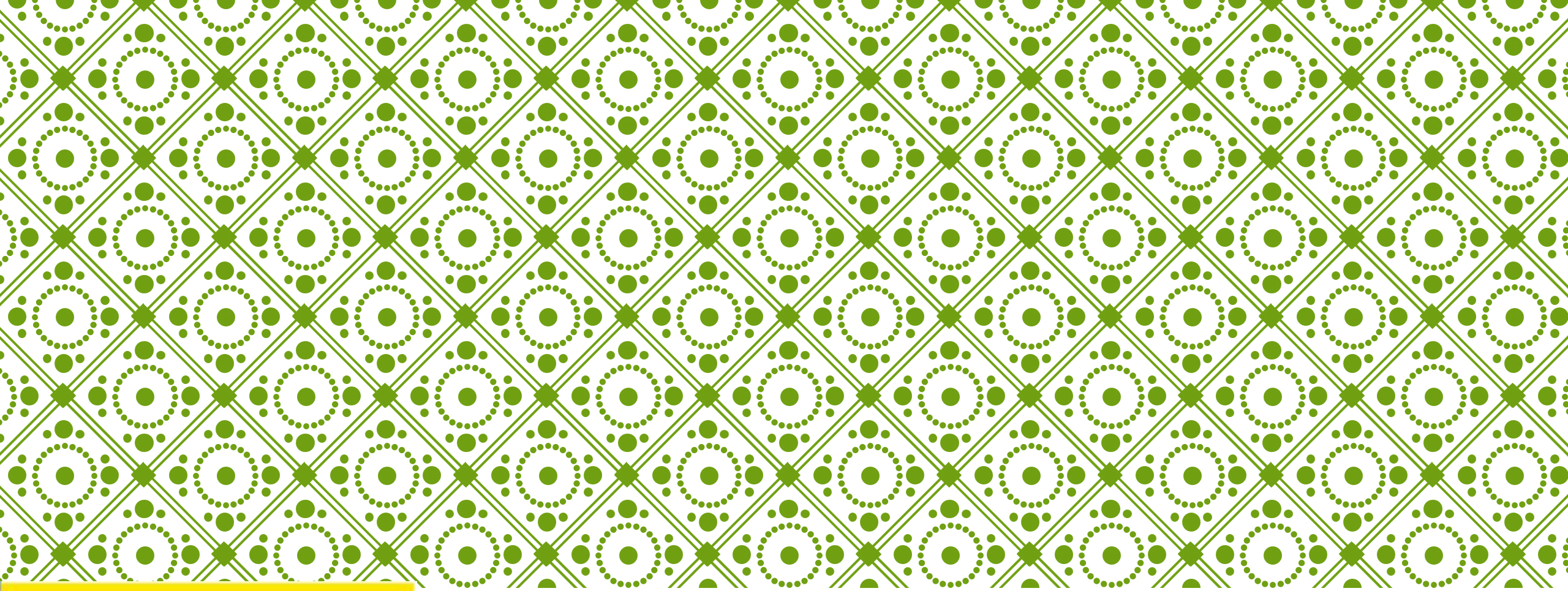

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CHEM1011 LECTURE 2

Dr Shannan Maisey

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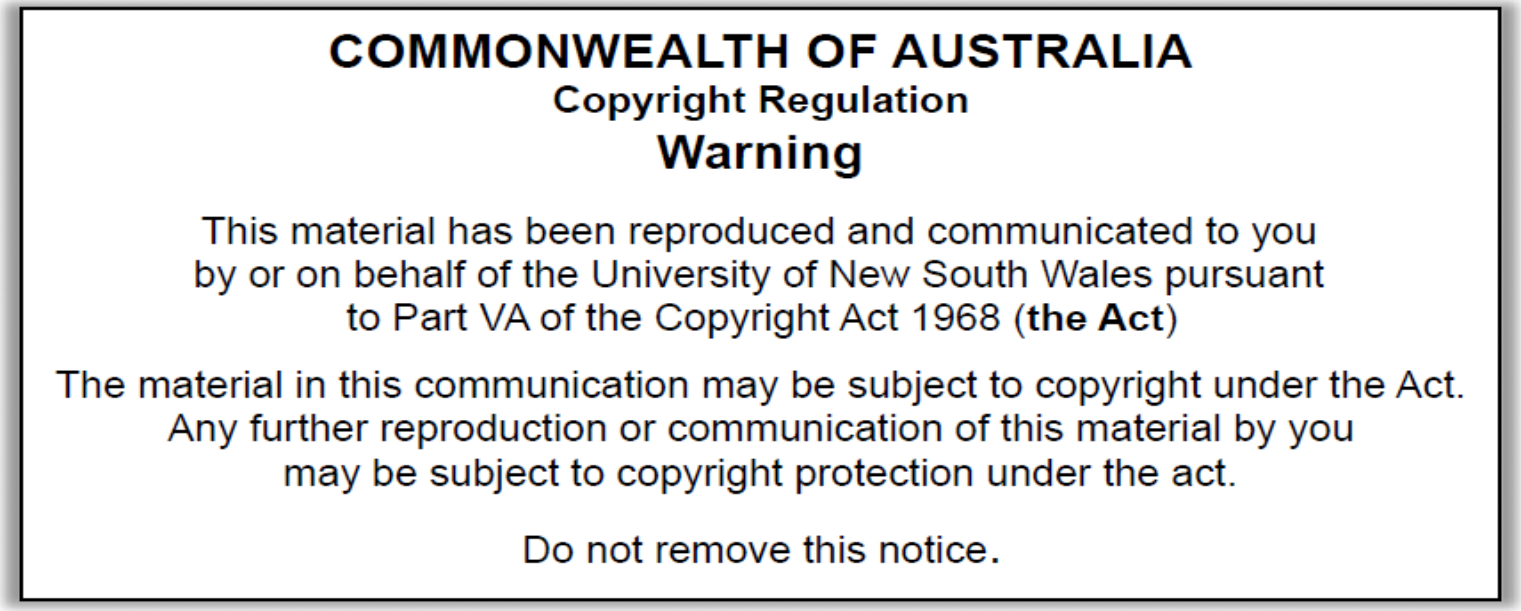

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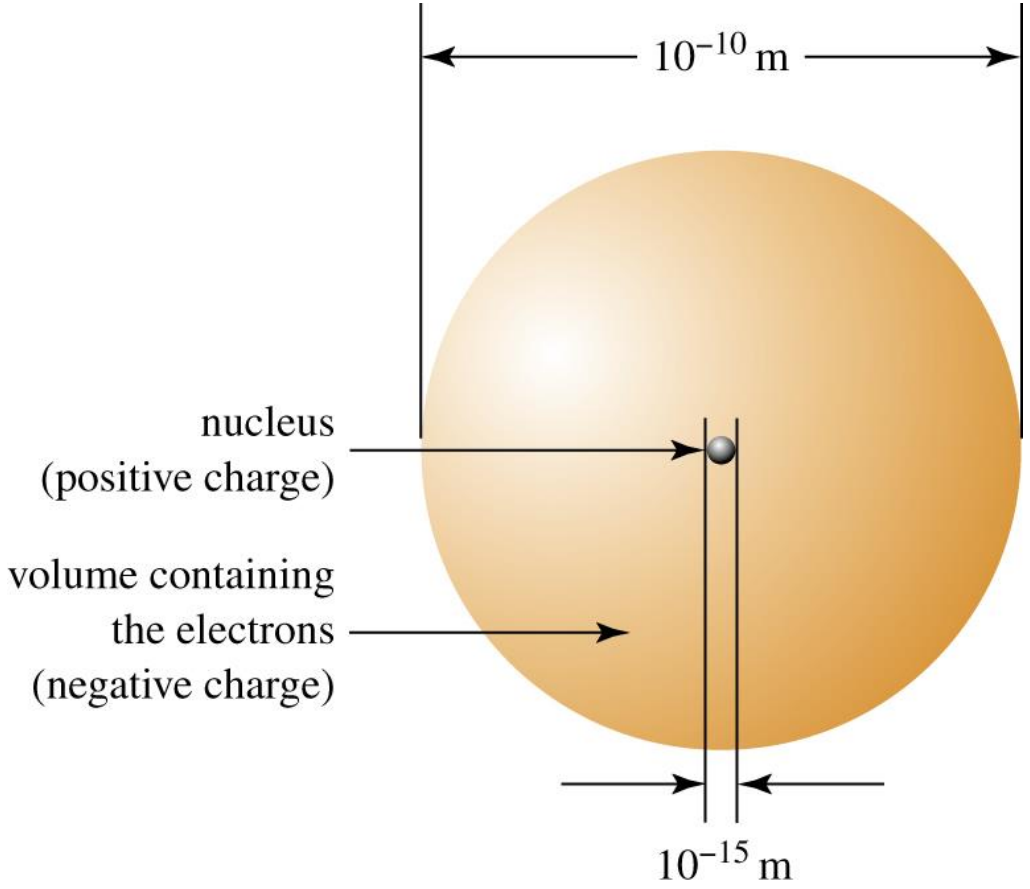
DIMENSIONS OF THE ATOM

The H atom's electron cloud is 10,000 times larger than its nucleus.

