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Chapter 2

Chemical Compounds

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Atomic Structure & Subatomic Particles

Atoms are composed of three subatomic particles:

- electrons (e^-)
- protons (p^+)
- neutrons (n^0).

These particles were discovered in a series of important experiments which began in the 1890's.

Radioactivity

Becquerel (1896)

- U ore emits rays that “fog” a photographic plate.

Marie and Pierre Curie (1898)

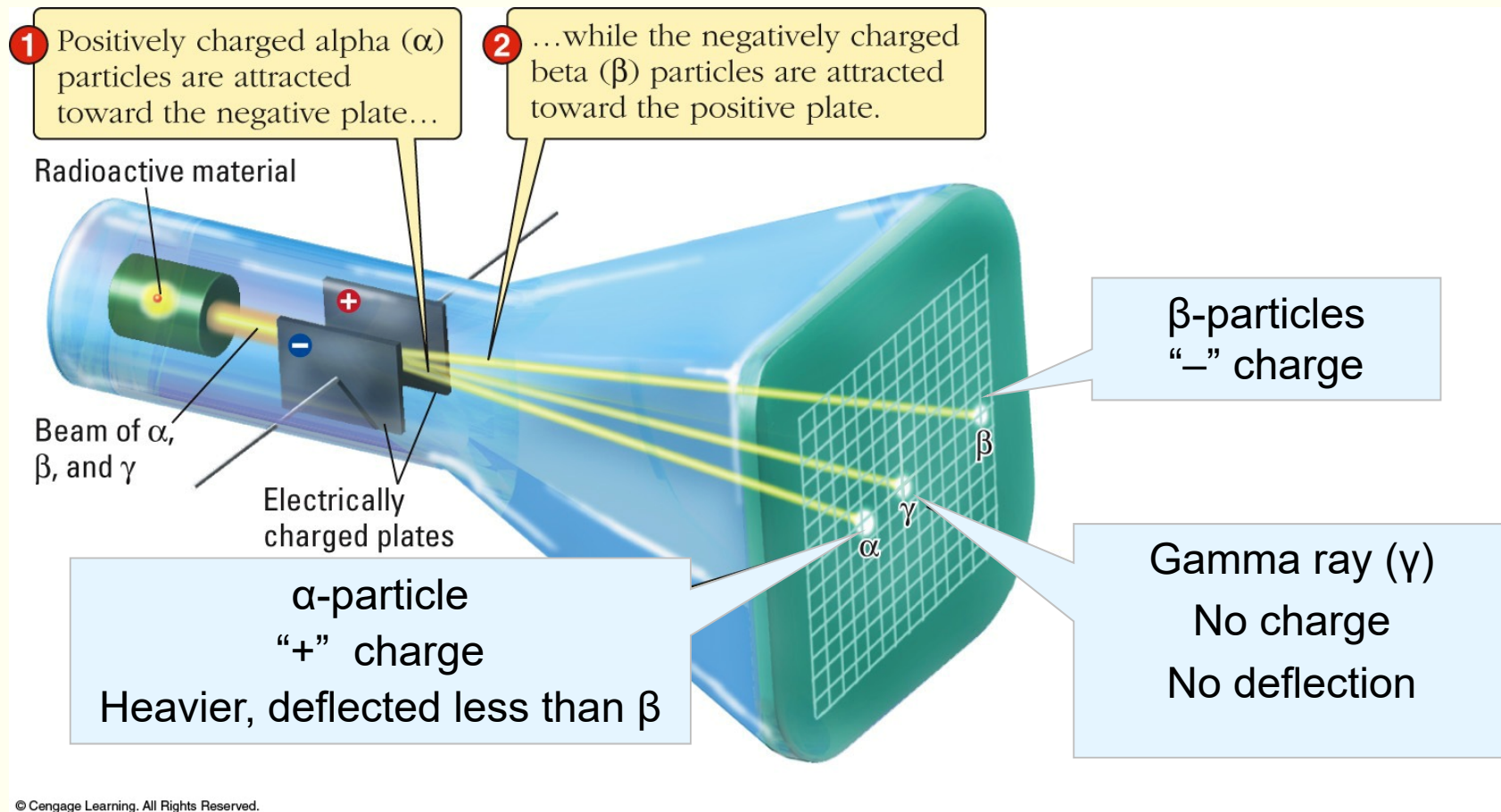
- Isolated new elements (Po & Ra) that did the same.
- Marie Curie called the phenomenon **radioactivity**.

Are these “rays” electrically charged? Scientists used a well known property:

- Like charges repel; opposite charges attract.
- Uncharged particles are unaffected.

Radioactivity

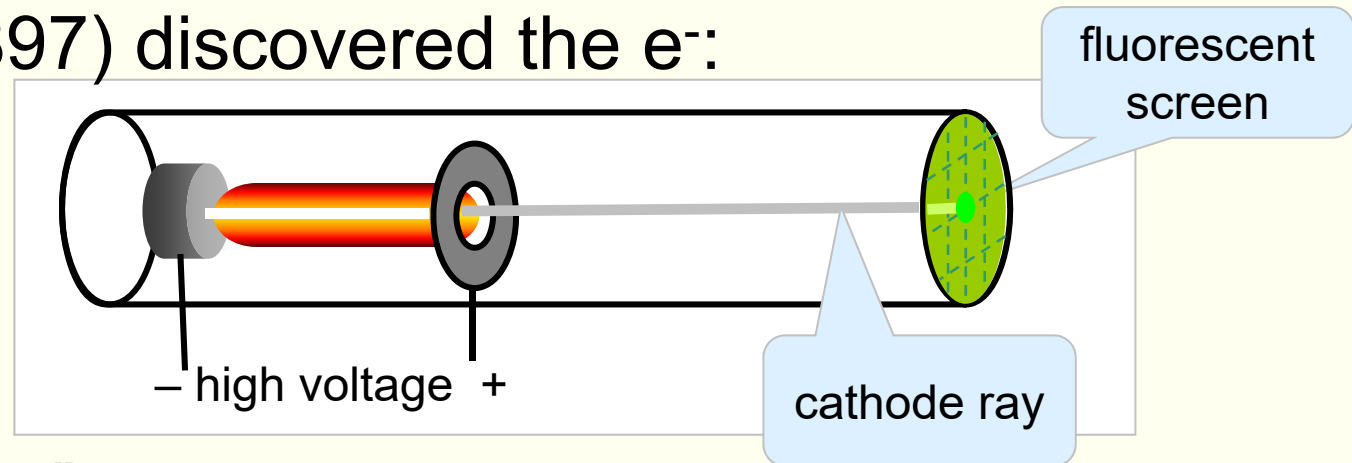
Three distinct types of radiation were discovered:



Atoms must contain smaller sub-units.

Electrons

Thomson (1897) discovered the e^- :



“Cathode rays”

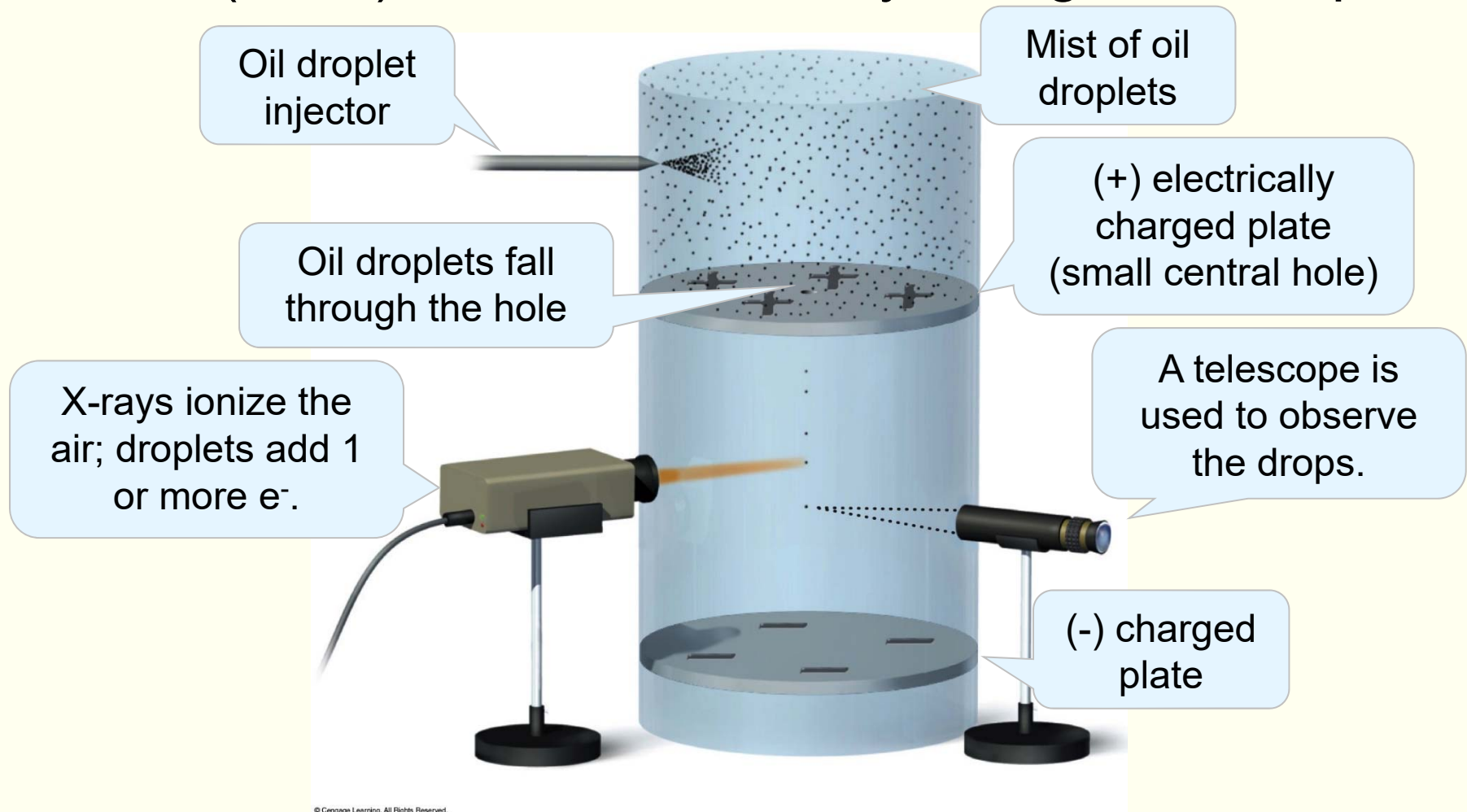
- Travel from cathode (-) to anode (+).
- Negative charge (e^-).
- Emitted by cathode metal atoms.

