Chapter 2: Atomic Structure and Chemical Bonding

- Materials → Molecules → Atoms
- Atoms = protons (p) + neutrons (n) + electrons (e)
- Protons and neutrons are made of quarks
- Quantitative measurements need units: *metric* or *S.I.* (Systeme International) or *mks* (meter-kilogram-second) units

meter	(m)	for length
cubic meter	(m^3)	for volume
kilogram	(kg)	for mass
Kelvin	(K)	for temperature
second	(s)	for time
mole	(mol)	for amount of substance

Typical parameters: atoms are small

	Mass (kg)	Charge (coulomb)
Proton	1.673×10^{-27}	$+1.602 \times 10^{-19}$
Neutron	1.675×10^{-27}	0
Electron	9.109×10^{-31}	-1.602×10^{-19}

- Nuclear radius is measured in 10^{-15}m = fm
- Electron radii measured in Å = 0.1 nm = 10^{-10} m
- Fundamental charge = e = -1.602×10^{-19} C

2.1 The Structure of Atoms

- Atomic number **Z**

In neutral atom:

# of protons = # of electrons = atomic number **Z**

Value of Z is different for each element H (Z = 1), O (Z = 8), Fe (Z = 26)

- Isotopes *Mass number* → A *Atomic number* → Z $^{A}_{Z}X$ ← *Element*

Same element (same Z) might have different # of neutrons (**N**)

Same chemistry (same # of electron)

Hydrogen: "protium" H-1; $^{1}_{1}H$ "deutiruim" H-2 or D $^{2}_{1}H$ "tritium" H-3 or T $^{3}_{1}H$

- Atomic mass unit (amu): 1/12 of C-12 (<1% of C-13, isotopically pure)
- Atomic mass **A** **A ≈ Z + N**
- Atomic weight (periodic table) – weighted average of all isotopes

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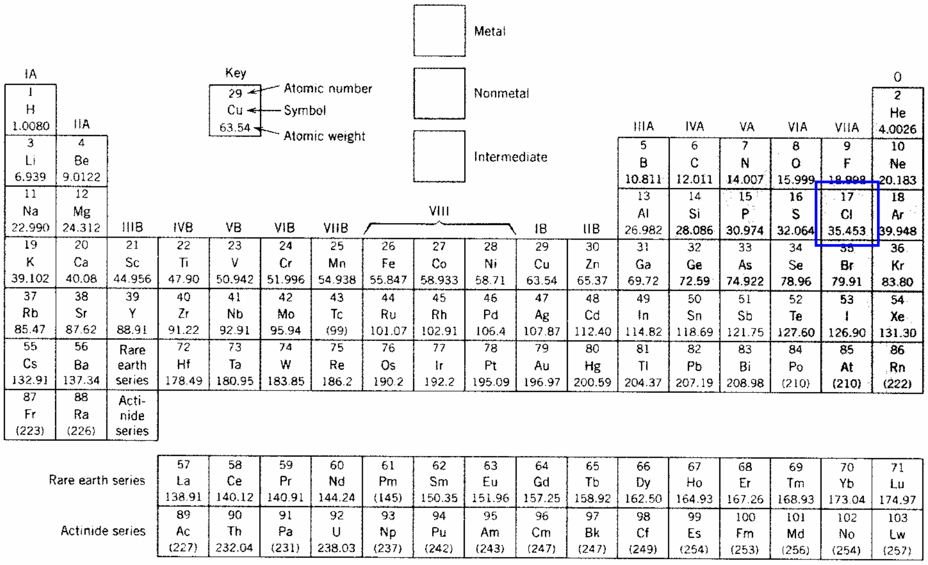
2.2 Periodic Table of Elements



☐ Metal

☐ Nonmetal

☐ Intermediate

Key

29 ← Atomic number

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19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.54	30 Zn 65.37	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.91	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.34	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)
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2.3 Electrons in Atoms

- One of the first models: Bohr atom

Bohr assumed that electrons orbited the nucleus due to Coulomb forces
Electrons could only be in one of infinitely many discrete states
Explained spectra of H, He^+, Li^{2+}

- Not working for atoms with >1 electron
- Need a quantum mechanics approach → Will summarize main points

1. Particles can have wave-like properties

de Broglie suggested that any particles with momentum p(=m×V, non-relativistically) displays wave-like properties:

$$\lambda = h/p$$

2. Wave can have particle-like properties

Light as a propagating wave of electric and magnetic fields
Wavelength determines the colour
Einstein showed that light is divided into packets of E (so called "photons")

$$E = h f$$

The Heisenberg Uncertainty Principle

3. We can no longer describe a particle as having a **precise position x and momentum p**

4. The Heisenberg Uncertainty Principle

We cannot know both x and p simultaneously with arbitrary precision
There is a limit ! $\delta x \, \delta p \geq h/2\Pi \equiv \hbar$
We do know exactly where an electron is, we can't know how fast it is moving

