26020 Chemistry (Polytechnical Foundation)

Plan for today:

1. About the course
2. Chemistry in society
3. Atoms, molecules, ions, and stoichiometry
4. The Periodic table
5. Energies of reactions
6. A bit of naming of compounds
7. Size of molecules

Overview of the course

Book:

Chang, Goldsby: ***General Chemistry: The Essential Concepts,*** McGraw-Hill. 7th Ed.

Exercises: Monday 8:00-10:00 in building 324 rooms 20, 40, 50, 60, 70 and the surrounding lobby (areas 3, 4, 5, and 8). Building 306 room 31. We have 324 seats in 324 and 58 in 306. We are 386 registered students (as of Wednesday 24.8.)

Bhaskar Reddy Sudireddy bhsu@dtu.dk
Ming Chen minc@dtu.dk

Lecture: Monday 10:15-12 in Building 306. auditorium 34 (194 seats) in each auditorium

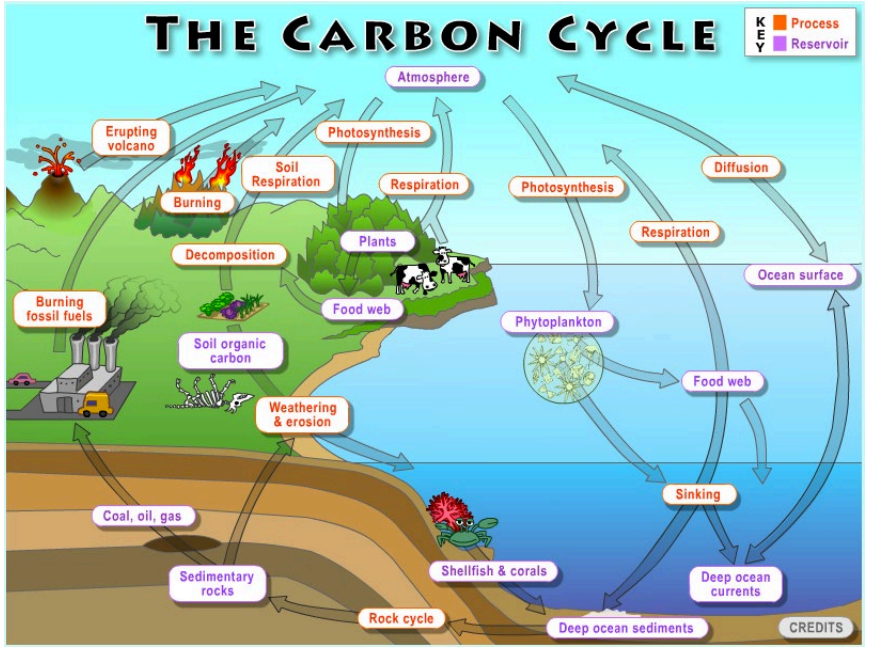
Stream: live streaming in Building 306 auditorium 35 or elsewhere go the course DTUlearn homepage and go into Video & Streaming.
Afterwards available on panopto in the 26020 folder

Course responsible

Kristoffer Almdal kral@dtu.dk

Flipped classroom

- We do exercises in the subject in front of the lectures that deal with them
- The TA will help communicate subjects to receive special attention in the lecture to the lecture – we will use slido for this
- We will use the circulation of carbon on earth to illustrate how chemistry can be used to evaluate current debates an gain chemistry based quantitative and qualitative insights



Science Education Resource Center. Retrieved 31-7-2023 from https://serc.carleton.edu/download/images/56944/global_carbon_cycle_1427132279.jpg under CC BY-NC-SA license

