}$

(0.3 kj/mol)



H-O (H_2O

432 kj/mol

I

	Pentane	Iso-pentane (2-methyl butane)	Neo-pentane (2,2-dymethyl propane)
Boiling point (°C)	36	28	9.5
ΔH vap [kj/mol]	25.8	24.7	22.8

CH_3F $-78°C$

CH_3OH $65°C$

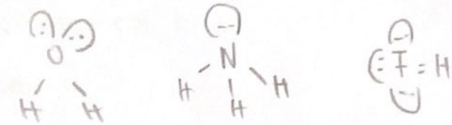
C_5H_{12}

CH_4

$CHCl_3$

C_4C_9OH

	H_2O	NH_3	HF
Boil. p.	100°C	−33,34°C	19.5°C



2 1 3 lone pairs of e^-

radius ratio, $\rho = \frac{r\ smaller}{r\ larger} =$

$FeO = \frac{0.077}{0.14} = 0.55 \Rightarrow 6 \Rightarrow$ octahedral

$CaO = 0.71$ octahedral

$NaCl = 0.56$ octahedral

$TiO_2 =$ - -

Theoretical density (ρ)

$\rho = \frac{n \cdot A}{V_c \cdot N_A} = \frac{63.55 \cdot n_{atom}}{V_c \cdot 6{,}023 \cdot 10^{23}} = \frac{63{,}55\ g/mol \cdot 4\ atoms}{(2\sqrt{2} \cdot 0{,}128 \cdot 10^{-7})^3 \cdot 6{,}023 \cdot 10^{23}\ atoms/mol} = \frac{254{,}2}{28{,}5}$
cm^3

$= 8{,}89\ g/cm^3$ teoretical

Length $4R = \sqrt{2}a$

$\boxed{4}\ \boxed{\frac{4}{3}\pi(\sqrt{2}a/4)^3}$ ← volume atom

8,94 g/cm³ exp

Course (10/11?)

States of Matter

→ solid, liquid, gas, plasma

	0.7142 g
	0.7072 g
1/1 Pasc	0.6977 g
1-30	0.7045 g
22	0.7243 g
1/2	0.6985 g
MBL	0.7322 g
Noir	0.738 g
Venom	0.713 g

magnesium : $\rho m =$ ~~.92 77~~

$\rho m = \frac{24 \cdot 30 + 27 \cdot 70}{100} = 26{,}1$

$\frac{26{,}1}{27} = 0{,}96606$

202 torr / 56.2°C

Acetone

$CH_3-\overset{\overset{O}{\|}}{C}-CH_3$

Methanol

CH_3-OH

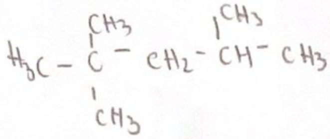
108 torr 65°C

H_2O

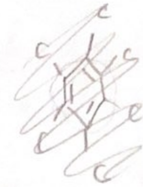
H–O–H

19.8 torr / 100°C

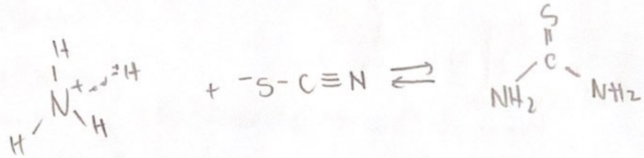
a)

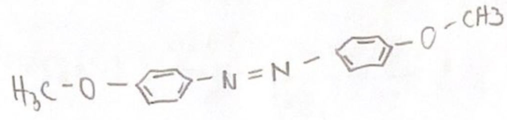


NH_2^-



b)





Course 11

→ In main cases, including) gases need to be treated as non-ideals
→ this term adjusts the volume occupied by the gas particles...
→ Correcting the ideal gas eq.: $\boxed{p \cdot V = n \cdot R \cdot T}$
→ the volume correction: $V - n b$ a, b – Van der Waals consts for diff. gases

$- a \left(\frac{n}{V}\right)^2$

→ "a" accounts the attraction between particles
- frequency of the collision
- intensity of the collision

$$p = \frac{n \cdot R \cdot T}{V - nb} - a\left(\frac{n^2}{V^2}\right) ; \boxed{\left(p + a\left(\frac{n}{V}\right)^2\right) \cdot (V - nb) = n \cdot R \cdot T}$$

Van der Waals eq. for real gases

Gas	a [atm L² mol⁻²]	b [L · mol⁻¹]
O_2	1.360	0.03153
H_2	0.244	0.0266
Water	5.464	0.0304
	2.253	0.0427

1) CH_4
$V = 49\ dm^3$ (L)
m_1 tank (empty) = 55.85 kg
m_2 (filled) = 62.07 kg
$T = 21°C$
What is the % correction by using the more realistic Van der Waals eqs?

filled $n = \frac{6.22}{16} = \frac{\Delta m}{M} = 0.388\ kmol = 388\ mols$

$T = 294\ K$

$\Delta m = 6.22\ kg$

$p = \frac{nRT}{V} = \frac{388 \cdot 8.31 \cdot 294}{49 \cdot 10^{-3}} = 19\,345 \cdot 10^{+3} = 193.45 \cdot 10^5\ Pa$

$p = \frac{388 \cdot 0.082 \cdot 294}{49}\ atm = 190\ atm$