Electric and magnetic fields deflect the beam.

- Gives mass/charge of $e^- = -5.60 \times 10^{-9} \text{ g/C}$.
- Coulomb (C) = SI unit of charge.

Electrons

Millikan (1911) studied electrically-charged oil drops.



(+) and (-) plate charges are adjusted until a drop is stationary.

Electrons

Droplet charges obeyed:

$$n (-1.60 \times 10^{-19} \text{ C}) \quad \text{with } n = 1, 2, 3, \dots$$

multiple e^-
per drop

$$n (e^- \text{ charge})$$

$$\text{Modern value} = -1.602176487 \times 10^{-19} \text{ C.}$$

$$= -1 \text{ "atomic units".}$$

$$m_e = \cancel{\text{charge}} \times \frac{\text{mass}}{\cancel{\text{charge}}}$$

$$= (-1.60 \times 10^{-19} \text{ C})(-5.60 \times 10^{-9} \text{ g/C}) = 8.96 \times 10^{-28} \text{ g}$$

$$\text{Modern value} = 9.10938215 \times 10^{-28} \text{ g}$$

Protons

Atoms gain a positive charge when e^- are lost.

- Implies a positive fundamental particle.

Hydrogen ions had the lowest mass.

- Hydrogen nuclei assumed to have “unit mass”
- Called **protons**.

Modern science: $m_p = 1.672621637 \times 10^{-24} \text{ g}$

$$m_p \approx 1800 \times m_e$$

Charge = $-1 \times (e^- \text{ charge})$

$$= +1.602176487 \times 10^{-19} \text{ C}$$

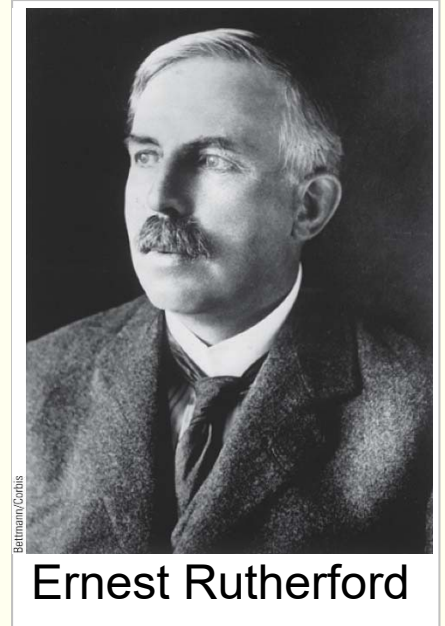
= +1 atomic units

The Nuclear Atom

How are the p^+ and e^- arranged?

Thompson:

- Ball of uniform positive charge, with small negative dots (e^-) stuck in it.
- The “plum-pudding” model.



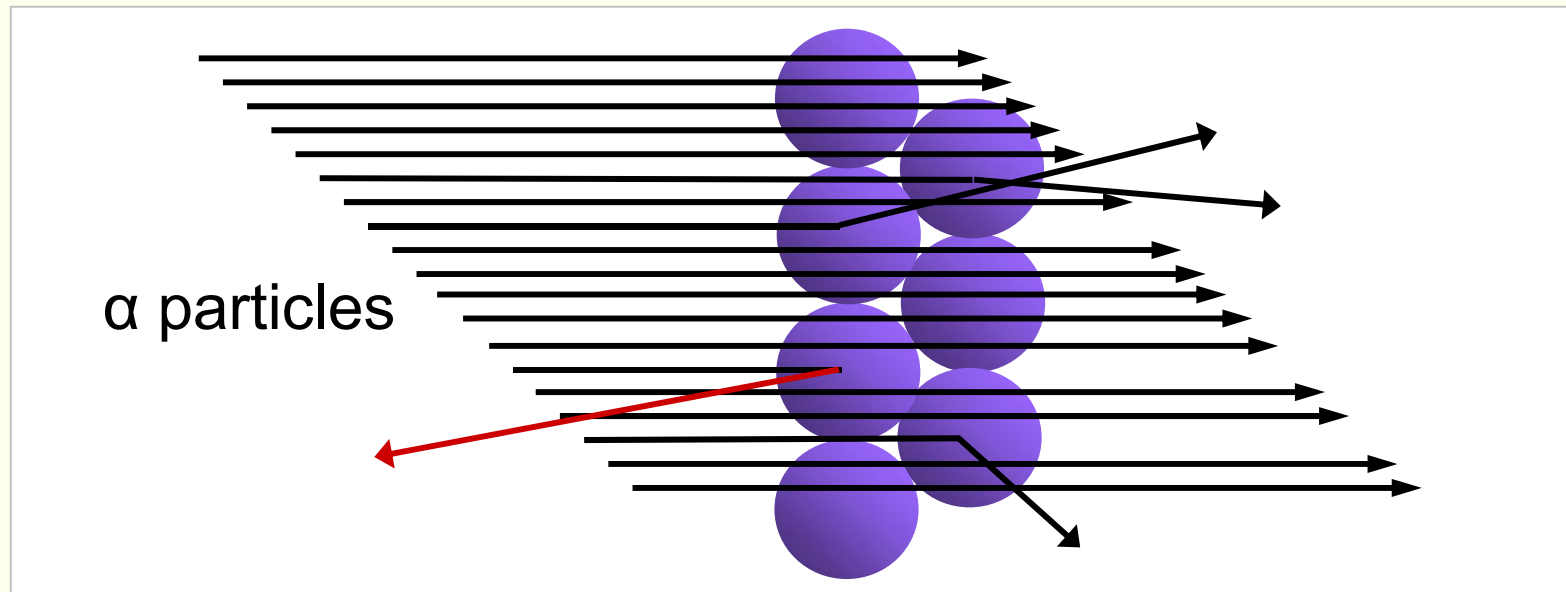
1910

Rutherford fired α -particles at thin metal foils

- Expected them to pass through with minor deflections.

The Nuclear Atom

But ... some had large deflections.

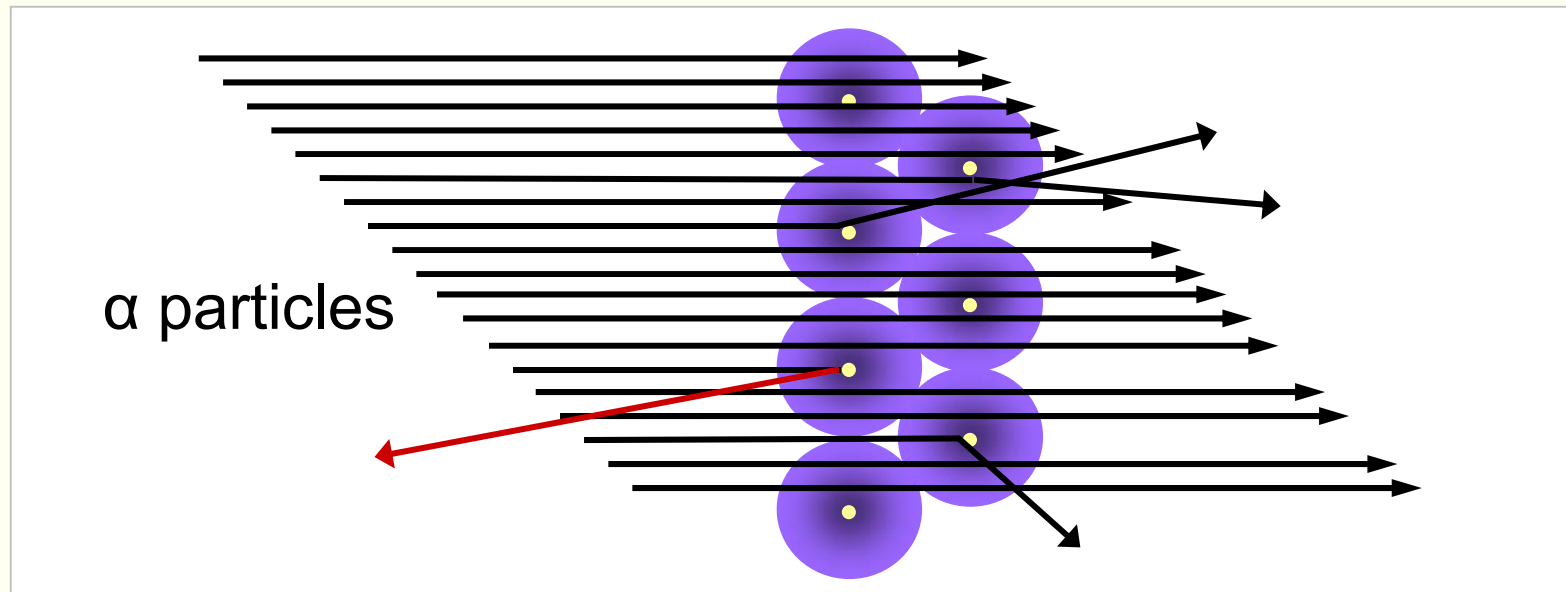


Rutherford

“It was about as credible as if you had fired a 15-inch shell at a piece of paper and it came back and hit you.”