Kristoffer Almdal

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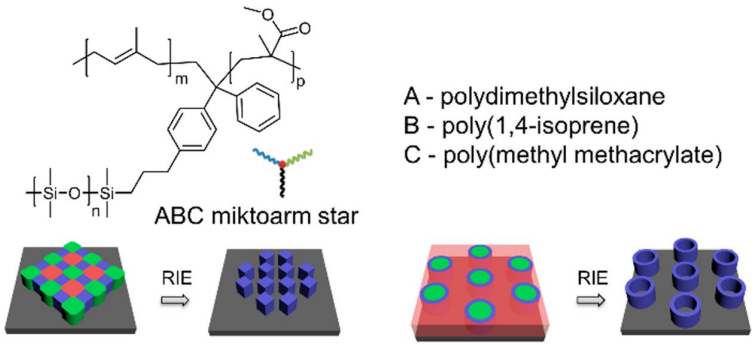
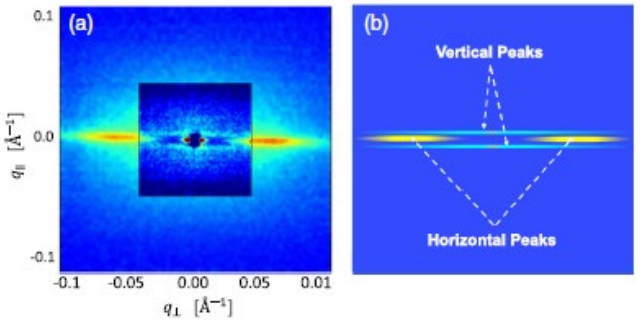
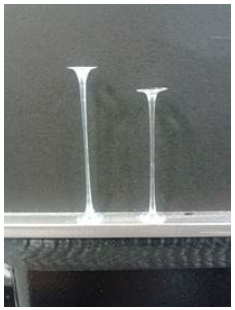
DTU Chemistry,
Building 206 room 042



Teaches:

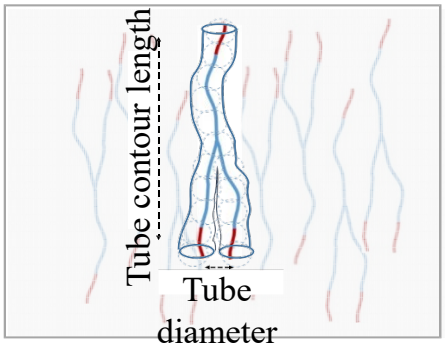
- Several Materials Science courses
- Chemistry (polytechnical foundation)
- Polymer physics and chemistry





Research:

- Self-organizing soft materials
- Polymer syntheses
- Block copolymer and applications of them
- Structuring of surfaces
- Polymer degradation
- Extensional flow



Course plan

Course plan - 26020 Chemistry (Polytechnical Foundation)

Lecturer: Krisotffer Almdal, E-mail: kral@dtu.dk

Exercises: Bhaskar Reddy Sudireddy bhsu@dtu.dk

Book: Chang, General Chemistry: The Essential Concepts, 7th Ed., McGraw-Hill.

Exercises: Monday 08-10, B324: rooms 20, 40, 50, 60, 70 and the surrounding lobby (areas 3, 4, 5, and 8). Building 306 room 31.

Lectures: Mondays 10:15-12. Aud. 34, B306 and streaming in Aud 35

Lecture	Chapters and topics	Keywords
1	**Ch. 2+3:** Atoms, molecules, stochiometry	atoms, elements, periodic table, formula, molar weight, nomenclature, stoichiometry
2		to be announced
3		to be announced
4		to be announced
5		to be announced
6		to be announced
7		to be announced
8		to be announced
9		to be announced
10		to be announced
11		to be announced
12		to be announced
13	Repetition: Highlights: What did we learn?	Reptition of difficult topics questions in class

Chapter 1 is presumed known.

What is Chemistry 1?

Encyclopedia Britannica:

the science that deals with the properties, composition, and structure of substances (defined as elements and compounds), the transformations they undergo, and the energy that is released or absorbed during these processes

Wikipedia:

Chemistry is the scientific study of the properties and behavior of matter

this definition is very broad – materials science - solid state physic - chemistry

Common perception:

You easily find statements:

chemical free beauty tips

On the WEB

A paper was submitted to Nature Chemistry with the title

A comprehensive overview of chemical-free consumer products

(it was not published)

What is Chemistry 2?

Historical:

developed from alchemy – concerned with several objectives, most known is the wish to produce gold

Modern view:

Chemistry is the science of the behavior of substances and their reactions and the effort to rationalize this behavior based on experimental observations and theoretical considerations

Organic chemistry:	Chemistry involving the element carbon
Inorganic Chemistry:	Chemistry of all the other molecules and compounds – often compounds containing elements that are metals
Physical Chemistry:	Laws describing the properties of chemical compounds and their state of matter. A physical approach to chemistry – includes thermodynamics and quantum mechanics
Biochemistry:	Chemistry related to processes in living organisms
Analytical Chemistry:	Development and use of method to identify and quantify elements and compounds

Chemistry can achieve many things – good and less good

Here are some of the positives:

- Clean **drinking water** for everybody
- Effective, healthy, and sustainable **food**
- Plenty, cheap, and clean **energy** for all
- **Materials** for houses, tools, devices (yes, incl. your smartphone!), etc.
- Effective use of **resources**, e.g. metals,
- Cleaner and more ”green” ways to **produce**
- Medical challenges and **health**
- **Climate** and **environment**

Resources on a global scale:

- Plastics use 5% of all crude oil produces
- Chemical industry (besides the polymers) use ~ another 5%
- Production of ammonia (for fertilizers production) use 1-3% of the worlds energy consumption
- Most of the rest is used for transportation and heating and cooling of houses

Chemistry is important for all engineers

- Chemistry is a fundamental part of our understanding of our world and thus required to understand the phenomena of our society and surroundings.