5. Electrons in atoms can only be in certain "states"

The energy is "quantized" – only certain levels are permitted
The level can change, but only if exactly the correct energy is emitted or absorbed

6. 4 quantum numbers: The state of an electron in an atom is described by a set of 4 quantum numbers

principle	quantum number	n =	1, 2, 3, …n
subsidiary or azimuthal number		L =	0, 1, 2, … n-1
magnetic	quantum number	m_L=	0, ±1, ±2, … ±n-1
spin	quantum number	m_S =	±½

7. The Pauli Exclusion Principle: Two electrons in an atom can never have exactly the same set of all 4 quantum numbers (n, L, m_L, m_S)

Possible electron states

- So … what are the possible combinations of states?
- Notation

n		L	
1	K	0	s
2	L	1	p
3	M	2	d
4	N	3	f

- We can describe an electron state as 1s or 3p or 5f

Energy levels of the electron states

- the energy of an electron is determined by its state
- If there is only **one** electron in the atom, the energy depends on n alone
- If there are more electrons, they interact (repel each other), and so different states have different energies

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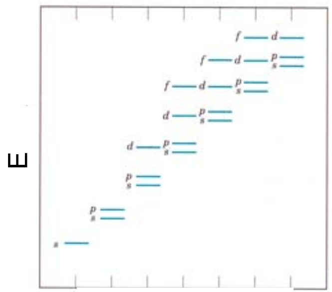
Shell and Subshell Energies



Principle quantum number, n

Schematic representation of the relative energies of the electrons for various shells and subshells (adopted from Callister, Figure 2.4)

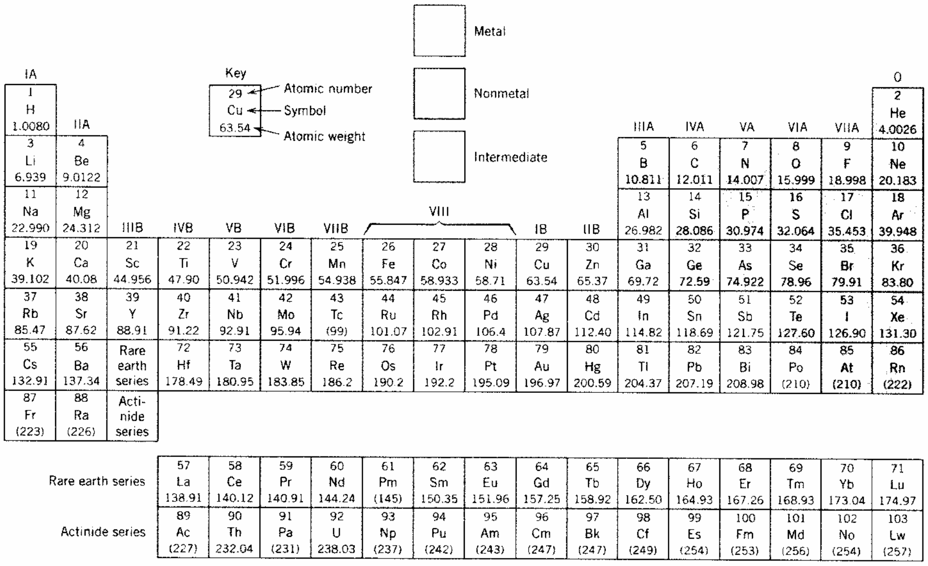
Valence electrons

- The electrons in the outer shell (largest n) are called valence electrons
- Very important for chemical reactions and holding matter together
- If the outer shell is filled, the atom is inert
- If not, there is a tendency for the outer shell to become filled

Electronegative – if it is almost full, the atom has a tendency to gain enough electrons to fill the shell

Electropositive – if it is almost empty, it easily losses the electrons in the outer shell

Periodic Table of Elements



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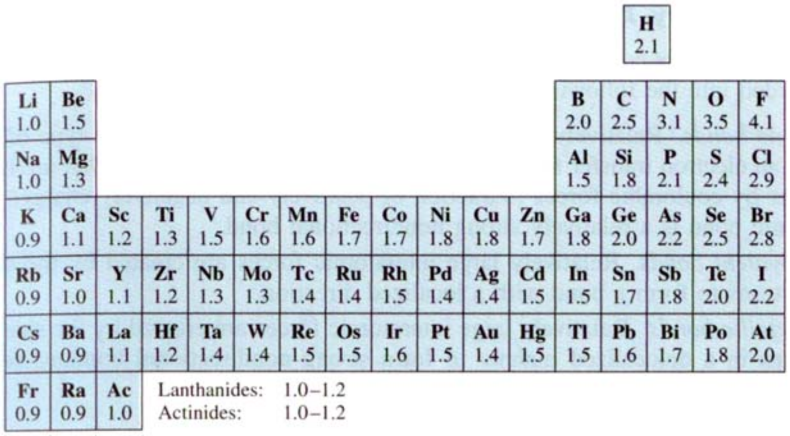
Electronegativity