The Nuclear Atom

Most of the mass and all “+” charge is concentrated in a small core, the **nucleus**.



- A gold nucleus is $\approx 10,000$ x smaller in diameter than a gold atom.
- e^- occupy the remaining space.

Neutrons

Measured atomic masses were too large:

- Larger than the sum of the p^+ and e^- masses.
- Rutherford proposed a neutral particle.

Chadwick (1932) fired α -particles at Be atoms.

- Neutral particles, **neutrons** (n^0), were ejected.
- The n^0 beam ejected p^+ from other atoms, allowing detection.

$$m_n \approx m_p \text{ (0.1\% larger).}$$

$$m_n = 1.674927211 \times 10^{-24} \text{ g.}$$

n^0 are present in all atoms (except normal H).

The Nuclear Atom

Nucleus

- Contains p^+ and n^0 .
- Most of the atomic mass.
- Compact.
- Positive (each p^+ has +1 charge).

Electrons

- Tiny low mass particles surrounding the nucleus.
- Occupy most of the volume.
- Charge = -1.

Atoms are neutral:

Number of e^- = Number of p^+

Atomic sizes

How many copper atoms lie across the diameter of a penny? A penny has a diameter of 1.90 cm, and a copper atom has a diameter of 256 pm.

$$1 \text{ pm} = 1 \times 10^{-12} \text{ m} \quad ; \quad 1 \text{ cm} = 1 \times 10^{-2} \text{ m}$$

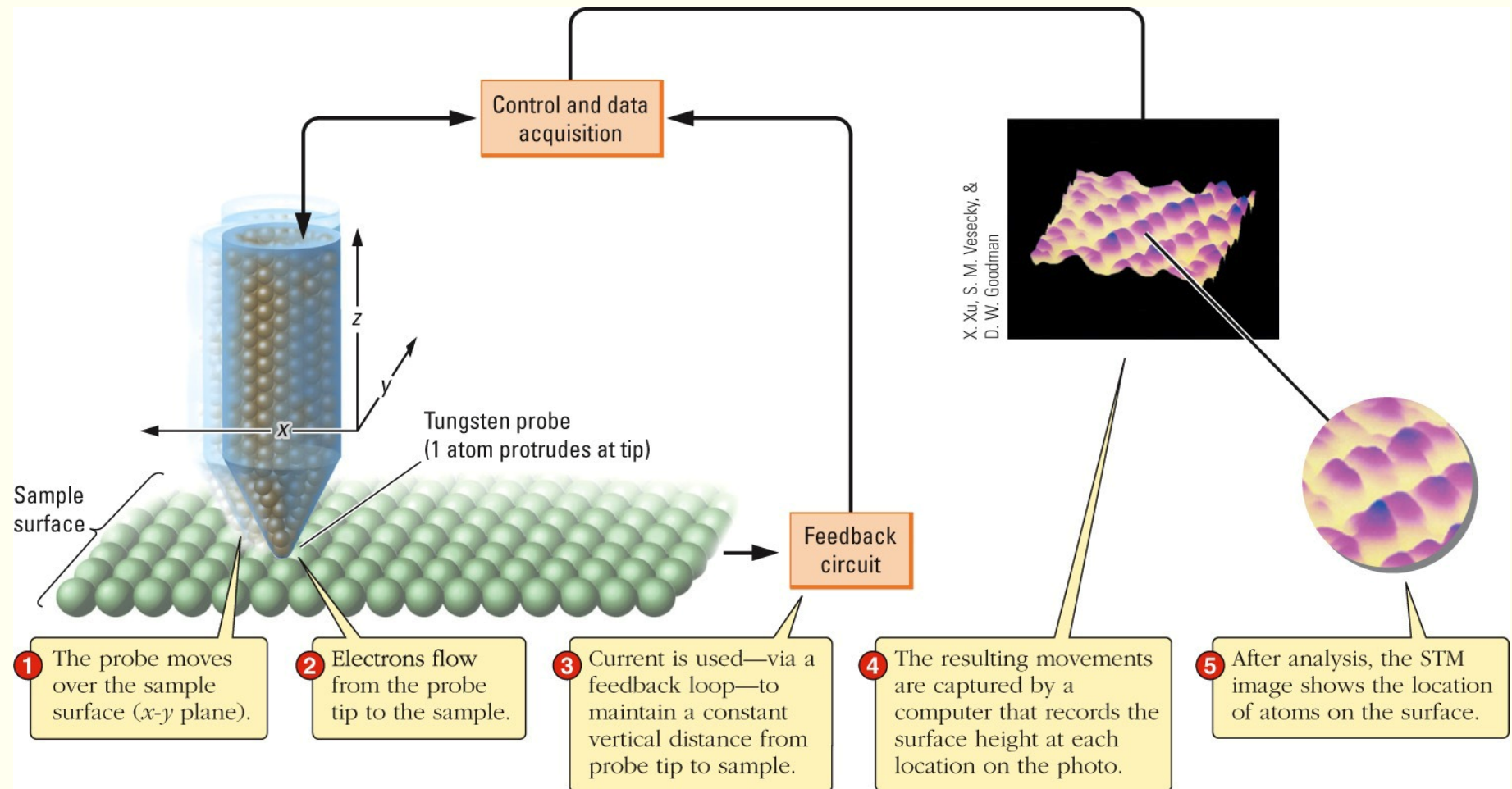
$$1.90 \text{ cm} \times \frac{1 \times 10^{-2} \text{ m}}{1 \text{ cm}} \times \frac{1 \text{ pm}}{1 \times 10^{-12} \text{ m}} = 1.90 \times 10^{10} \text{ pm}$$

Number of atoms across the diameter:

$$1.90 \times 10^{10} \text{ pm} \times \frac{1 \text{ Cu atom}}{256 \text{ pm}} = 7.42 \times 10^7 \text{ Cu atoms}$$

Scanning Tunneling Microscopy

The scanning tunneling microscope allows us to “see” individual atoms:



Atomic Numbers & Mass Numbers

All atoms of the same element have the same number of protons:

Atomic number (Z) = number of p^+

The mass number (A) = number of p^+ + number of n^0

For element X, write: A_ZX e.g. ${}^{12}_6C$

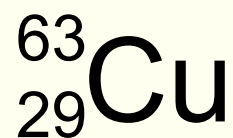
or AX e.g. ${}^{12}C$

or X-A e.g. carbon-12

(Z is constant for a given element)

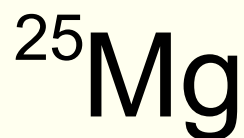
Atomic Numbers & Mass Numbers

How many p^+ , n^0 and e^- are in the following elements:



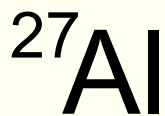
$$29 p^+ = 29 e^- \text{ (neutral atom: } e^- = p^+)$$

$$63 - 29 = 34 n^0$$



$$12 p^+ = 12 e^- \text{ (periodic table; neutral)}$$

$$25 - 12 = 13 n^0$$



$$13 p^+ = 13 e^-$$

$$27 - 13 = 14 n^0$$

Isotopes & Average Atomic Mass

Atoms are very small.

- 1 tsp of water contains 3x as many atoms as there are tsp of water in the Atlantic Ocean!

They are so small is difficult to measure their mass.