The nucleus of H is 1833 times heavier than its electron.

THEREFORE:

- The size of the atom's electron cloud defines the atom's size.
- The composition of the atom's nucleus defines the atom's weight.



Not to scale!

If it were the nucleus would be invisible!

ELEMENTS

A **chemical element** is a substance consisting of one *type* of atom distinguished by its atomic number: the number of protons in its nucleus.

So, it is the number of protons in the nucleus that determine the element

- 1 proton => hydrogen
- 6 protons => carbon
- 79 protons => gold

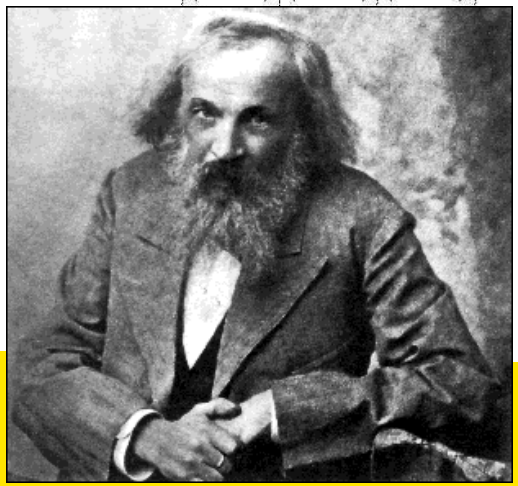
- **Chemistry is just a counting exercise!**

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

The Periodic Table

1 **H** 1.008																	2 **He** 4.003
3 **Li** 6.941	4 **Be** 9.012											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.88	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.39	31 **Ga** 69.72	32 **Ge** 72.59	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	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** (98.91)	44 **Ru** 101.1	45 **Rh** 102.9	46 **Pd** 106.4	47 **Ag** 107.9	48 **Cd** 112.4	49 **In** 114.8	50 **Sn** 118.7	51 **Sb** 121.8	52 **Te** 127.6	53 **I** 126.9	54 **Xe** 131.3
55 **Cs** 132.9	56 **Ba** 137.3	57 **La** 138.9	72 **Hf** 178.5	73 **Ta** 180.9	74 **W** 183.9	75 **Re** 186.2	76 **Os** 190.2	77 **Ir** 192.2	78 **Pt** 195.1	79 **Au** 197.0	80 **Hg** 200.6	81 **Tl** 204.4	82 **Pb** 207.2	83 **Bi** 209.0	84 **Po** (210.0)	85 **At** (210.0)	86 **Rn** (222.0)
87 **Fr** (223.0)	88 **Ra** (226.0)	89 **Ac** (227.0)															

58 **Ce** 140.1	59 **Pr** 140.9	60 **Nd** 144.2	61 **Pm** (144.9)	62 **Sm** 150.4	63 **Eu** 152.0	64 **Gd** 157.3	65 **Tb** 158.9	66 **Dy** 162.5	67 **Ho** 164.9	68 **Er** 167.3	69 **Tm** 168.9	70 **Yb** 173.0	71 **Lu** 175.0
90 **Th** 232.0	91 **Pa** (231.0)	92 **U** 238.0	93 **Np** (237.0)	94 **Pu** (239.1)	95 **Am** (243.1)	96 **Cm** (247.1)	97 **Bk** (247.1)	98 **Cf** (252.1)	99 **Es** (252.1)	100 **Fm** (257.1)	101 **Md** (256.1)	102 **No** (259.1)	103 **Lr** (260.1)



Dimitri Mendeleev, 1834-1907

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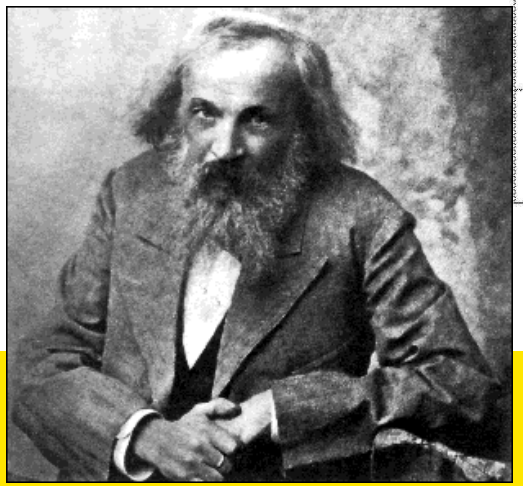

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NUCLEAR (ATOMIC) ARITHMETIC

Formalism: $${}^{M}_{Z}A^{\pm n}$$

A = symbol of element

M = mass number (protons plus neutrons)

Z = number of protons (atomic number)

Examples: $${}^{12}_{6}C$$ 6 protons, 6 neutrons, 6 electrons

$${}^{13}_{6}C^{2+}$$ 6 protons, 7 neutrons, 4 electrons

WHAT ARE ISOTOPES?

Isotopes of a given element always have a **different** number of _____?

Isotopes of a given element always have the **same** number of _____?

- A Protons and neutrons
- ✓ B Neutrons and protons
- C Protons and electrons
- D Electrons and protons
- E Don't know

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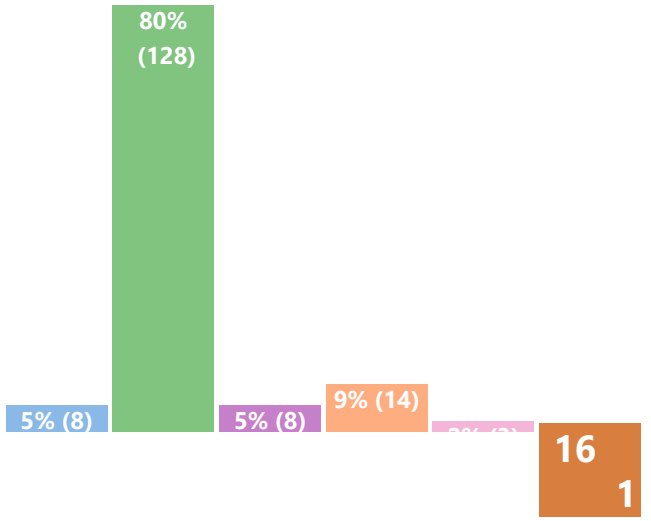

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WHAT ARE ISOTOPES?

Not all atoms of an element are identical…

ISOTOPES:

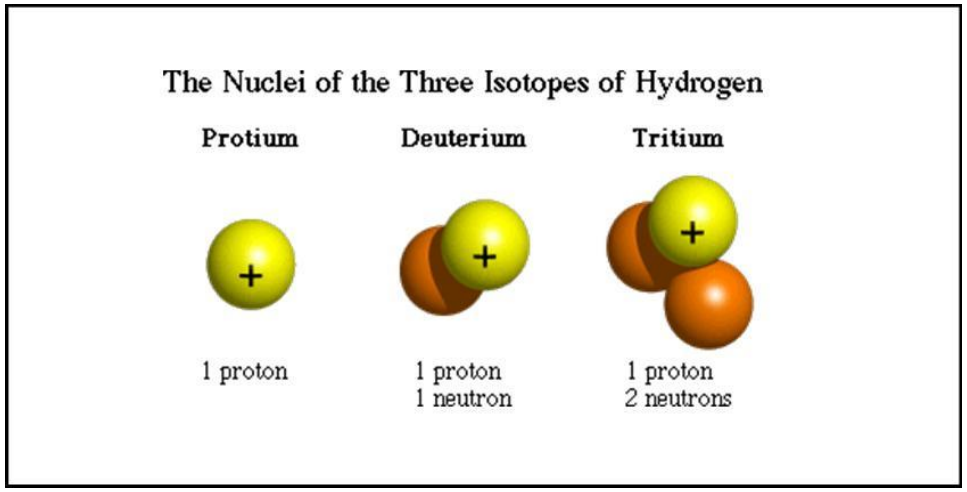
- have same number of protons
- different numbers of neutrons
- different atomic mass numbers.