Electronegativity is a degree to which an atom attracts electron to itself



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Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.1	O 3.5	F 4.1
Na 1.0	Mg 1.3											Al 1.5	Si 1.8	P 2.1	S 2.4	Cl 2.9
K 0.9	Ca 1.1	Sc 1.2	Ti 1.3	V 1.5	Cr 1.6	Mn 1.6	Fe 1.7	Co 1.7	Ni 1.8	Cu 1.8	Zn 1.7	Ga 1.8	Ge 2.0	As 2.2	Se 2.5	Br 2.8
Rb 0.9	Sr 1.0	Y 1.1	Zr 1.2	Nb 1.3	Mo 1.3	Tc 1.4	Ru 1.4	Rh 1.5	Pd 1.4	Ag 1.4	Cd 1.5	In 1.5	Sn 1.7	Sb 1.8	Te 2.0	I 2.2
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Lanthanides: 1.0–1.2
Actinides: 1.0–1.2

The electronegativity of the elements, adapted from Smith&Hashemi

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Chemical reactivity: valence e-s

Noble gases: s^2p^6 configuration

Ne: $1s^22s^2p^6$

Electronegative – if it is almost full, the atom has a tendency to gain enough electrons to fill the shell

Cl: $1s^22s^2p^63s^2p^5$ or [Ne] $3s^2p^5$

$Cl + 1e = Cl^-$ negative ion (anion)

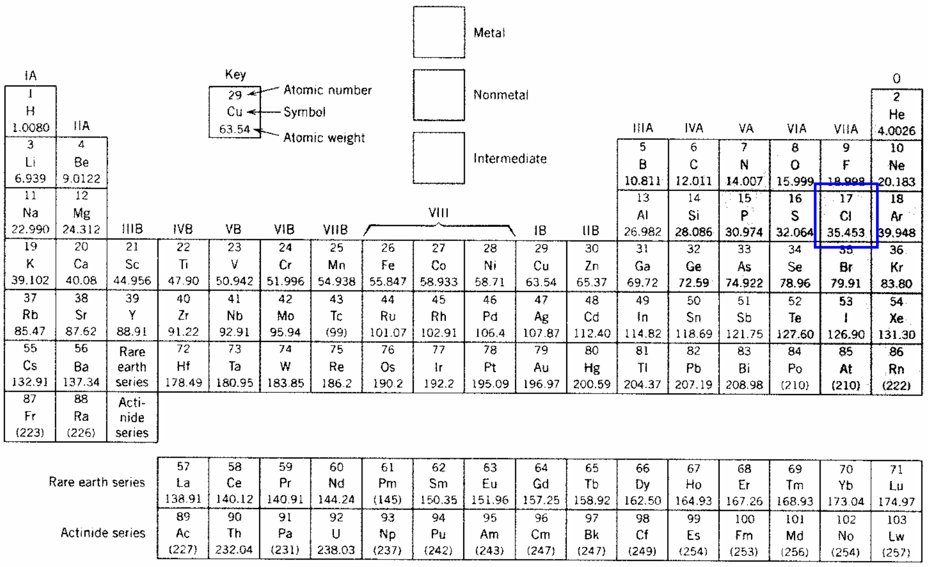
Electropositive – if it is almost empty, it easily losses the electrons in the outer shell (typically metals)

K: $1s^22s^2p^63s^2p^64s^1$ or [Ar] 4s

$K – 1e = K^+$ positive ion (cation)

Oxidation number or oxidation state - not all allowed!!!