Relative masses were determined experimentally

- When H and F combined to form HF, they reacted in a 1:19 mass ratio
- Implied $m_F = 19 m_H$

Isotopes & Average Atomic Mass

Absolute atomic masses refer to the mass of a single ^{12}C atom:

or amu or
dalton (Da)

1 Unified atomic mass unit (u) = $\frac{1}{12}$ (mass of ^{12}C)

$$1 \text{ u} = 1.66054 \times 10^{-24} \text{ g}$$

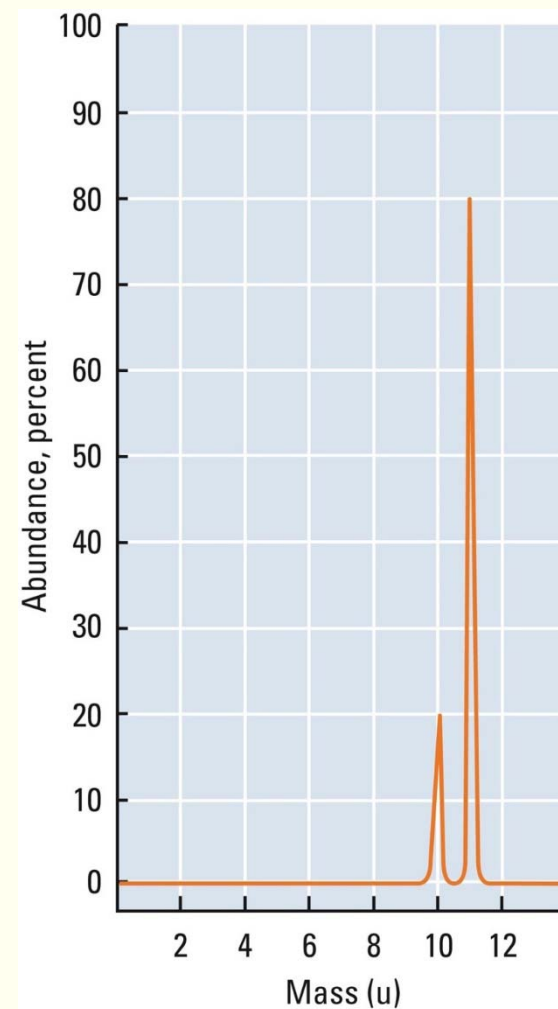
Particle	Mass			Charge a.u.
	g	u	~u	
e^-	9.1094×10^{-28}	0.000548579	0	-1
p^+	1.6726×10^{-24}	1.00728	1	+1
n^0	1.6749×10^{-24}	1.00866	1	0

Mass Spectrometer

A mass spectrometer measures the mass to charge ratio of charged atoms and molecules.

Pure neon result:

- Three peaks: 3 different types of Ne.
- Peak areas give relative amounts of each.



Isotopes & Average Atomic Mass

Atoms of the **same element** with different mass (different A) are called **isotopes**. They have:

- equal numbers of p^+
 - different numbers of n^0
-

Neon isotopes:	${}_{10}^{20}\text{Ne}$	10 p^+ and 10 n^0
	${}_{10}^{21}\text{Ne}$	10 p^+ and 11 n^0
	${}_{10}^{22}\text{Ne}$	10 p^+ and 12 n^0

Isotopes & Atomic Weight

Most elements occur as a mixture of isotopes.

Magnesium is a mixture of:

	²⁴ Mg	²⁵ Mg	²⁶ Mg
Number of p ⁺	12	12	12
Number of n ⁰	12	13	14
Mass (amu)	23.985	24.986	25.983
Abundance	79 %	10 %	11 %
Atomic weight	24.305		

$$\text{Atomic wt} = \sum (\text{fractional abundance})(\text{isotope mass})$$

Sum of...

fraction of
each isotope

Average Atomic Mass

Boron contains ^{10}B and ^{11}B (10.0129; 11.0093 u). ^{10}B is 19.91% abundant. Calculate the atomic mass of B.

$$^{10}\text{B} \quad \frac{19.91}{100} (10.0129 \text{ u}) = 1.994 \text{ u}$$

fraction mass

Abundance of ^{11}B = 100% - 19.91% = 80.09%

$$^{11}\text{B} \quad \frac{80.09}{100} (11.0093 \text{ u}) = 8.817 \text{ u}$$

fraction mass

$$\text{Atomic weight of B} = 1.994 + 8.817 \text{ u}$$
$$= 10.811 \text{ u}$$

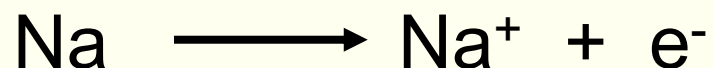
5
B
Boron
10.811

Ions & Ionic Compounds

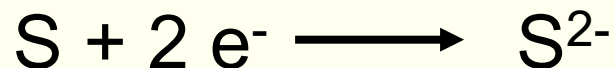
Ions - charged units

- formed by transfer of e^- between elements.

Cation = positive ion. Metals form cations



Anion = negative ion. Nonmetals form anions

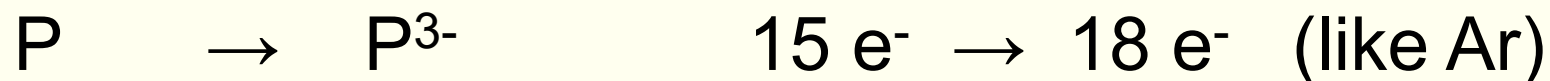
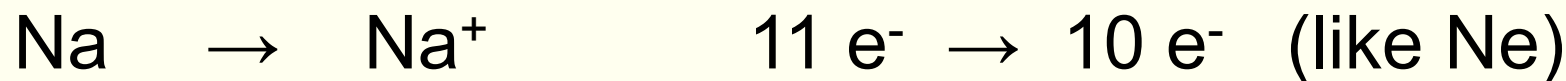
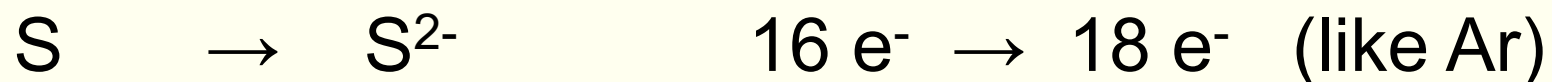


Monatomic Ions

Main group elements

Add/lose enough e^- to “get to” the nearest noble gas.

- Charge on ion = group A# or (grpA# - 8)
- Each e^- lost produces one positive charge
- Each e^- gained adds one negative charge



Monatomic Ions

Transition metals:

- lose varying number of e⁻.
- old (and new) group number not very helpful.

Ti	Ti ²⁺	(grp 4B)
Cr	Cr ²⁺ or Cr ³⁺	(grp 6B)
Fe	Fe ²⁺ or Fe ³⁺	(grp 8B)
Cu	Cu ⁺ or Cu ²⁺	(grp 1B)
Mn	Mn ²⁺ Mn ⁵⁺ or Mn ⁷⁺	(grp 7B)

Monatomic Ions

Number of e⁻ lost varies.

Hydrogen appears twice because H can lose or gain an electron.

Negative charges for Groups 5A, 6A, and 7A equal 8 - A-Group number.

1A (1)		2A (2)		Transition metals									3A (13)		4A (14)	5A (15)	6A (16)	7A (17)	8A (18)
H ⁺																	H ⁻		
Li ⁺																			
Na ⁺	Mg ²⁺																		
K ⁺	Ca ²⁺																		
Rb ⁺	Sr ²⁺																		
Cs ⁺	Ba ²⁺																		

Positive charges for Groups 1A and 2A equal the Group number.

Transition metals can lose varying numbers of electrons, forming cations with different charges. Most transition metals form 2+ ions and many form 3+ ions.

Positive charge for Group 3A equals A-Group number.

Legend:
 Main-group metals (grey)
 Transition metals (blue)
 Metalloids (orange)
 Nonmetals, noble gases (purple)

Polyatomic Ions

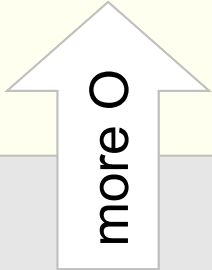
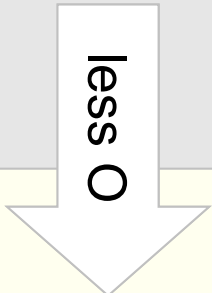
Multiple atom “units” with a net electrical charge.

Ion	Name
NH_4^+	ammonium ion
OH^-	hydroxide ion
SO_4^{2-}	sulfate ion
HSO_4^-	hydrogen sulfate ion
CN^-	cyanide ion
NO_3^-	nitrate ion

Memorize all the ions in Table 2.2

Oxoanions

A series of related names:

				
				ClO_4^- perchlorate
PO_4^{3-} phosphate	SO_4^{2-} sulfate	NO_3^- nitrate		ClO_3^- chlorate
PO_3^{3-} phosphite	SO_3^{2-} sulfite	NO_2^- nitrite		ClO_2^- chlorite
				ClO^- hypochlorite

If they begin with H, add a prefix “hydrogen”

HSO_4^- hydrogen sulfate ion
(common name: bisulfate ion)

HCO_3^- hydrogen carbonate ion
(common name: bicarbonate ion)

Ionic Compounds

Ionic compounds are:

- Held together by electrostatic forces.
- Always electrically neutral.

Cation	Anion	Compound	Charge Balance
Mg^{2+}	F^-	MgF_2	$(+2) + 2(-1) = 0$
Mg^{2+}	SO_4^{2-}	MgSO_4	$(+2) + (-2) = 0$
Mg^{2+}	PO_4^{3-}	$\text{Mg}_3(\text{PO}_4)_2$	$3(+2) + 2(-3) = 0$
NH_4^+	CO_3^{2-}	$(\text{NH}_4)_2\text{CO}_3$	$2(+1) + (-2) = 0$

Recognizing Ionic Compounds

Compounds are ionic when they contain:

- A *metal* cation + a non-metal anion
- One (or more) *polyatomic ion*(s)

Ionic Compound	non ionic
CaCl_2	CH_3OH
Na_2SO_3	BrF_5
$\text{Sr}_3(\text{PO}_4)_2$	H_2O
NH_4NO_3	SO_3

Naming Ions & Ionic Compounds

Positive ions

Most are metal ions (exception: ammonium NH_4^+).

- metal ion with only one charge state?
 - Use *metal name + ion*.
- metal ion with multiple charge states?
 - Use *metal name + (Roman numeral)* to show charge.

Na^+ sodium ion

Ca^{2+} calcium ion

Fe^{2+} iron(II) ion

Fe^{3+} iron(III) ion

no
space

Naming Ions & Ionic Compounds

Negative ions

- Monatomic ion?
 - Add “-ide” to the name stem.
- Polyatomic ion?
 - Memorize these.