They have similar chemical properties but slightly different physical properties.

ISOTOPES OF THE HYDROGEN ATOM

e.g., The three common isotopes of hydrogen are written:

$$H_{1}^{1} \qquad H_{1}^{2} \qquad H_{1}^{3}$$



Alternative names for these isotopes are protium, deuterium and tritium (respectively).

(Don't have alternative names for other elements just name the isotope number, e.g. carbon-14)

RADIOCARBON DATING USING ISOTOPES

Determining the ages of old things

- Carbon-14 is a radioactive isotope of carbon found in all living things

- It decays at a steady rate, so we can determine the age of things that lived between 2000-50,000 years ago

Sample being removed from bone for carbon dating

Credit: Laura Marschke

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RADIOCARBON DATING ÖTZI THE ICEMAN

"Only the back of the head, the bare shoulders and part of his back jutted out of the ice and melt water. The corpse lay with its chest against a flat rock and its face obscured. Beside the corpse the two hikers noticed several pieces of rolled-up birch bark. Before leaving the scene, they took a photograph of what they thought to be the unfortunate victim of a mountaineering accident a few years back."

Undisputable proof of the authenticity and extraordinary age of the Iceman and his possessions was provided by C-14 analysis

Four different scientific institutions analyzed tissue samples from the corpse and the finds. The results were unequivocal: **the Iceman lived between 3350 and 3100 BC**

Reconstruction of Otzi's face!

Credit: Laura Marschke

ATOMS VS IONS

NEUTRAL ATOM: number of protons = number of electrons

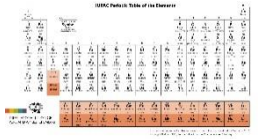
(Individual atoms are electrically neutral)

ION: Charged particle (single atom or group of atoms)

- ANION: Negatively charged species, protons < electrons
- CATION: Positively charged species, protons > electrons

Fundamental Property of elements:

The number of protons in each atom of a specific element is constant



MASS NUMBER & ATOMIC NUMBER

An isotope contains 16 protons, 18 electrons and 16 neutrons. What is the identity of the isotope?

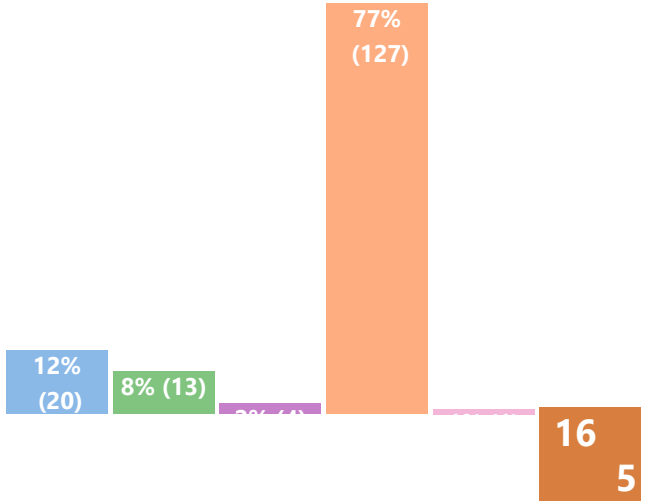
A $^{34}S^{2-}$

B $^{32}Ar^{2-}$

C $^{34}Ar^{2-}$

✓ D $^{32}S^{2-}$

E Don't know



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Atomic Mass:

To find mass of an atom? - Experimentally!

ATOMIC MASS: average mass in amu of the atoms of the naturally occurring mixture of isotopes.

ATOMIC MASS UNIT: 1/12 th of the mass of a carbon-12 atom

Example: Calculate the (average) atomic mass of naturally occurring magnesium.

Isotope Mass Number	Abundance	Isotopic Weight
24	78.99%	23.98504
25	10.00%	24.98584
26	11.01%	25.98259

Atomic Mass = …

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26	11.01%	25.98259

Atomic Mass = 24.30505 amu

WORKED EXAMPLE

Copper occurs naturally as a mixture of two isotopes: ^{63}Cu (abundance 69.09%) and ^{65}Cu (30.91%). Their atomic masses are 62.930 amu and 64.928 amu, respectively. Calculate the average atomic mass of copper.

Lets consider you have 10000 atoms of natural copper (2 decimal places)

Of these, 6909 atoms will be ^{63}Cu, of weight = 6909 x 62.930 amu.
Similarly the weight of the ^{65}Cu atoms will be = 3091 x 64.928 amu.
Thus, the total weight of all 10000 atoms …
= [6909 x 62.930 + 3091 x 64.928] amu.
= 635480 amu.

Thus, the average atomic mass of one atom = 635480 /10000
= 63.55 amu.

WHERE DO ELEMENTS COME FROM?

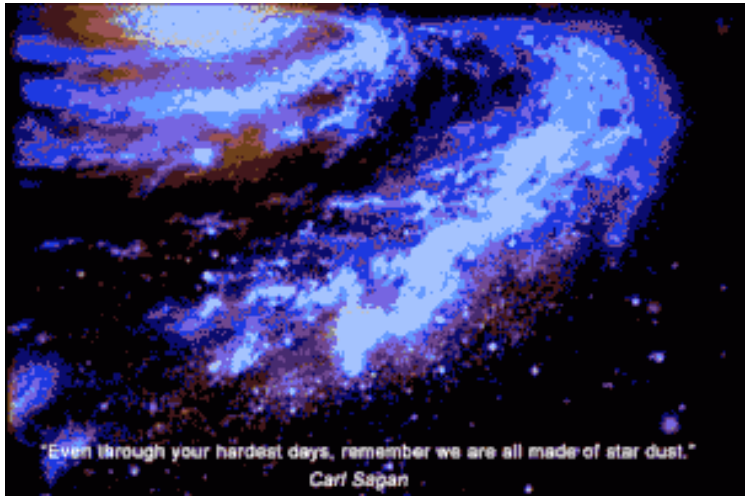
They come from stars (and the death of stars)

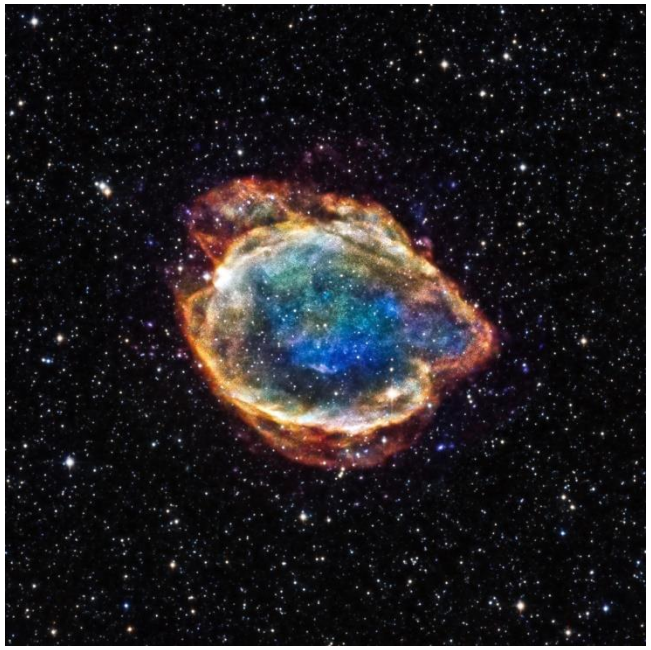
Hydrogen formation and some light elements - the big bang