Periodic Table of Elements



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2.4 Types of atomic and molecular bonds

- Primary atomic bonds

1. Ionic (large interatomic forces, nondirectional, electron transfer, coulombic forces)
2. Covalent (large interatomic forces, localized (directional), electron sharing)
3. Metallic (large interatomic forces) nondirectional

- Secondary atomic and molecular bonds

1. Permanent dipole bonds
2. Fluctuating dipole bonds

Examples and characteristics of 5 types of bonds

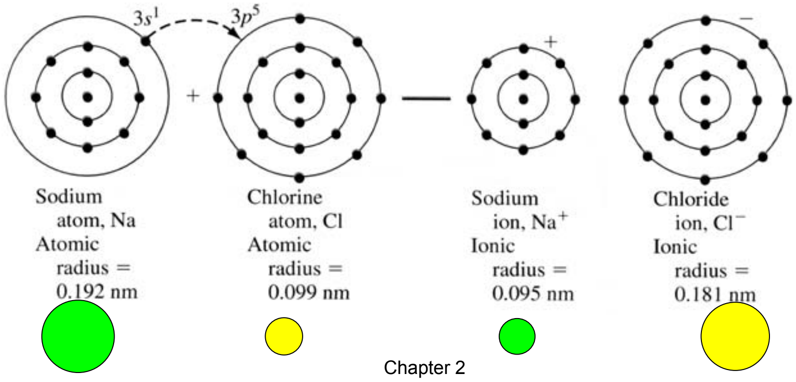
Bond type	Examples	Typical energies, eV/atom	Distinct characteristics
Ionic	**LiF, NaCl, CsCl**	**5-10**	**Nondirected bonding, giving structures of high coordination; no electrical conductivity at low temperature**
Covalent	**Diamond, Si, Ge**	**3-8**	**Spatially directed bonds, structures with low coordination; low conductivity at low temperature for pure crystals**
Metallic	**Li, Na, Cu, Ta**	**0.7-1.6**	**Nondirected bond, structures of very high coordination and density; high electrical conductivity; ductility**
Fluctuating or permanent dipole	Ne, Ar,Kr, Xe, $CHCl_3$	0.05-0.2	Low melting and boiling points
Hydrogen	H_2O, HF	0.25-0.6	Increase in bonding energy over similar molecules without hydrogen bonds

2.5 Ionic bonding

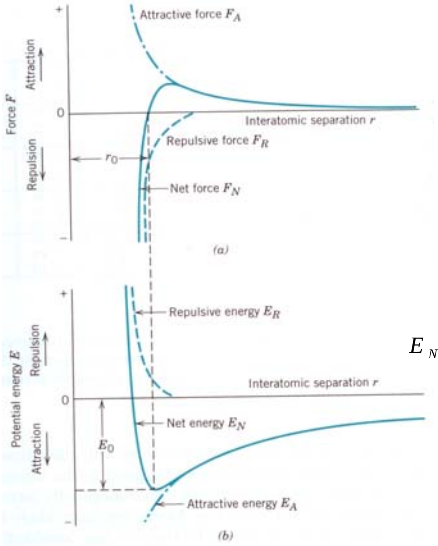
Typically between highly electropositive (metallic) and electronegative (nonmetallic) elements

NaCl Na $1s^22s^2p^63s$ Cl $1s^22s^2p^63s^2p^5$

Na^+ $1s^22s^2p^6$ Cl^- $1s^22s^2p^63s^2p^6$



Force and Energy Diagram



$F_{net} = F_{attactive} + F_{repulvise}$

The **interionic energy** can be defined as the energy needed to rip a compound into its components placed ∞ far apart ($E_{NET}(\infty) = 0$)

$$E_{NET} = E_{attractive} + E_{repulsive} = +\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_o a} + \frac{b}{a^n}$$

- Q.: Calculate attractive force between Na^+ and Cl^- ion at equilibrium interionic separation distance

Interionic Energies

- the energy needed to rip a compound into its components placed ∞ far apart ($E_{net}(\infty) = 0$

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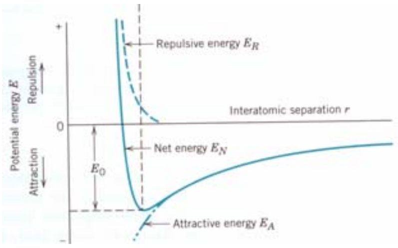


- Q2.: Calculate the net potential energy of a simple Na^+ Cl^- ion pair in equilibrium (using the equation above) and assuming that n = 9

Bonding Energies in Ionic Solids

- Typically large lattice energies (Table 2.6)

  600-3000 kJ/mol
- High melting temperatures

  801°C for NaCl

For NaCl: $E_{Na+Cl-} = -7.42 \times 10^{-19}$J = 4.63eV (2.315 per ion)
Compare to 3.3eV (elsewhere): big difference…!