P	phosphorus	P^{3-}	phosphide ion
S	sulfur	S^{2-}	sulfide ion
		SO_3^{2-}	sulfite ion

Naming Ionic Compounds

Name the ions and add together...

... cation then anion (drop "ion" from both).

Single charge metal-ion examples

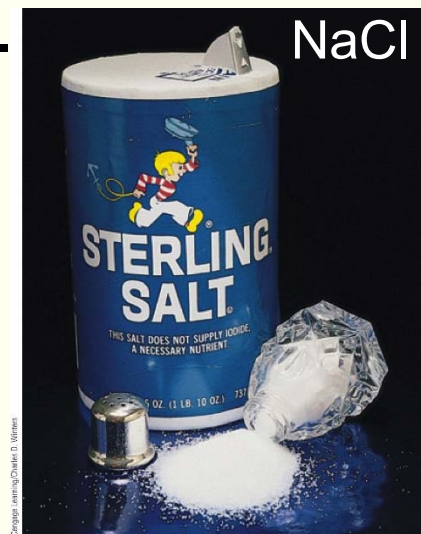
NaCl sodium chloride

MgCO₃ magnesium carbonate

SrO strontium oxide

Mg(OH)₂ magnesium hydroxide

K₂Cr₂O₇ potassium dichromate



Naming Ionic Compounds

Multiple charge examples

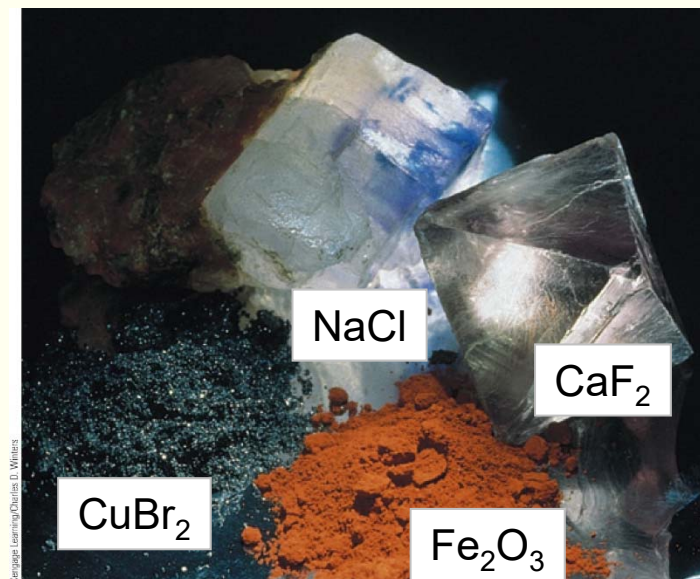
FeCl_2 iron(II) chloride

FeCl_3 iron(III) chloride

Cu_2O copper(I) oxide

CuO copper(II) oxide

Fe_2O_3 iron(III) oxide



Naming Ionic Compounds

When are Roman numerals used?

Main block metals form one type of ion:

- equal to A group number
- omit Roman numerals.
- **exceptions**: lead (Pb^{2+} , Pb^{4+}) and tin (Sn^{2+} , Sn^{4+}).

Transition metals form multiple ions

- use Roman numerals.
- **exceptions**: silver (Ag^+) and zinc (Zn^{2+}).

Naming Compounds

Li_2SO_3 lithium sulfite

CuSO_4 copper(II) sulfate

AlCl_3 aluminum chloride

AgF silver fluoride

Na_2S sodium sulfide

PbO_2 lead(IV) oxide

Naming Compounds

sodium hypochlorite



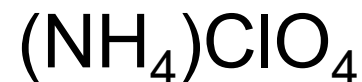
chromium(III) sulfate



potassium dichromate



ammonium perchlorate



potassium chloride



Ionic Compound Properties

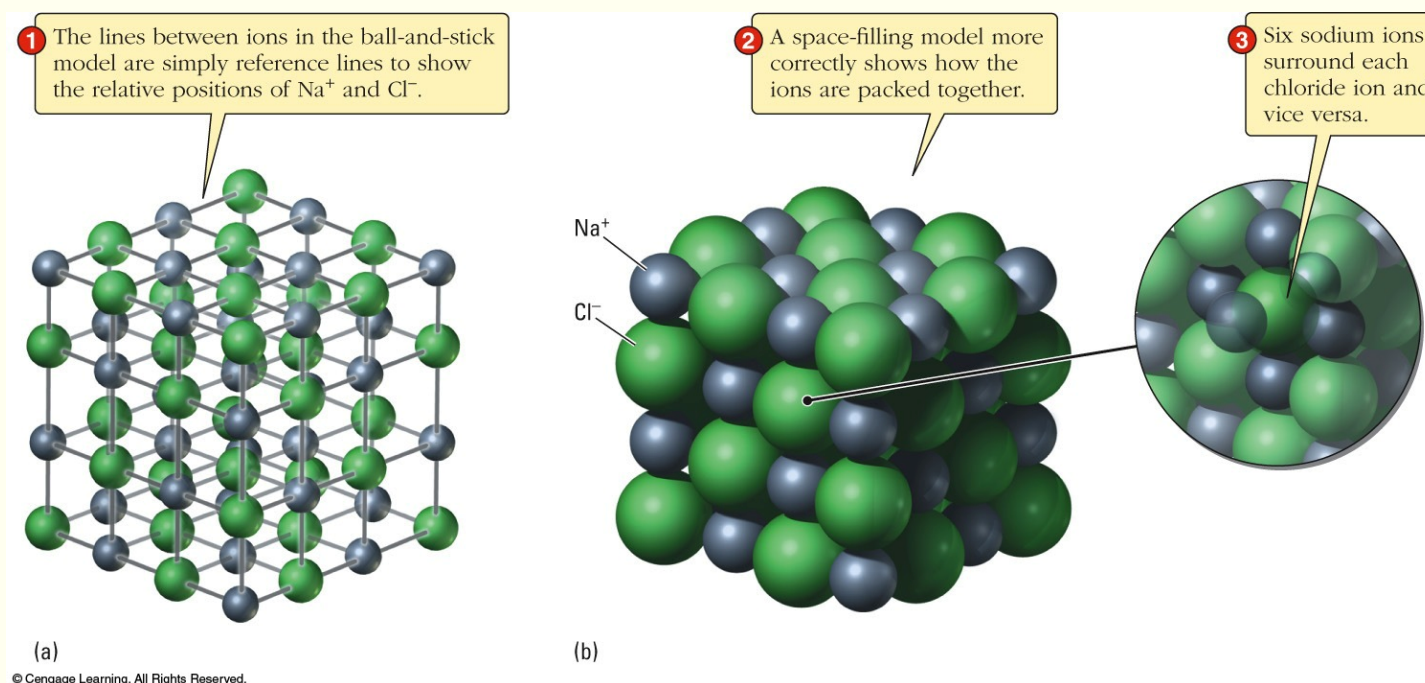
Ionic compounds are generally:

- Solids at room temperature with high melting and boiling temperatures.
- Hard
- Brittle (and easily cleaved).
- Poor heat conductors.
- Poor electrical conductors (unless molten).

The Crystal Lattice

Ionic compounds exist as **Crystal lattices**

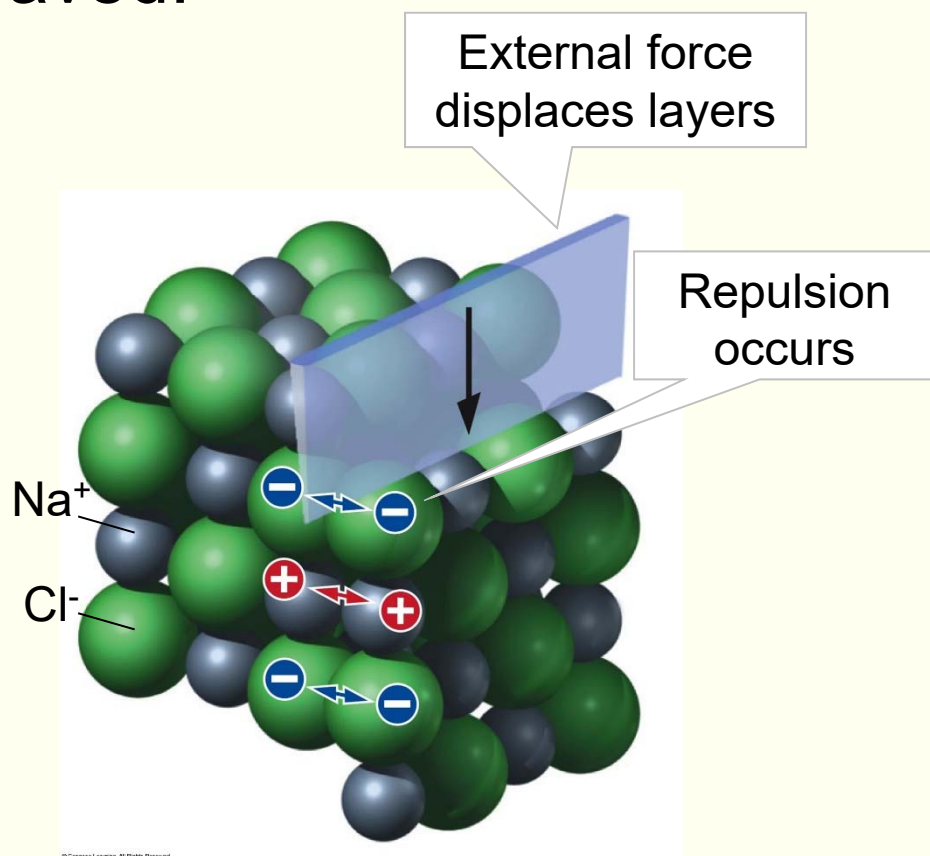
- Each ion is surrounded by many others.
- Sodium chloride:



Formula unit = smallest ratio of anions to cations

Properties of Ionic Compounds

Ionic crystals have distinctive shapes and can be cleaved:



Ionic Compound Properties

Ionic compounds are held together by strong Coulombic forces:

The diagram shows the equation $F = k \frac{Q_1 Q_2}{d^2}$ with callouts for each term: F is labeled 'Force between ions', k is labeled 'constant', Q_1 is labeled 'Charge on ion 1', Q_2 is labeled 'Charge on ion 2', and d^2 is labeled 'Distance between ions'.

$$F = k \frac{Q_1 Q_2}{d^2}$$

A lot of energy is required to disrupt the crystal lattice, and so melting and boiling points are high.