Elements carbon to iron form inside stars

Many elements heavier than iron formed by exploding stars (supernovae)

Elements heavier than uranium are man made





Names of elements

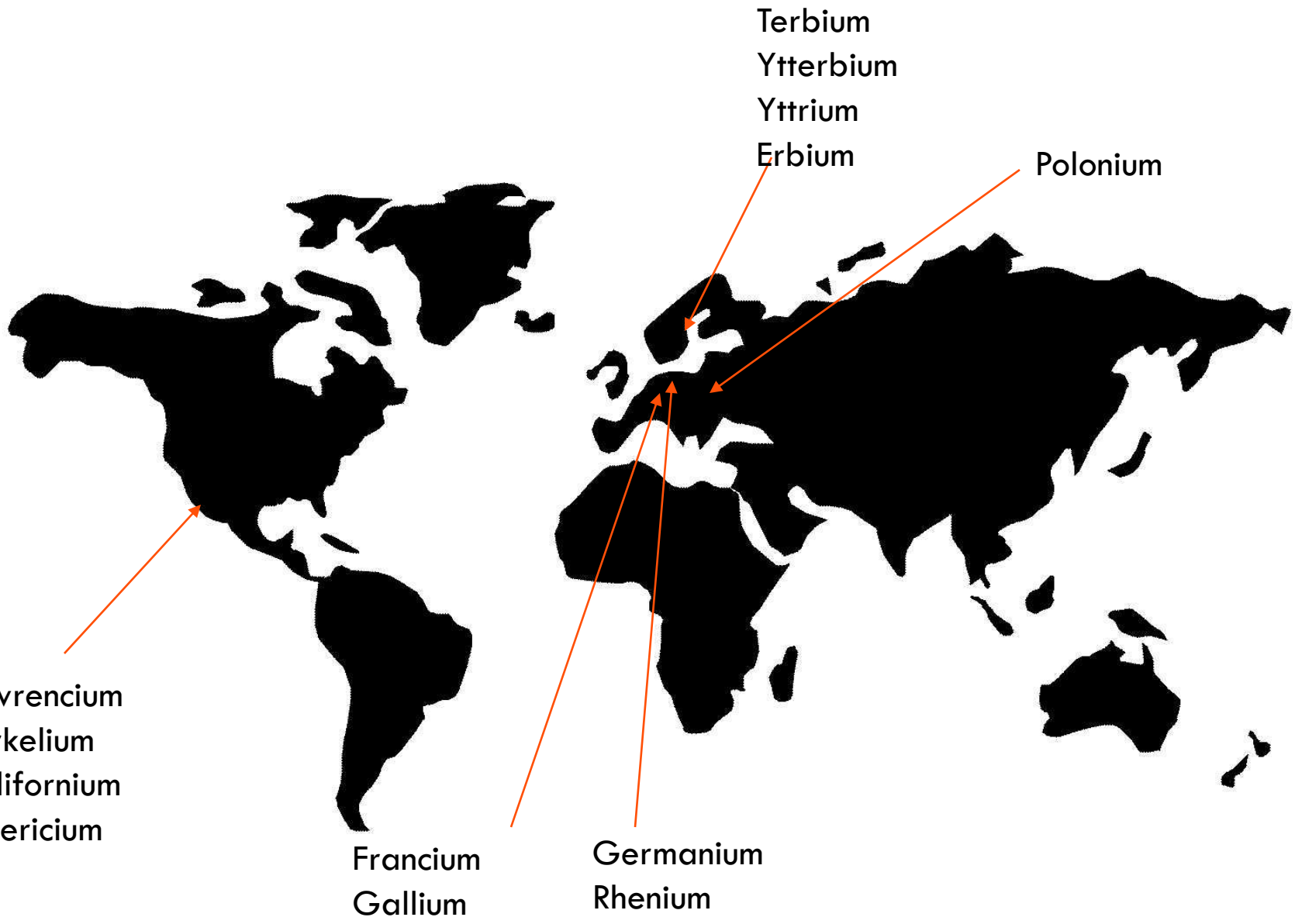
Some from antiquity: Carbon, Copper, Gold, Antimony, Iron, Lead, Silver, Mercury, Sulfur

Some named from mythology: Thorium, Promethium, Niobium, Tantalum

Some named after people: Meitnerium, Curium, Fermium, Einsteinium, Nobelium, Gadolinium

Greek:
- Hydrogen - water former
- Oxygen - acid former
- Iodine - violet
- Osmium – smell
- Nitrogen - soda former
- Chlorine - greenish yellow
- Bromine - stench

Some are named after places……


Terbium
Ytterbium
Yttrium
Erbium
Polonium
Lawrencium
Berkelium
Californium
Americium
Francium
Gallium
Germanium
Rhenium

Beyond Elements – some definitions

Compound: atoms of 2 or more elements combined chemically

Molecule: independent structural unit of 2 or more atoms combined chemically. Held together by covalent bonds
- may be of the same element

Binary Compound: contains 2 element types - A_xB_y.

Formula: Empirical - simplest whole number ratio in which elements combine.

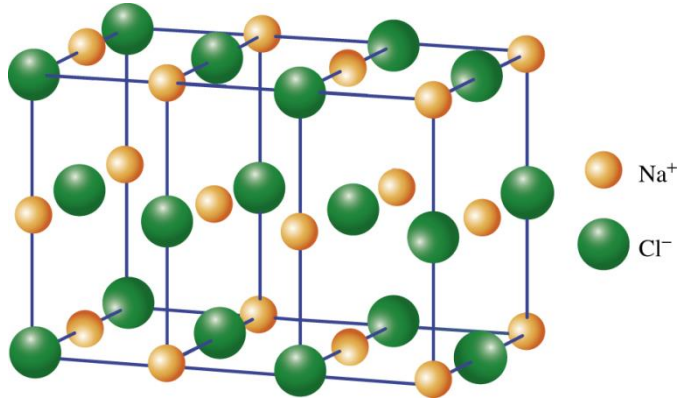
Molecular - number of atoms of each element type per molecule