Ionic Packing

- X-ray crystallography tells us most of ionic compounds (NaCl, CsCl, LiF, etc) are crystals
- Ionic radii of selected ions are listed in the table below (note increase in size, as their principle quantum number increases)
- No preferred orientation (nondirectional character of the ionic bond)
- Geometrical arrangements (coordination) and neutrality is maintained

Cation	Ionic radius (nm)	Anion	Ionic radius (nm)
Li+	0.060	F-	0.136
Na+	0.095	Cl-	0.181
K+	0.133	Br-	0.195
Rb+	0.148	I-	0.216
Cs+	0.169		

Coordination and neutrality in ionic crystals

CsCl:

8 Cl^- ions can pack around Cs^+

$R(Cs^+)/R(Cl^-)=$

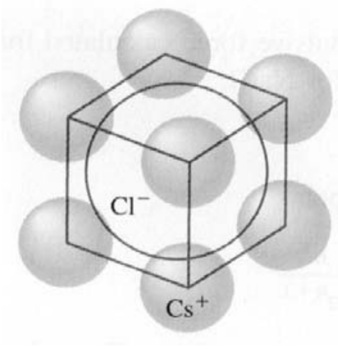
$= 0.169 / 0.181 = 0.934$

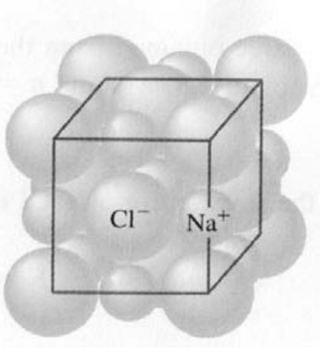
NaCl:

6 Cl^- ions can pack around Na^+

$R(Na^+)/R(Cl^-)=$

$= 0.095 / 0.181 = 0.525$





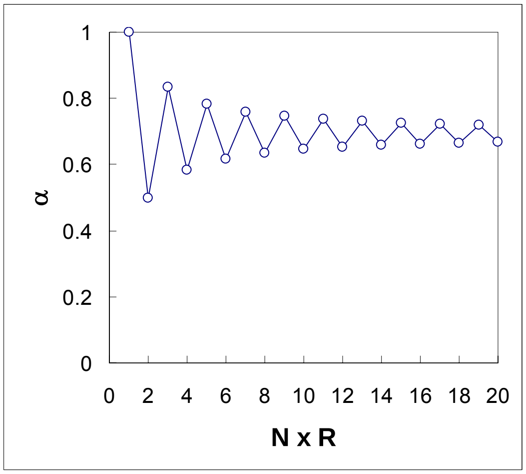
Evaluation of the Madelung Constant

1. Consider a cube of 8 ions
2. Consider a line of alternating in sign ions, with distance R between ions
3. Consider a lattice: lattice sum calculation can be used to estimate Madelung constant, α

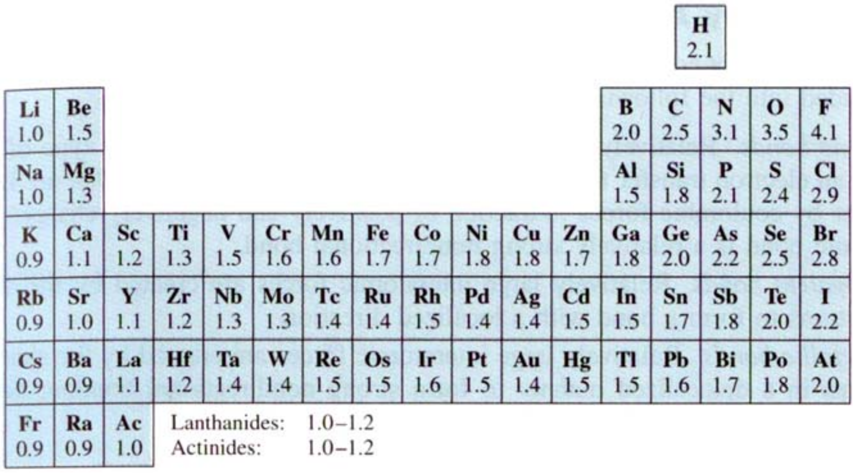
$$\alpha = \sum_j \frac{\pm}{R_{ij}}$$

Structure	α
NaCl	1.7475
CsCl	1.7626
ZnS	1.6381

Madelung constant for line of ions



Electronegativity



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Actinides: 1.0–1.2

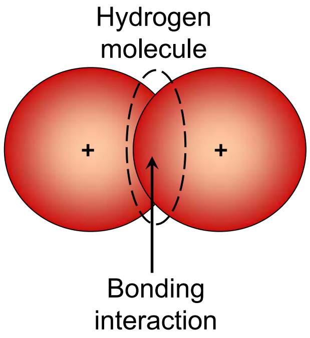
2.6 Covalent bonding

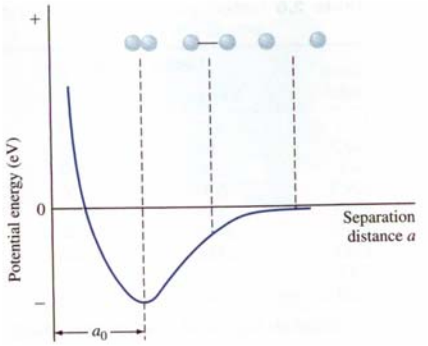
- Takes place between elements with small difference in electronegativity
  - F, O, N, Cl, H, C, Si…
- *s* and *p* electrons are commonly shared to attain noble-gas electron configuration
- Multiple bonds can be formed by one atom