Ionic Compound Properties

$$F = k \frac{Q_1 Q_2}{d^2}$$

Forces are stronger when:

- the ion charges (Q_1 and Q_2) are large
- The ions are small (d is small)

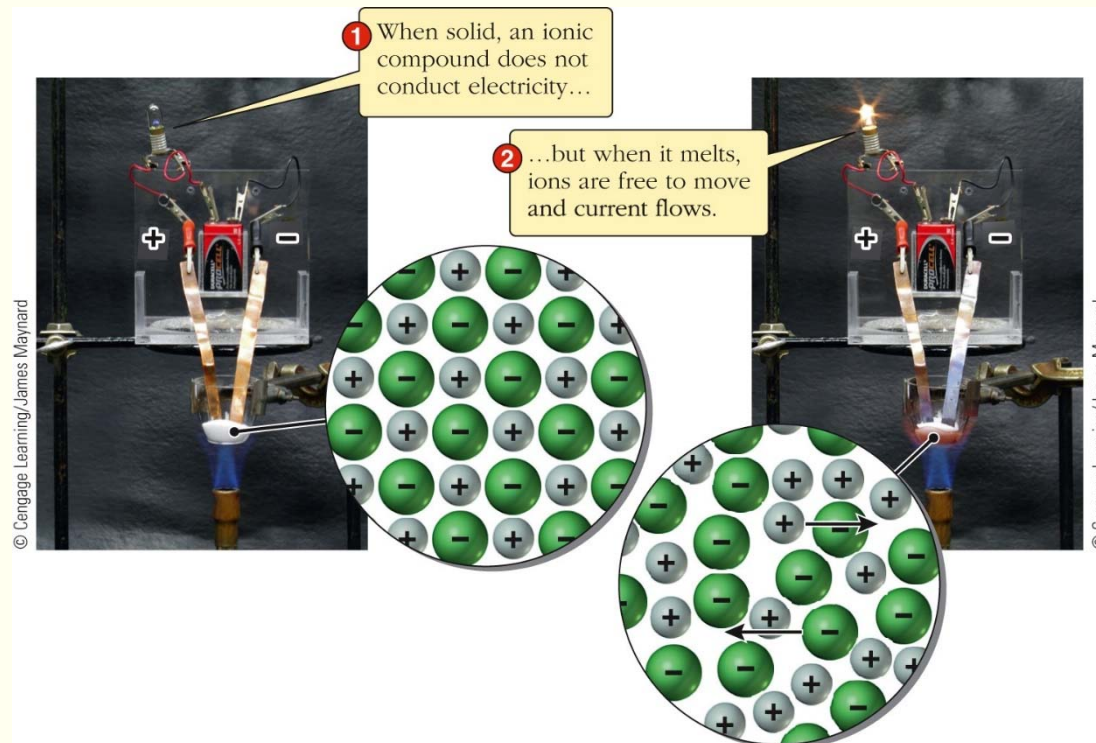
Ionic Compound	Q_1 & Q_2	Melting Point
NaF	+1 & -1	993 °C
NaI	+1 & -1	651 °C
CaO	+2 & -2	2572 °C

I⁻ is larger than F⁻

Properties of Ionic Compounds

Ionic compounds are electrical insulators when **SOLID**

- will conduct if molten



Many are soluble in water

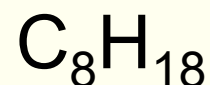
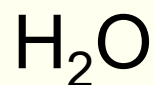
Molecular Compounds

Ionic compounds contain metal ions. Compounds formed exclusively with non-metal atoms are usually **molecular**.

At the nanoscale:

- 2 or more elements combine
- Individual, independent units (molecules) form

The molecular formula shows the number and kind of elements combined:



Molecular & Ionic Compounds

Property	Molecular Compounds	Ionic Compounds
Composition	Mostly non-metal combinations	Metal/non-metal combinations
Nanoscale	Individual molecules	Ions in a crystal lattice
Physical state	Gas, liq. or solid Brittle & weak or soft & waxy	Crystalline solid Hard & brittle
Melting point	Low	High
Boiling point	Low	High
Heat transport	Low	Low
Electrical conductivity	Low	Low (but high if molten)

Molecular Compounds

Inorganic compounds

- Do not contain C or (C and H)

e.g. water = H_2O ammonia = NH_3
 carbon dioxide = CO_2

Organic compounds

- Always contain C, usually H
- May contain many other elements

e.g. benzene = C_6H_6 ethanol = $\text{C}_2\text{H}_6\text{O}$

- Most (but not all) are molecular.

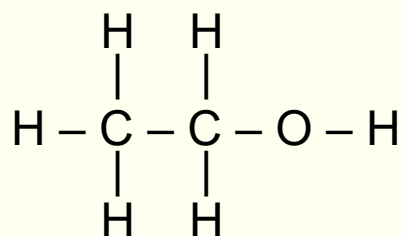
Molecular Formulas

Ethanol has the formula C_2H_6O ...

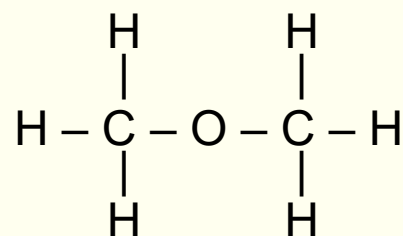
- Doesn't show atom connections.
- A **structural formula** does.

C_2H_6O may not be ethanol.

- Two C_2H_6O structural formulas:



ethanol



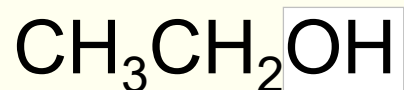
dimethyl ether

Molecular Formulas

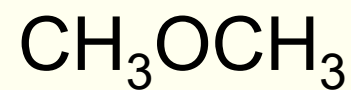
Condensed formula

Similar information, but in a more compact form.

C, what's attached to it, C ...



ethanol



dimethyl ether

Groups of atoms attached to C (like OH) are called
functional groups

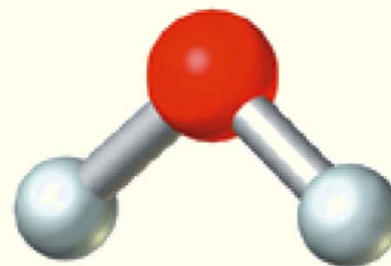
–OH is the alcohol group.

Molecular Formulas

More elaborate models of ethanol:



Space-filling
model



Ball-and-stick
model

Naming Binary Molecular Compounds

Binary compounds contain two different elements.

If one element is hydrogen:

- It is written first in the formula and named first
- The other element is renamed with an “-ide” ending

HCl	hydrogen chloride
H ₂ S	hydrogen sulfide
HF	hydrogen fluoride

Naming Binary Molecular Compounds

Other **binary** compounds (without H):

- Name elements in formula order.
 - The 2nd element's name ends in “-ide”
- Prefixes show the number of each atom present.

N_2F_4 = dinitrogen tetrafluoride

#	Prefix
1	Mono
2	Di
3	Tri
4	Tetra
5	Penta
6	Hexa
7	Hepta
8	Octa
9	Nona
10	Deca

Naming Binary Molecular Compounds

Mono is optional for the 1st element (usually omitted):

CO	carbon monoxide*
NO ₂	nitrogen dioxide
N ₂ O	dinitrogen monoxide
P ₂ O ₅	diphosphorus pentaoxide
PBr ₅	phosphorus pentabromide
SF ₆	sulfur hexafluoride
P ₄ O ₁₀	tetraphosphorus decaoxide

*Monoxide would also be correct.

Naming Binary Molecular Compounds

There are several common names in wide-spread use that you should know:

H_2O	water	NO	nitric oxide
NH_3	ammonia	N_2O	nitrous oxide
PH_3	phosphine	N_2H_4	hydrazine

Hydrocarbons

Binary molecules containing (C and H) are known as **hydrocarbons**.