CH = empirical formula for C_2H_2 and C_6H_6

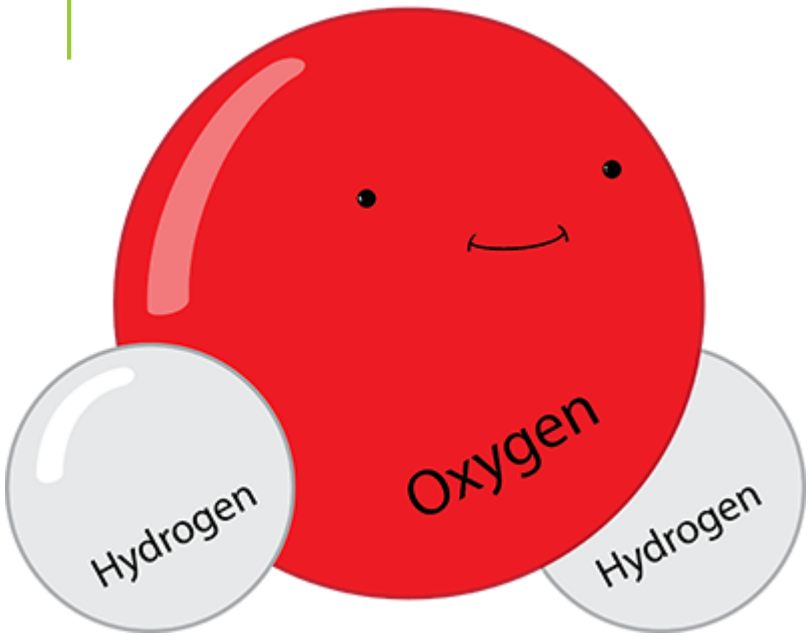
A LOOK AT SOME COMPOUNDS

Most materials are made of combinations of elements – we call these compounds

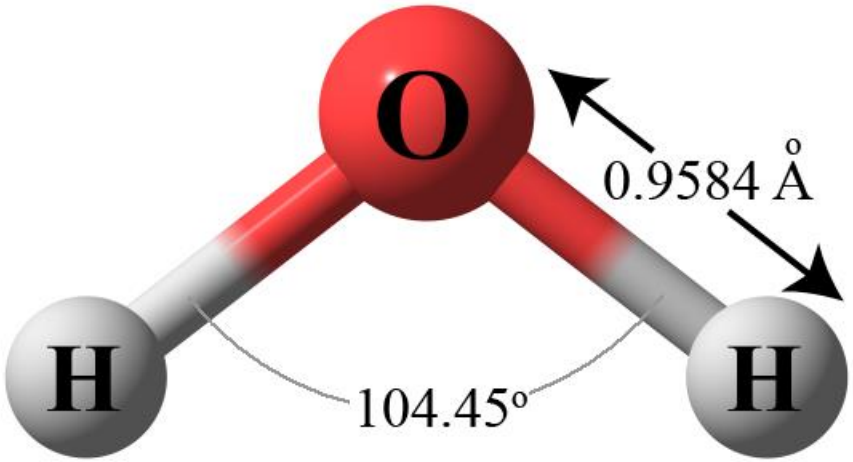
- Compounds may be composed of individual molecules, ionic lattice or a covalently bonded network of atoms
- Individual 'molecules' of an ionic compound don't exist…
  - Sodium chloride, NaCl, simply represents the smallest repeating unit in an enormous 3D array of Na^+ and Cl^- ions
  - Ionic compounds have a cation (+ve) and an anion (-ve). Overall charge for a solid is neutral – charges balance.

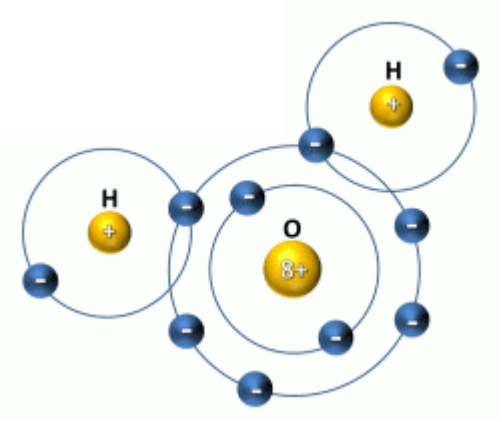


Chemists use various representations for the same compounds….



H_2O





Source: clipartfox.com, Climate Science Investigations (CSI), NASA,

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THE TREACHERY OF IMAGES

Image taken from a University of Alabama site, **"Approaches to Modernism"**

REPRESENTATIONS OF ATOMS AND MOLECULES

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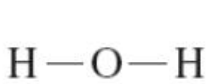
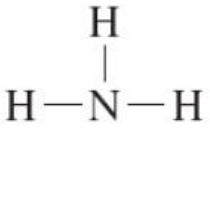
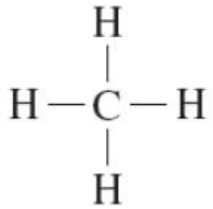
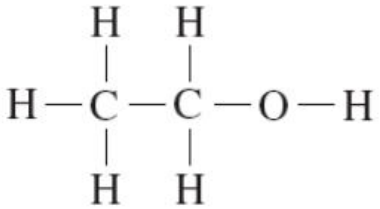
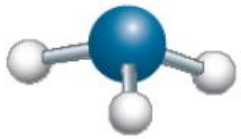
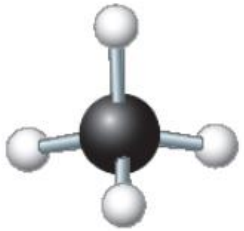
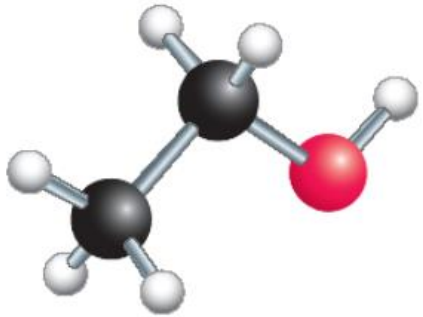
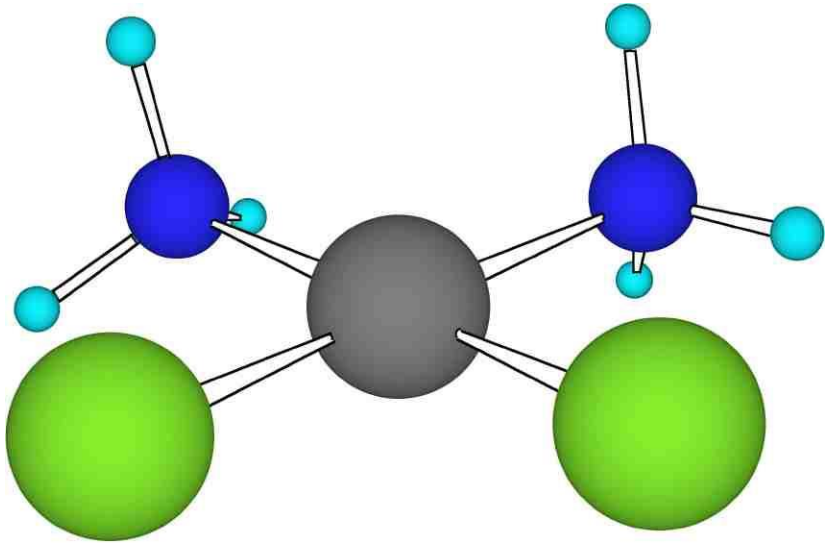
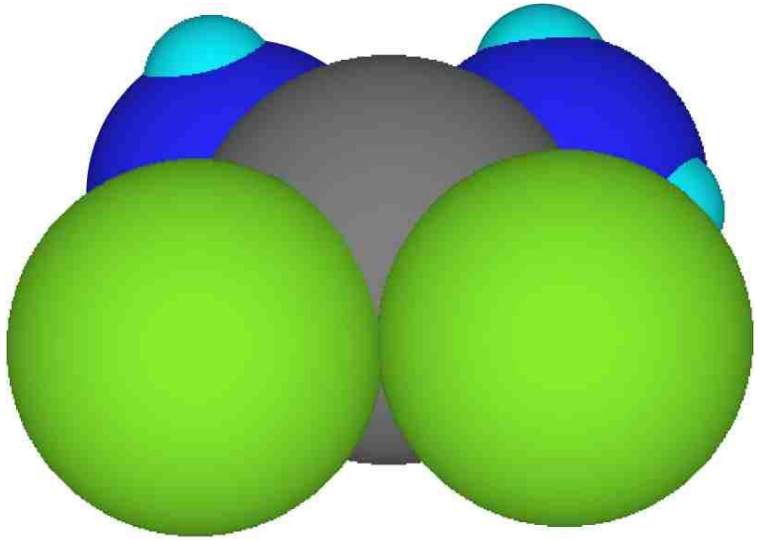
Molecule	water	ammonia	methane	ethanol
Chemical formula	H_2O	NH_3	CH_4	C_2H_6O
Structural formula				
Ball-and-stick model				
Space-filling model				

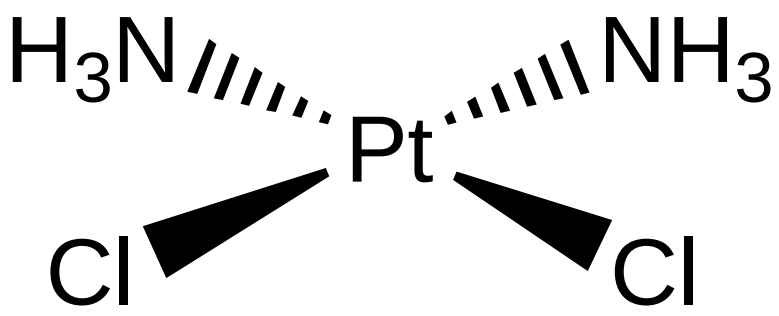
The language of Chemistry – six representations of Cisplatin