Hydrogen molecule

2 H: 1s $\rightarrow$ H_2 $1s^2$

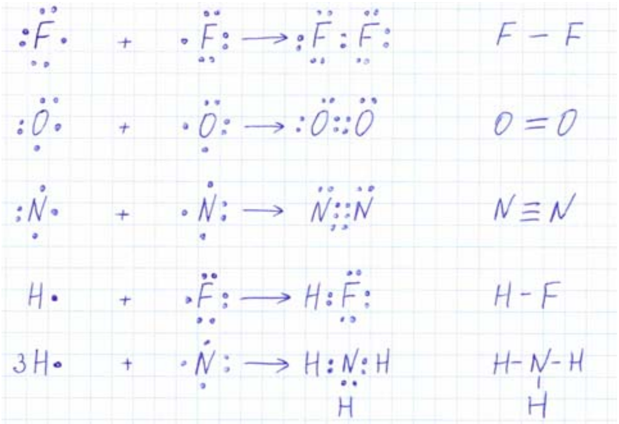
H· + H· $\rightarrow$H : H (electron –pair covalent bond)





Other Covalent Molecules

- F $2s^22p^5$
- O $2s^22p^4$
- N $2s^22p^3$

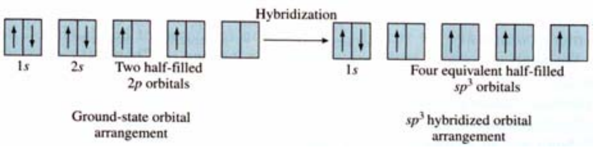


Bond energies and bond lengths of selected covalent bonds

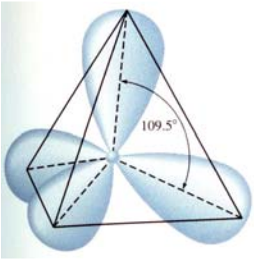
150 - 890 kJ/mol (or ~1.5-9.1eV) 0.074nm (H_2) – 0.18nm (C-Cl)

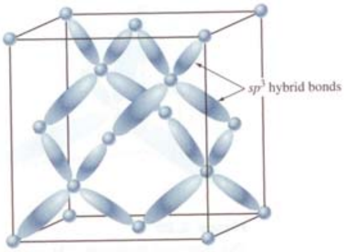
Covalent bonding by carbon

- C $1s^2 2s^2 2p^2$
- Formation of 4 equal covalent bond: hybridization
- *sp^3* hybridization



- other hybridizations..? → sp^2, sp





Carbon-containing molecules

- C and H: *hydrocarbons*
- Structural formulas: CH_4 (methane), C_2H_6 (ethane), and C_4H_{10} (normal butane)

- Saturated C_nH_{2n+2}

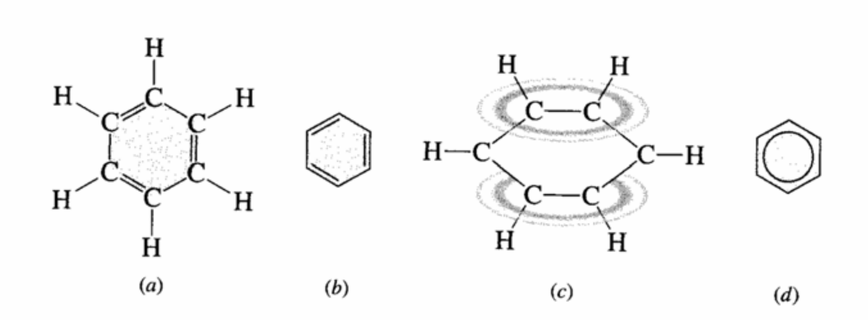
- strong bonds inside molecule, weak between molecules

- Unsaturated C_nH_{2n}, C_nH_{2n-2}

- generally more reactive

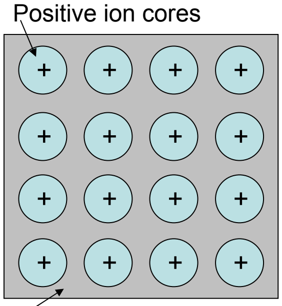
Benzene (C_6H_6)

important for some polymeric materials



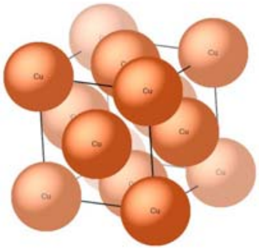
2.7 Metallic Bonding

- Consider Na metal: what holds it together?
- In solid state metal atoms are packed in a systematic pattern or crystal structure
- The valence electrons are weakly bonded to the positive-ion cores and can readily move as “free electrons”