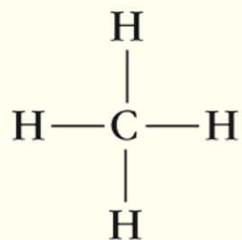
Alkanes

Hydrocarbons with C-C **single** bonds only:

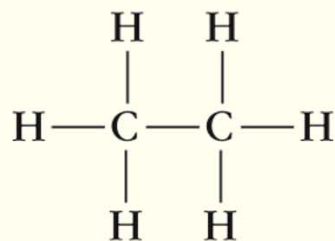
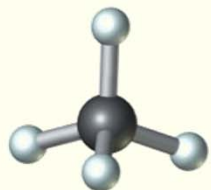
- Use an **-ane** ending.
- Linear and branched molecules
 - formula C_nH_{2n+2}
- Cyclic molecules
 - formula: C_nH_{2n}



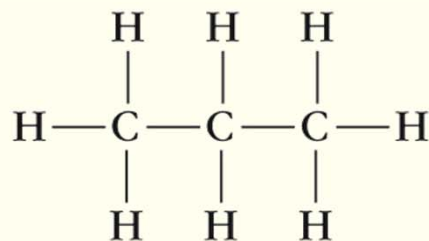
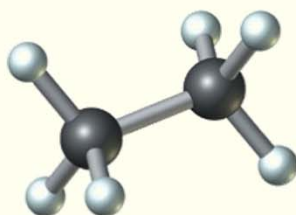
Hydrocarbons



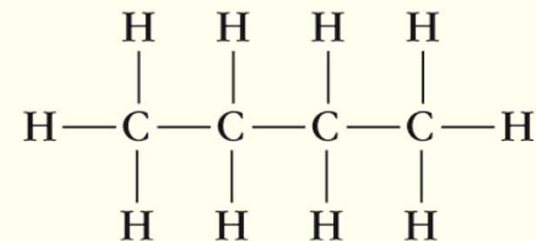
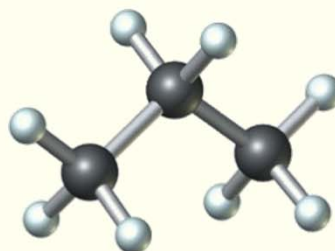
methane



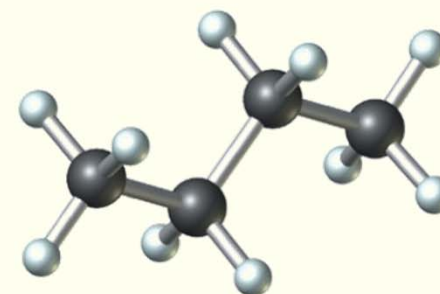
ethane



propane



butane



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Boiling points (°C)

-162

-88

-42

-1

Larger mass = higher b.p.

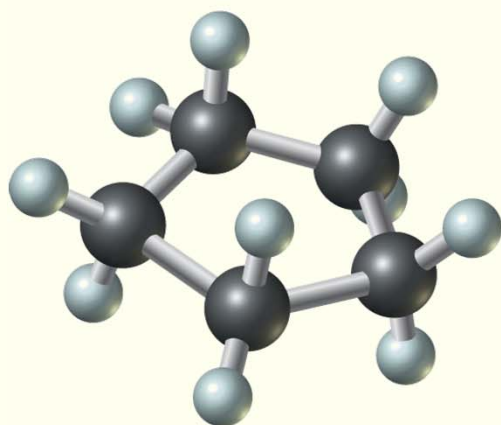
Hydrocarbons

C_8H_{18} = octane

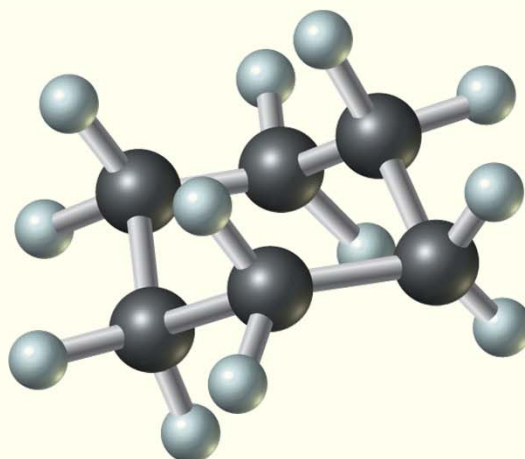
C_5H_{12} = pentane

Rings use a “cyclo-” prefix.

Examples:



cyclopentane, C_5H_{10}



cyclohexane, C_6H_{12}

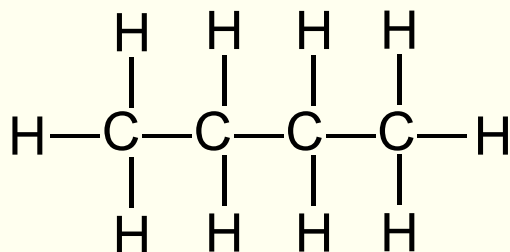
# of C	Prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Dec

Isomers

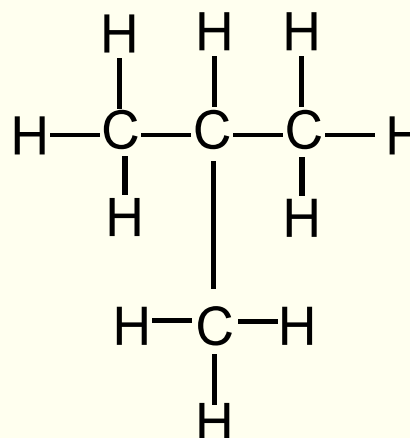
Isomers: Two or molecules with the same formula, but with different atom arrangements.

Branched alkanes are isomers of the linear forms.

butane C_4H_{10}



methylpropane C_4H_{10}



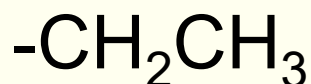
Alkanes & Their Isomers

Alkyl functional groups

- An alkane with a H atom removed.
- Named by replacing “-ane” with “-yl”



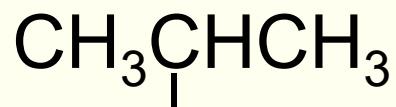
methyl



ethyl

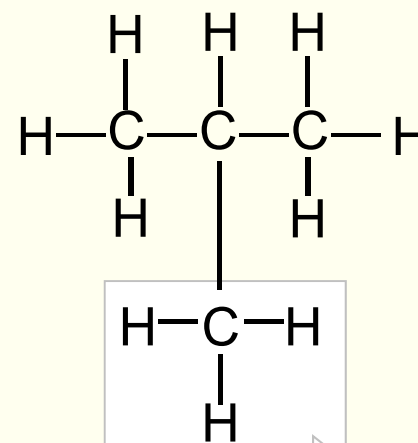


propyl



isopropyl

methylpropane C_4H_{10}



a methyl
group

Alkanes & Their Isomers

Formula	Isomers	Formula	Isomers
CH_4	1	C_9H_{20}	35
C_2H_6	1	$\text{C}_{10}\text{H}_{22}$	75
C_3H_8	1	$\text{C}_{11}\text{H}_{24}$	159
C_4H_{10}	2	$\text{C}_{12}\text{H}_{26}$	355
C_5H_{12}	3	$\text{C}_{15}\text{H}_{32}$	4,347
C_6H_{14}	5	$\text{C}_{20}\text{H}_{42}$	366,319
C_7H_{16}	9	$\text{C}_{30}\text{H}_{62}$	4.1×10^9
C_8H_{18}	18	$\text{C}_{40}\text{H}_{82}$	6.9×10^{13}

Amount of Substance: The Mole

A counting unit – a familiar counting unit is a “dozen”:

1 dozen eggs = 12 eggs

1 dozen peas = 12 peas

1 mole (mol) = Number of atoms in 12 g of ^{12}C

- Latin for “heap” or “pile”
- 1 mol = $6.02214179 \times 10^{23}$ “units”
- Avogadro's number

1 mole eggs = 6.02×10^{23} eggs

1 mole peas = 6.02×10^{23} peas

Amounts of Substances: The Mole

A green pea has a $\frac{1}{4}$ -inch diameter. 48 peas/foot.

$$(48)^3 / \text{ft}^3 \approx 1 \times 10^5 \text{ peas/ft}^3.$$

$$\begin{aligned} V \text{ of 1 mol} &\approx (6.0 \times 10^{23} \text{ peas}) / (1 \times 10^5 \text{ peas/ft}^3) \\ &\approx 6.0 \times 10^{18} \text{ ft}^3 \end{aligned}$$

$$\begin{aligned} \text{U.S. surface area} &= 3.0 \times 10^6 \text{ mi}^2 \\ &= 8.4 \times 10^{13} \text{ ft}^2 \end{aligned}$$

height = V / area , 1 mol would cover the U.S. to:

$$\frac{6.0 \times 10^{18} \text{ ft}^3}{8.4 \times 10^{13} \text{ ft}^2} = 7.1 \times 10^4 \text{ ft} = 14 \text{ miles !}$$

Amounts of Substances: The Mole

1 mole of an atom = atomic weight in grams.

1 Xe atom has mass = 131.29 u

1 mol of Xe atoms has mass = 131.29 g

1 He atom has mass = 4.0026 u

1 mol of He has mass = 4.0026 g

There are 6.022×10^{23} atoms in 1 mol of He **and** 1 mol of Xe – but they have different masses.

... 1 dozen eggs is much heavier than 1 dozen peas!

Amounts of Substances: The Mole

Cu 63.55 g

Al 26.98 g

Hg 200.6 g



C 12.01 g

Ag 107.9 g

Fe 55.84 g

Gram-Mole Calculations

Example

How many moles of copper are in a 320.0 g sample?