Ball and stick model



Space filling model





Structure drawing

Names:
Cisplatin - common name

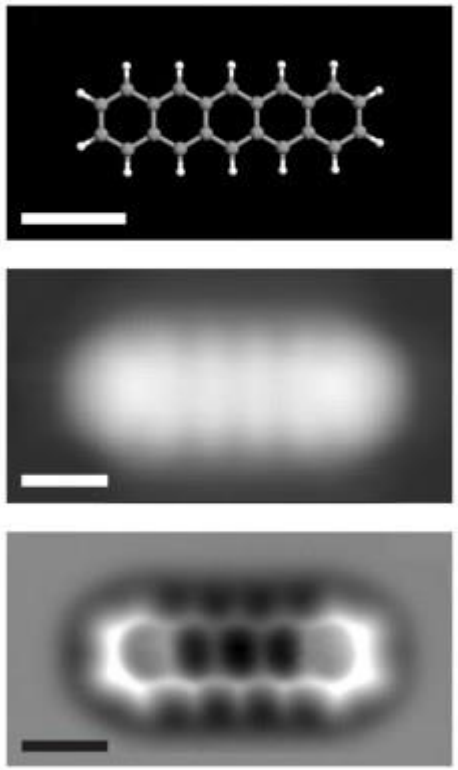
cis-diamminedichloroplatinum(II)
-formal name

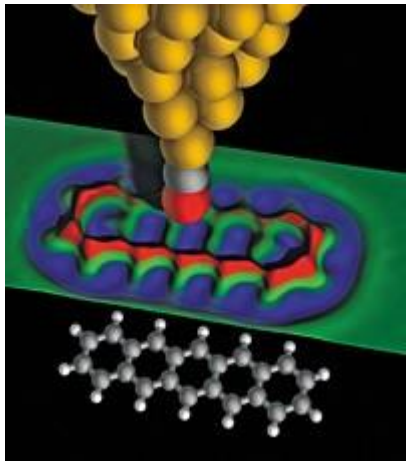
Formula: $Pt(NH_3)_2Cl_2$

Cisplatin is a **molecular** compound

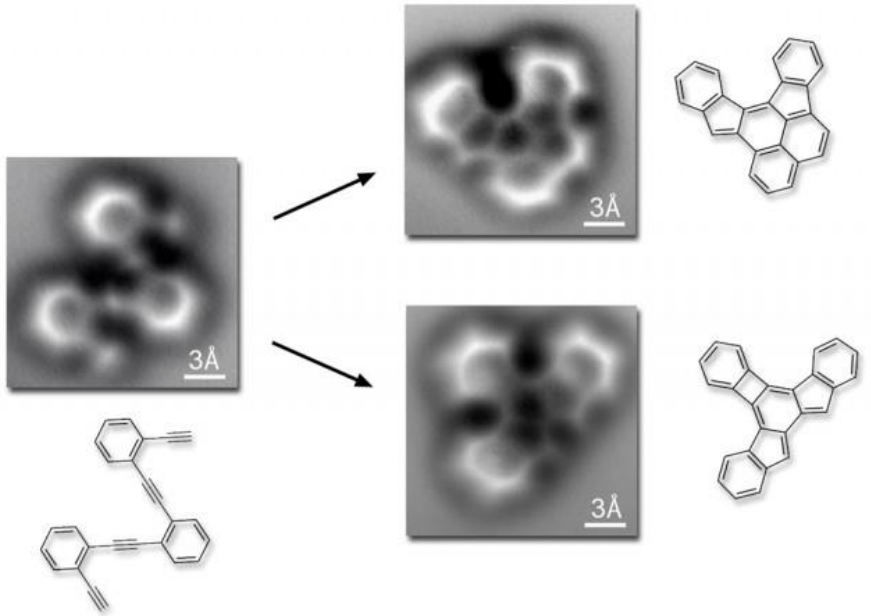
SO WHAT DO MOLECULES ACTUALLY LOOK LIKE?

…not too far removed from how we represent them actually





Atomic force microscopy



Learn more about this here!

http://cen.acs.org/articles/87/i35/Molecules-Atoms-Bonds-Visualized.html

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CHEMICAL FORMULAE (BLACKMAN 2.2)

Chemical formulae

- Subscript shows the relative number of each type of atom present in a substance
  - H_2O
  - $C_{30}H_{34}AuBClF_3N_6O_2P_2PtW$
- A molecular formula is a chemical formula that refers to a discrete molecule
- There is a standardised way of writing chemical formulae

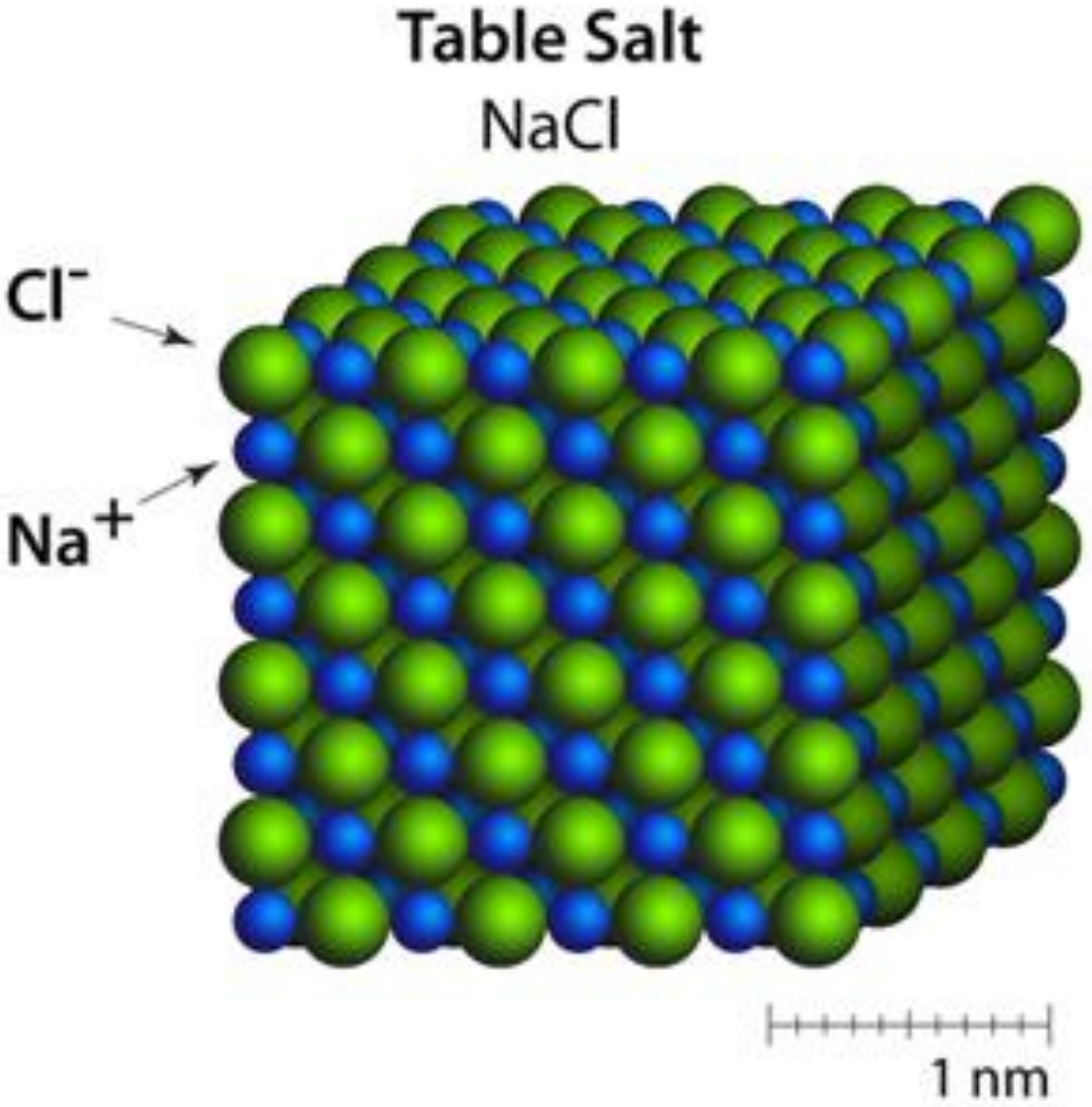
CHEMICAL FORMULAE - BINARY COMPOUNDS

- Element further to the left of the periodic table appears first
  - KCl, Al_2S_3
- Hydrogen is the exception to this rule
  - LiH, NH_3, H_2O_2, HCl
    - Hydrogen written last except when with group 16 or 17
- If both elements are from the same group the lowest element appears first
  - SiC, BrF_3

CHEMICAL FORMULAE – BINARY IONIC COMPOUNDS

- In ionic compounds are written as the simplest proportion of the two ions.
- The cation is written first followed by the anion
  - NaBr, $MgCl_2$

Remember: a subscripted number refers ONLY to the atom immediately preceding it UNLESS the number comes after a species enclosed in brackets



CHEMICAL FORMULAE – BEYOND BINARY COMPOUNDS

Writing chemical formulae for compounds containing more than two elements requires some knowledge of the bonding within the compound.