Positive ion cores

Valence electrons in the form of electron charge clouds or “electron gas”



Nonlocalized behavior of electrons in metals

- **High electrical conductivity**

- electrons move easily when E-field applied

- **High thermal conductivity**

- the electrons can carry energy through metal

- **High density**

- outer shell removed from atoms, so can be packed together

- **High ductility**

- if metal distorted, bent, electrons can quickly move to compensate
- metal bond is not directional

2.8. Secondary Bonding

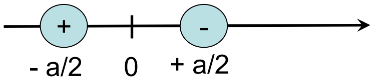
- Fluctuating or permanent dipoles (also called ***physical bonds, or van der Waals bonds or forces)***

- weak relatively to the primary bonding (2-5eV/atom or ion)
    ~ 0.1eV/atom or ~ 10 kJ/mol

- always present, but overwhelmed by other interaction
    most easily observed in inert gases

- dipoles to be considered…

Electric dipole



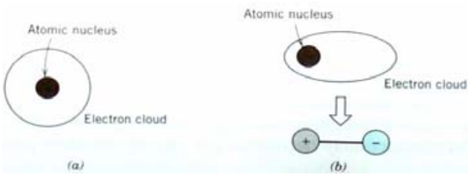
consider a “+” and “-” charge (e) separated by a distance ***a***

Dipole moment [debye]: $\mu = e \times a$

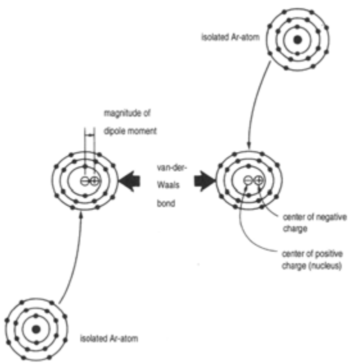
What is the PE (U) of two dipoles in a distance *x* apart?

$$U = -\frac{ke^2}{x-a} + 2\frac{ke^2}{x} - \frac{ke^2}{x+a}$$

Fluctuation Dipole

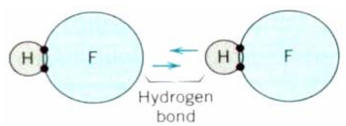


- Noble-gas elements: s^2p^6
- Stronger effect for larger electron shells → Boiling temperature increases as a function of Z



Schematic representation of how the van-der-Waals bond is formed by interaction of induced dipoles.

Permanent Dipoles



- When a covalent molecule has permanent dipole? Depends on geometry of the molecule…
- CH_4 ? CH_3Cl ? H_2O ?

Q.: Calculate the dipole moment associated with the ionic model of the water molecule. The length of the O-H bond is 0.097nm and the angle between the bonds is 104.5°.

- Hydrogen bond: permanent dipole-dipole interaction for the molecules with a hydrogen atoms bonded to a highly electronegative element (F, Cl, O, N)

e.g.: H_2O, polymeric materials

Permanent dipole bond: a secondary bond created by the attraction of molecules that have permanent dipoles

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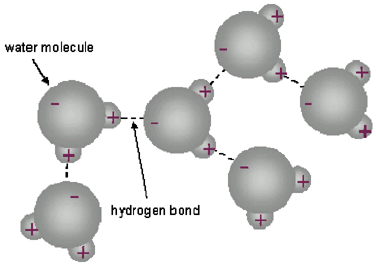
Q.: Calculate the dipole moment associated with the ionic model of the water molecule. The length of the O-H bond is 0.097nm and the angle between the H-O-H bonds is 104.5°.



2.9 Mixed Bonding

- Ionic - Covalent Mixed Bonding

AB: $$\%\_ionic\_character = 100\% \times \left(1 - e^{\left(-\frac{1}{4}\right)(X_A - X_B)^2}\right)$$

where X_A and X_B are the electronegativity of the atoms A and B (Table above) e.g. ZnSe, GaAs

- Metallic - Ionic Mixed Bonding

Typical for intermetallic compounds between elements with significant difference in electronegative

e.g.: $NaZn_{13}$

Summary

- Primary atomic bonds

1. Ionic (large interatomic forces, nondirectional, electron transfer, coulombic forces)

$$\boxed{E_{net} = E_{attraction} + E_{repulsion} = +\frac{Z_1 Z_2 e^2}{4\Pi \varepsilon_o a} + \frac{b}{a^n}}$$