Cu-atom mass = 63.546 g/mol (periodic table)

Conversion factor: $\frac{1 \text{ mol Cu}}{63.546 \text{ g}} = 1$

$$n_{\text{Cu}} = 320.0 \text{ g} \times \frac{1 \text{ mol Cu}}{63.546 \text{ g}} = 5.036 \text{ mol Cu}$$

n = number of moles

Gram-Mole Calculations

Calculate the number of atoms in a 1.000 g sample of boron.

$$n_{\text{B}} = (1.000 \text{ g}) \frac{1 \text{ mol B}}{10.81 \text{ g}} = 0.092507 \text{ mol B}$$

$$\text{B atoms} = 0.092507 \text{ mol B} \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol}}$$

$$= 5.571 \times 10^{22} \text{ B atoms}$$

Moles of Compounds

A mole of $X_m Y_n$ contains:

m moles of atom X and n moles of atom Y

1 mol of H_2O contains:

2 mol of H atoms and 1 mol of O atoms

Molar mass = sum of the atomic masses

Mass of 1 water molecule:

$$= 2(1.008 \text{ u}) + 1(15.999 \text{ u}) = 18.015 \text{ u}$$

Molar mass of water:

$$= 2(1.008 \text{ g/mol}) + 1(15.999 \text{ g/mol}) = 18.015 \text{ g/mol}$$

Molar Mass of Ionic Compounds

Ionic compounds do not contain molecules.

Formula weight (or molar mass) should be used to describe the mass of an ionic compound.

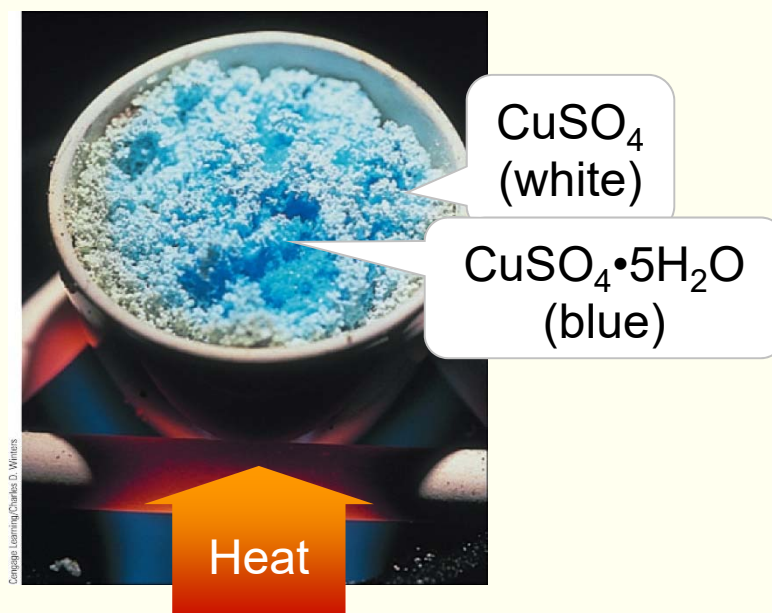
Compound	Atomic Masses, Formula mass	Molar mass
NaCl	$22.99 \text{ u} + 35.45 \text{ u} = 58.44 \text{ u}$	58.44 g/mol
$\text{Ca}(\text{NO}_3)_2$	$40.08 + 2(14.01) + 6(16.00) = 164.10 \text{ u}$	164.10 g/mol

Ionic Hydrates

Ionic hydrate: ionic compound with water trapped in the crystal

- the water of hydration.
- use “hydrate” with a Greek prefix for the number.
- heat can remove some, or all, of this water.

$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
copper(II) sulfate pentahydrate



Gram-Mole Calculations

How many moles of $\text{Ca}_3(\text{PO}_4)_2$ are in 10.0 g of the compound?

$$\begin{aligned}\text{Molar mass} &= 3(40.08) + 2(30.97) + 8(16.00) \\ &= 310.18 \frac{\text{g}}{\text{mol}}\end{aligned}$$

$$\text{Moles of } \text{Ca}_3(\text{PO}_4)_2 = 10.0 \text{ g} \left(\frac{1 \text{ mol}}{310.2 \text{ g}} \right) = 0.0322 \text{ mol}$$

$$n_{\text{Ca}_3(\text{PO}_4)_2} = 0.0322 \text{ mol}$$

Gram-Mole Calculations

Find the mass of cobalt in 3.49 g of cobalt(II) sulfate.

$$\begin{aligned}\text{Molar mass CoSO}_4 &= 58.93 + 32.07 + 4(16.00) \\ &= 155.00 \text{ g mol}^{-1}\end{aligned}$$

$$n_{\text{Co}} = 3.49 \text{ g } \cancel{\text{CoSO}_4} \left(\frac{1 \text{ mol } \cancel{\text{CoSO}_4}}{155.0 \text{ g } \cancel{\text{CoSO}_4}} \right) \left(\frac{1 \text{ Co}}{1 \cancel{\text{CoSO}_4}} \right)$$

$$n_{\text{Co}} = 0.02252 \text{ mol Co}$$

$$\text{mass of Co} = 0.02252 \cancel{\text{ mol Co}} \frac{58.93 \text{ g Co}}{1 \cancel{\text{ mol Co}}} = 1.33 \text{ g Co}$$

Composition & Chemical Formula

Two names used:

percent composition by mass, or
mass percent of the compound.

Example

What is the mass percent of each element in sodium chlorite, NaClO_2 ?

$$\begin{aligned}\text{Molar mass} &= 22.990 + 35.453 + 2(15.999) \text{ g mol}^{-1} \\ &= 90.441 \text{ g mol}^{-1}\end{aligned}$$

Percent Composition

$$\begin{aligned}\% \text{Na} &= \frac{\text{mass of Na in 1 mol NaClO}_2}{\text{mass of NaClO}_2 \text{ in 1 mol NaClO}_2} \times 100 \% \\ &= \frac{22.990 \text{ g}}{90.441 \text{ g}} \times 100 \% = 25.42\%\end{aligned}$$

$$\begin{aligned}\% \text{O} &= \frac{\text{mass of O ...}}{\text{mass of NaClO}_2 \text{ ...}} \times 100 \% \\ &= \frac{2(15.999) \text{ g}}{90.441 \text{ g}} \times 100 \% = 35.38\%\end{aligned}$$

Percent Composition

$$\%Cl = \frac{\text{mass of Cl ...}}{\text{mass of NaClO}_2 \dots} \times 100 \%$$

$$= \frac{35.453 \text{ g}}{90.441 \text{ g}} \times 100 \% = 39.20\%$$

Check your work:

$$\%Na + \%O + \%Cl = 25.42 + 35.38 + 39.20 = 100\%$$

Empirical & Molecular Formulas

Last example:

molecular formula \longrightarrow percent composition

The process can be reversed:

percent composition \longrightarrow empirical formula

Not molecular
formula

Empirical formula = the simplest ratio of atoms in a compound.

Empirical & Molecular Formulas

Compound	Mol. formula	Emp. formula
Hydrogen peroxide	H_2O_2	HO
Borane (boron trihydride)	BH_3	BH_3
Diborane (diboron hexahydride)	B_2H_6	BH_3
Octene	C_8H_{16}	CH_2
Butene	C_4H_8	CH_2

Empirical & Molecular Formulas

Example

An orange compound is 26.6% K, 35.4% Cr and 38.0% O. Determine its empirical formula.

Assume a 100.0 g sample.

- % becomes mass in grams

Divide each mass by its atomic mass.

- Gives the number of moles of each (in 100 g).

Divide each by the smallest answer found.

- The smallest integer ratio = empirical formula.

Empirical & Molecular Formulas

Unknown: 26.6% K 35.4% Cr 38.0% O

In 100.0 g

$$26.6 \text{ g K} \left(\frac{1 \text{ mol K}}{39.10 \text{ g K}} \right) = 0.6803 \text{ mol K}$$

$$35.4 \text{ g Cr} \left(\frac{1 \text{ mol Cr}}{52.00 \text{ g Cr}} \right) = 0.6808 \text{ mol Cr}$$

$$38.0 \text{ g O} \left(\frac{1 \text{ mol O}}{16.00 \text{ g O}} \right) = 2.375 \text{ mol O}$$

Empirical & Molecular Formulas

Empirical formula = smallest integer ratio.

Divide by the smallest
(ratios stay the same!)

$$\text{K} \quad \frac{0.6803 \text{ mol}}{0.6803 \text{ mol}} = 1.000 \xrightarrow{\times 2} 2$$

$$\text{Cr} \quad \frac{0.6808 \text{ mol}}{0.6803 \text{ mol}} = 1.001 \xrightarrow{\times 2} 2$$

$$\text{O} \quad \frac{2.375 \text{ mol}}{0.6803 \text{ mol}} = 3.491 \xrightarrow{\times 2} 7$$

Choose a multiplier
to make integer

Empirical formula: $\text{K}_2\text{Cr}_2\text{O}_7$

Empirical & Molecular Formulas

The molecular formula can be determined if the molecular mass is known.

Example

Vitamin C has the empirical formula $C_3H_4O_3$ and molecular mass = 175 g/mol.

Empirical mass:

$$3(12.01) + 4(1.008) + 3(15.99) = 88.03 \text{ g/mol}$$

Empirical mass $\approx \frac{1}{2}$ (molecular mass)

Mol. formula = 2(emp. formula) = $C_6H_8O_6$