Categorise as:

- Ionic compounds
- Covalent compounds

CHEMICAL FORMULAE - IONIC COMPOUNDS

- **Write the cation followed by the anion**, e.g., $Ca(NO_3)_2$
- Note the positioning of the brackets around the NO_3^-
- Total charge zero, so two NO_3^- ions per Ca^{2+} in this case:
- Hydrate formation in the solid state is common among ionic compounds. The "water of crystallization" or other solvents that are present in the solid are written after the ionic formula separated by a full stop. e.g. $Ca(NO_3)_2.4H_2O$

- Dissolving in water, ionic compounds dissociate:

$$Ca(NO_3)_2(s) \rightarrow Ca^{2+}(aq) + 2NO_3^-(aq)$$

- The superscripts indicate the charge of the species

CHEMICAL FORMULAE - COVALENT COMPOUNDS

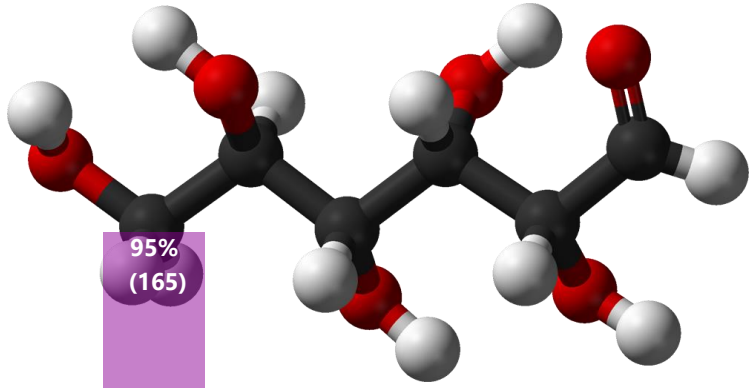
Covalent compounds

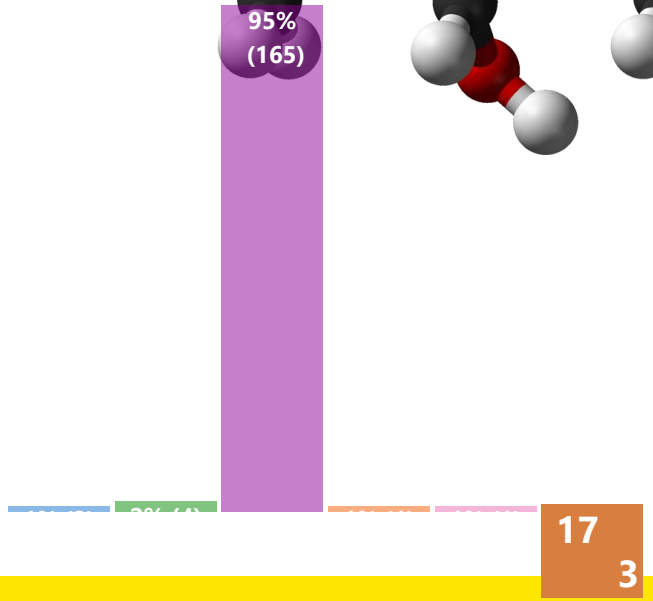
- Majority are carbon-based organic compounds
- Chemical formula often written carbon first, followed by hydrogen and then the remaining elements in alphabetical order, e.g. C_2H_6O, C_4H_9BrO
- Limited structural information in the chemical formula
- This will be looked at further in chemical bonding and Lewis structures.

MOLECULAR AND EMPIRICAL FORMULA

Molecules of glucose (blood sugar) contain 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms. What is the **molecular formula** of glucose?

	A	6C12H6O
	B	C6H12O6
✓	C	$C_6H_{12}O_6$
	D	$C_6.H_{12}.O_6$
	E	Don't know





vote at DrShan.participoll.com

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NOMENCLATURE (BLACKMAN 2.3)

- Nomenclature — the system for naming of compounds
- International Union of Pure and Applied Chemistry (IUPAC)
- Some compounds are better known by their common unsystematic name rather than their systematic IUPAC name
  - The systematic name of water is oxidane…

➢ **Make sure you work through the DIY naming tutorial!**

NOMENCLATURE – NAMING INORGANIC COMPOUNDS

Nonmetallic binary compounds

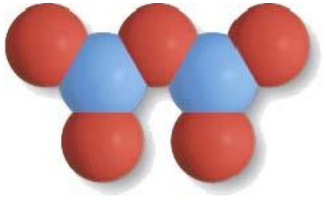
- Guidelines for naming:

NO

Nitrogen monoxide

NO_2

Nitrogen dioxide



N_2O_5

Dinitrogen pentoxide

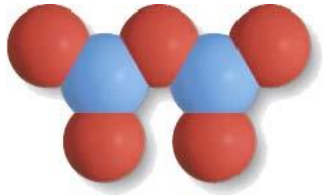
NONMETALLIC BINARY COMPOUNDS - NAMING GUIDELINES

NO

Nitrogen monoxide

NO_2

Nitrogen dioxide



N_2O_5

Dinitrogen pentoxide

1. The element closer to the left of the periodic table appears first.

   If both elements are from the same group of the periodic table, the lower one appears first.

2. The element that appears first retains its elemental name.
3. The second element begins with a root derived from its elemental name and ends with the suffix –*ide* in place of the usual ending.
4. When there is more than one atom of a given element in the formula, the name of the element usually contains a prefix that specifies the number of atoms present. prefixes - mono, di, tri, tetra, penta, hexa, *etc*.
5. Omit prefix if name is unambiguous without prefix *i.e.*, only one option for the ratio of those two elements

WHY YOU SHOULD  IUPAC

Pray tell…what are these ‘common’ chemical compounds?

Lampblack	Carbon
Jeweller's rouge	Iron oxide
Bitter salt	Magnesium sulfate
Ackey	Nitric acid
Permanent White	Barium sulfate
Oil of vitriol	Sulfuric acid
Chili saltpetre	Sodium nitrate

QUICK QUIZ

Name these compounds

PF_5

PBr_3

Make sure you practice naming till you get it! - see the course pack

QUICK QUIZ

Name these compounds

PF_5 phosphorus pentafluoride

PBr_3 phosphorus tribromide

NOMENCLATURE – IONIC COMPOUNDS

Cation : (element closer to the left of the periodic table) written first

Anion : (element closer to the right of the periodic table) written second, **with last syllable changed to -IDE**

NaBr	sodium bromide
K_2S	potassium sulfide
MgO	magnesium oxide
$BaCl_2$	barium chloride
Li_3N	lithium nitride

- Ionic species are expressed as the simplest ratio of cation: anion
- Note the space in the name between cation and anion
- Note no numbers in name for simple compounds where there is no option for the ratio of ions/atoms involved

QUICK QUIZ

Name these compounds

KCl

CaO

MgI_2

CsF

Al_2O_3

QUICK QUIZ

Name these compounds

KCl potassium chloride

CaO calcium oxide

MgI_2 magnesium iodide

CsF cesium fluoride

Al_2O_3 aluminium oxide (common name alumina)

Make sure you practice naming 'till you don't have to even think about!
(just think how popular you will be at parties!)