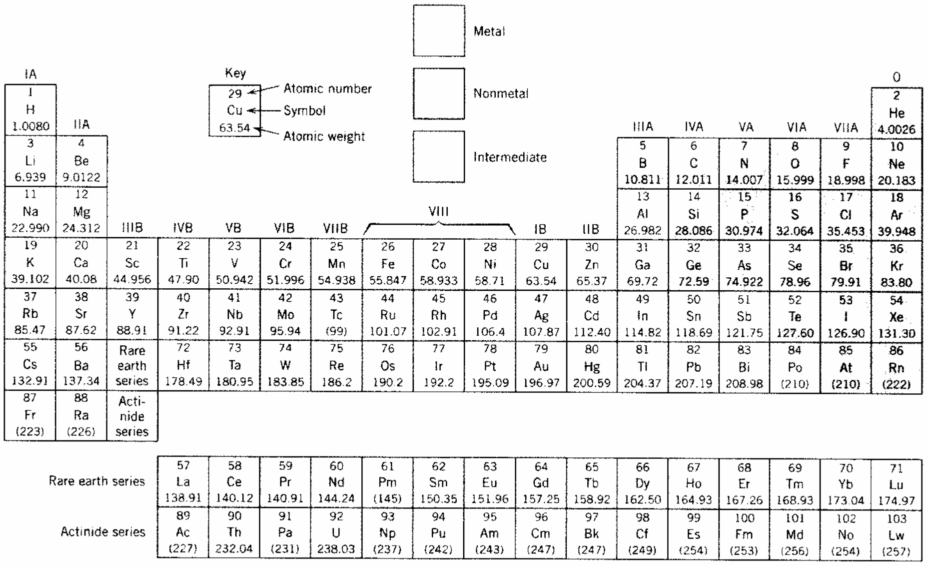
2. Covalent (large interatomic forces, localized (directional), electron sharing)
3. Metallic (large interatomic forces, nondirectional)

- Secondary atomic and molecular bonds

Dipole moment [debye]: $\mu = e \times a$

1. Permanent dipole bonds
2. Fluctuating dipole bonds

Periodic Table of Elements



Metal

Nonmetal

Intermediate

Key

29 ← Atomic number
Cu ← Symbol
63.54 ← Atomic weight

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080																	2 **He** **4.0026**
3 Li 6.939	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 **O** 15.999	9 F 18.998	10 **Ne** **20.183**
11 Na 22.990	12 Mg 24.312											13 Al 26.982	14 Si **28.086**	15 **P** **30.974**	**16** **S** **32.064**	17 **Cl** **35.453**	**18** **Ar** **39.948**
19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.54	30 Zn 65.37	31 Ga 69.72	32 **Ge** **72.59**	33 **As** **74.922**	34 **Se** **78.96**	35 **Br** **79.91**	**36** **Kr** **83.80**
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 **Te** **127.60**	**53** **I** **126.90**	**54** **Xe** **131.30**
55 Cs 132.91	56 Ba 137.34	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	**85** **At** **(210)**	**86** **Rn** **(222)**
87 Fr (223)	88 Ra (226)	Acti-nide series															

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa (231)	92 U 238.03	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lw (257)

Problems

2.1 How many atoms are there in 1 g of copper?

2.2. What is the mass in grams of one atom of copper?

2.3 The first Canadian pennies were made in 1858 and had a diameter of 25.4 mm and weight of 4.54 grams. Composition of the penny was 95% copper, 4% tin, 1% zinc (weight %) alloy.

(a) What are the atomic percentages of Cu, Sn and Zn in this alloy?

(b) Imagine that you found 1234 such pennies in your backyard. The current scrap copper value is ~ \$3.4/kg (Cu). How much will you gain, if you give “this treasure” away as a scrap copper metal?

2.4 What is the chemical formula of an intermetallic compound that consists of 15.68wt% Mg and 84.32wt % Al?

2.5 Calculate the energy in joules and electron volts of the photon whose wavelength is 303.4nm.

2.6 A hydrogen atom exists with its electron in the n = 6 state. The electron undergoes a transition to the n = 2 state. Calculate (*a*) the energy of the photon emitted, (*b*) its frequency, and (*c*) its wavelength in nanometers.

2.7 Write the electron configuration of the following ions using the spdf notation

(a) Mn^{2+}, Mn^{3+}, Mn^{7+}; (b) S^{4+}, S^{6+}, S^{2-}; (c) Mo^{3+}, Mo^{4+}, Mo^{6+}.

2.8 Carbon tetrachloride (CCl_4) has a zero dipole moment. What does this tell us about the C-Cl bonding arrangement in this molecule?