POLYATOMIC IONS

Ionic compounds may contain polyatomic ions:

Ammonium	NH_4^+
Nitrate	NO_3^-
Acetate	CH_3COO^-
Oxalate	$C_2O_4^{2-}$

Note: these won't exist on their own in the solid state – need an electrically neutral species, e.g.: Ammonium nitrate NH_4NO_3

Anions containing a central atom surrounded by oxygen atoms are known as oxoanions, e.g., CO_3^{2-} carbonate

NOMENCLATURE – OXOANIONS I

1. The name has a root taken from the name of the central atom
   - Carbonate CO_3^{2-}
   - Nitrite NO_2^-

2. When an element forms 2 different oxoanions, the one with fewer oxygen atoms ends in *–ite*, and the other ends in *–ate*

   - Sulfite SO_3^{2-}
   - Sulfate SO_4^{2-}

NOMENCLATURE – OXOANIONS II

3. Chlorine, bromine and iodine each form 4 different oxoanions that are distinguished by prefixes and suffixes
   - Hypobromite BrO^-
   - Bromite BrO_2^-
   - Bromate BrO_3^-
   - (Hy-)Perbromate BrO_4^-

4. A polyatomic anion with a charge more negative than 1- may add H^+ to give another anion. These anions are named from the parent anion by adding the word hydrogen
   - (mono)Hydrogen carbonate HCO_3^-
   - Dihydrogen phosphate $H_2PO_4^-$

NAMING INORGANIC COMPOUNDS

Protonation implies adding H^+

Protonated polyatomic oxyanions = oxyacids

-ate ions = -ic acid	e.g. H_2SO_4 = sulfuric acid
-ite ions = -ous acid	e.g. H_2SO_3 = sulfurous acid

When needed, specify number of protons attached.

e.g. HPO_4^{2-} = monohydrogenphosphate ion

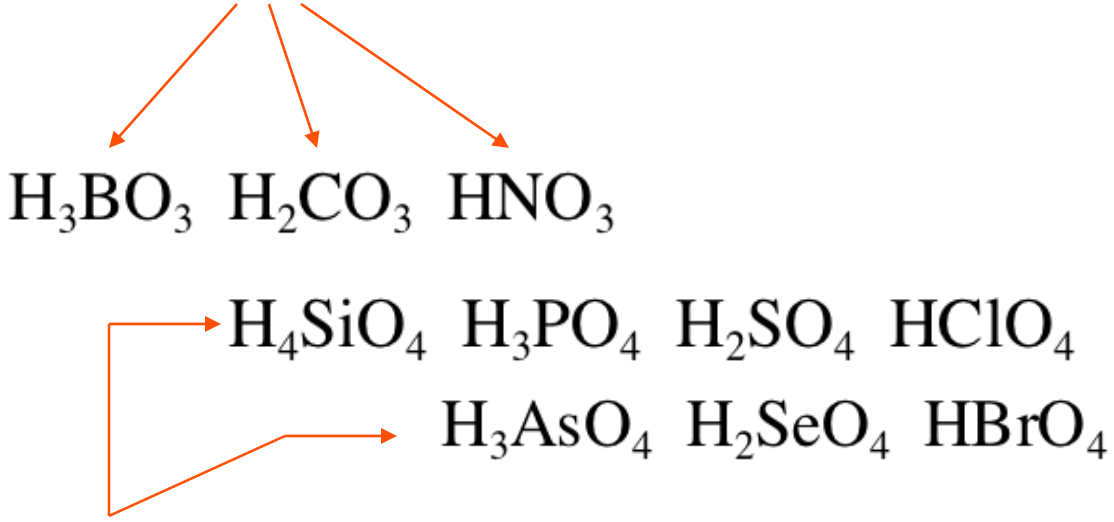
e.g. $H_2PO_4^-$ = dihydrogenphosphate ion

e.g. H_3PO_4 = phosphoric acid

e.g. PO_4^{3-} = phosphate ion

PATTERNS IN FORMULAE OF OXYACIDS

- Smaller central atom can fit around it a max. of three O atoms.



- Bigger central atom can fit around it a maximum of four O atoms.

					He
B	C	N	O	F	Ne
Al	Si	P	S	Cl	Ar
Ga	Ge	As	Se	Br	Kr
In	Sn	Sb	Te	I	Xn
Tl	Pb	Bi	Po	At	Rn

OXIDATION NUMBER (STATE) (BLACKMAN 12.1)

Oxidation states are sometimes written as a Roman numeral, e.g.; Fe(II), Cr(VI)

Definition: The number of charges an atom *would* have in a molecule (or ion) if the shared electrons were transferred completely to the more electronegative atom (see Blackman 12.1)

Much more on what electronegativity means and how to calculate oxidation numbers in weeks 4 and 5

Rules:

- Elements in their uncombined state = 0
- In neutral molecules, sum of ONs = 0
- In an ion, sum of ONs = charge on ion

Usually:

- Hydrogen: ON = +1 when combined with non-metals and = –1 with metals
- Oxygen: ON = –2 (except peroxides ON= –1)
- Fluorine: ON = – 1 (except in F_2)

Naming Inorganic Compounds – The alternative "systematic" approach

There are two ways of naming metal containing compounds when there is more than one possibility for the oxidation number of the metal

systematic nomenclature is useful for naming metal compounds,– with metal oxidation number in Roman numerals.

- $MnCl_2$ manganese(II) chloride (manganous chloride)
- $FeCl_2$ iron(II) chloride (ferrous chloride) contains Fe^{2+}
- $FeCl_3$ iron(III) chloride (ferric chloride) contains Fe^{3+}
- Hg_2Cl_2 mercury(I) chloride (mercurous chloride)
- $HgCl_2$ mercury(II) chloride (mercuric chloride)
- –ic and –ous nomenclature still appears (more or less!)

Usually only one space in name: separating cation from anion.

Naming Inorganic Compounds -the alternative "systematic" approach

- Can use for non-metals too
- SYSTEMATIC naming needs no numerical prefixes.
- Other naming uses numerical prefixes for ambiguous species.
- leftmost element first for non metals
- lower element first in same column
- -ide ending

	SYSTEMATIC	*COMMON*
NO	nitrogen(II) oxide	nitrogen monoxide
N_2O	nitrogen(I) oxide	dinitrogen oxide
N_2O_5	nitrogen(V) oxide	dinitrogen pentoxide
NO_2	nitrogen(IV) oxide	nitrogen dioxide
N_2O_4	nitrogen(IV) oxide	dinitrogen tetroxide
IF_5	iodine(V) fluoride	iodine pentafluoride

Quick Quiz - Naming Inorganic compounds

$FeSO_4$

$Fe(ClO_4)_3$

$Cr_2(CO_3)_3$

BrF_5

$HBrO$

Cl_2O_7

QUICK QUIZ - NAMING INORGANIC COMPOUNDS

$FeSO_4$	iron(II) sulfate	ferrous sulfate
$Fe(ClO_4)_3$	iron(III) perchlorate	ferric perchlorate
$Cr_2(CO_3)_3$	chromium(III) carbonate	chromic carbonate
BrF_5	bromine(V) fluoride	bromine pentafluoride
HBrO	hypobromous acid	
Cl_2O_7	chlorine(VII) oxide	dichlorine heptaoxide

NOMENCLATURE – HYDROGEN COMPOUNDS

Binary compounds of hydrogen

- Hydrogen requires special consideration
- It may appear first or second in the chemical formula of a compound, therefore first or second in the name
- Usually appears second when combined with a metallic element
- Examples: H first: groups 16 and 17; H second: groups 1 and 2

Lithium hydride	LiH
Hydrogen fluoride	HF
Hydrogen sulfide	H_2S
Calcium hydride	CaH_2

Groups 13, 14 and 15

- Unsystematic names e.g. B_2H_6 diborane

Oxygen forms two binary compounds with hydrogen. These have unsystematic names:

- water, H_2O (systematic name oxidane),
- hydrogen peroxide, H_2O_2 (systematic name dioxidane).

WHAT'S IN A NAME?

Often systematic names are of little practical use….

For example what do you think is the 'common' name for…..

0

(2*R*,3*R*,4*S*,5*S*,6*R*)-2-[(2*S*,3*S*,4*S*,5*R*)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol

A

Cocaine

B

Caffeine

C

Sucrose (Sugar)

D

DNA

MILLION $$ QUESTION

sulphur of sulfur?

Sulfur

Why?

Because IUPAC said so.