- Some examples where chemistry affects other areas of engineering science:

  - Building materials for houses and bridges
  - Sustainable food
  - Water quality and pollutants in environment
  - Medicine is chemical compounds
  - New designed proteins and enzymes
  - Corrosion of surfaces and materials
  - Electronic devices are chemical designs
  - Batteries for your laptop / smart phone
  - Climate science is very much about chemistry

The three states of matter

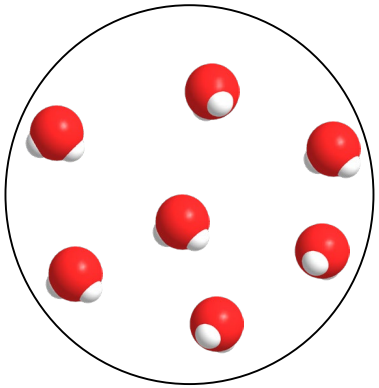
Most matter is either in the form of gas, solid, or fluid.

By changing temperature or pressure, one can convert from one to another.

These different macroscopic forms represent distinct molecular worlds.

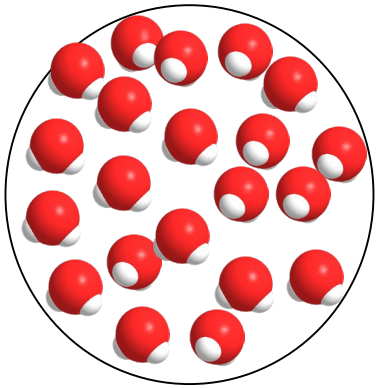
from:

steam



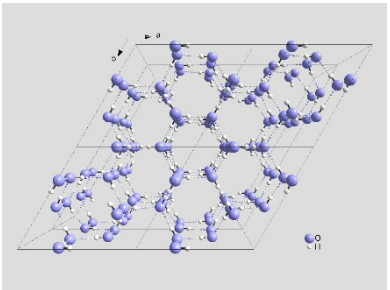
to

water



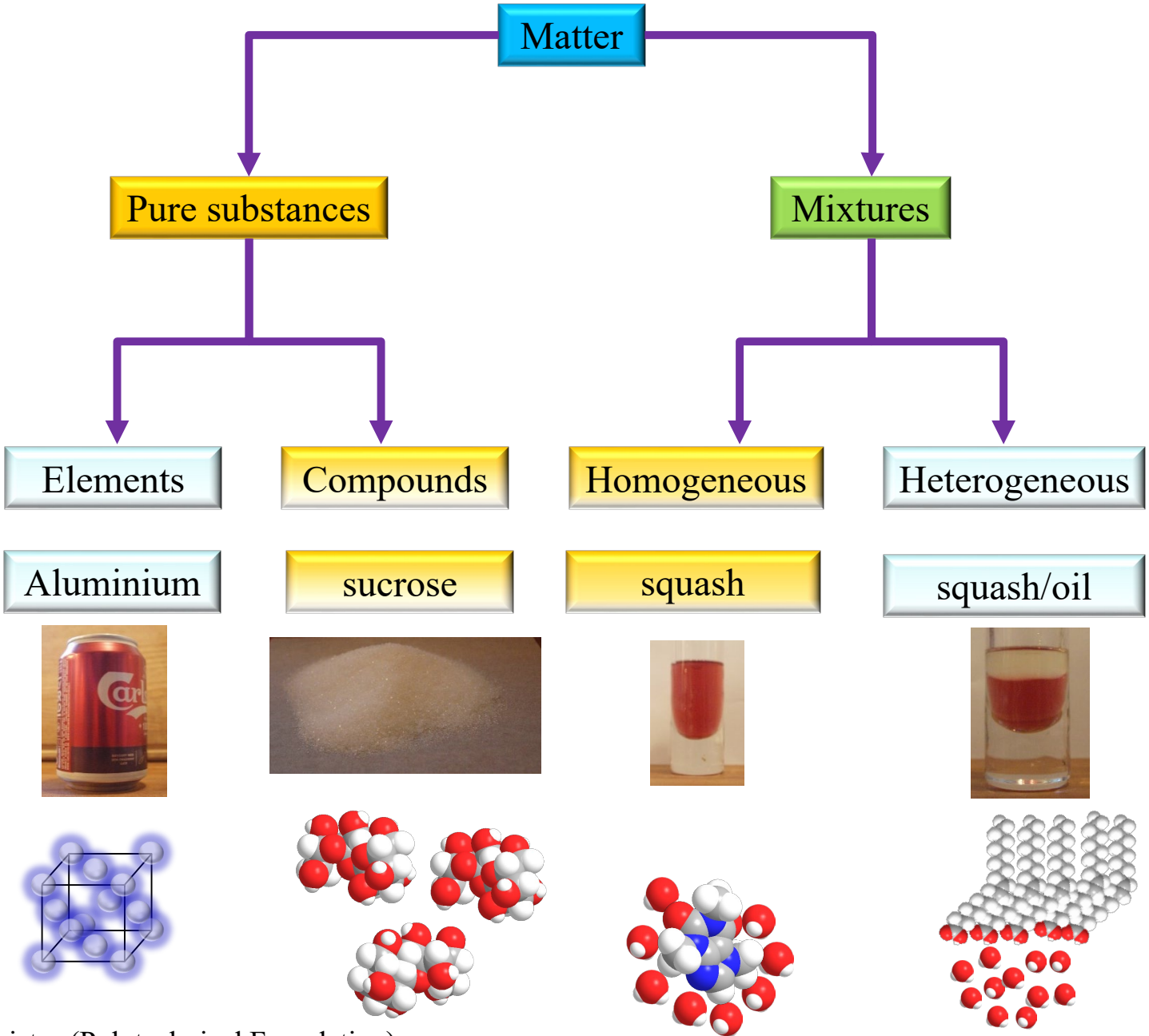
to

ice



https://en.wikipedia.org/wiki/Ice_Ih#/media/File:Crystal_struct_ice.png (CC BY-SA 3.0)

Classification of Matter



History of Chemistry up to the idea of atom

400 BC -1600
Alchemy:
'Pseudoscience'
Mystics/cheaters/…
Metallurgy
Mineralogy/medicine

late 1700
Antoine Lavoisier ('father of Chemistry')
- Combustion process
- Conservation of mass
- The first 'modern' chemistry textbook

~1800
John Dalton
- Father of the theory of atoms
- law of multiple proportions:

Mass of oxygen combined with 1g of carbon
compound 1: 1.33g
compound 2: 2.66g
i.e. 1 : 2 CO and CO_2

Middle 1800
Stanislao Cannizzaro
Measures relative atomic masses
(including C = 12×'M'$_H$)

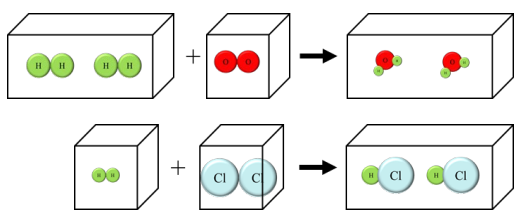
time

500 - 400 BC
Greeks
the 4 elements

Middle 1600
Robert Boyle ('the first chemist')
- Quantitative experiments
- Boyles law
- The idea of chemical elements

~1800
Joseph Proust
law of definite proportions
E.g. $CuCO_3$ Always: 5,3 parts cobber, ,4 parts oxygen, 1 part carbon (relative mass).

Early 1800
Avogadro and Gay-Lussac

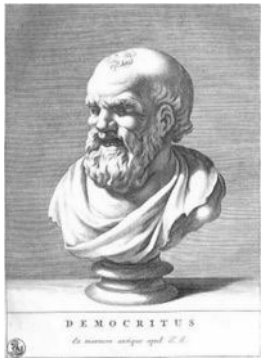


T and P = constant

atoms

Greek philosopher **Democritos**: "Everything is made of atoms."

A-tomos – indivisible



Democrit

(ca. 460 – 370)

In 1808 this theory was rediscovered by Dalton.

1. Elements consists of very small, elementary parts called atoms.
2. All atoms in an element are the same but differ from the atoms of other elements
3. Molecules consist of atoms. The distribution between different atoms is a simple relationship, e.g. 1:2 (like O:H in water)
4. A chemical reaction redistributes atoms among molecules, but does not create or destroy atoms themselves.

John Dalton

(1766-1844)

In the opinion of Nobel laureate Richard Feynman this is the most important scientific accomplishment ever

The atomic nucleus

Rutherford, 1910:

- When a beam of α-particles (He nuclei) are passed through a thin gold foil:

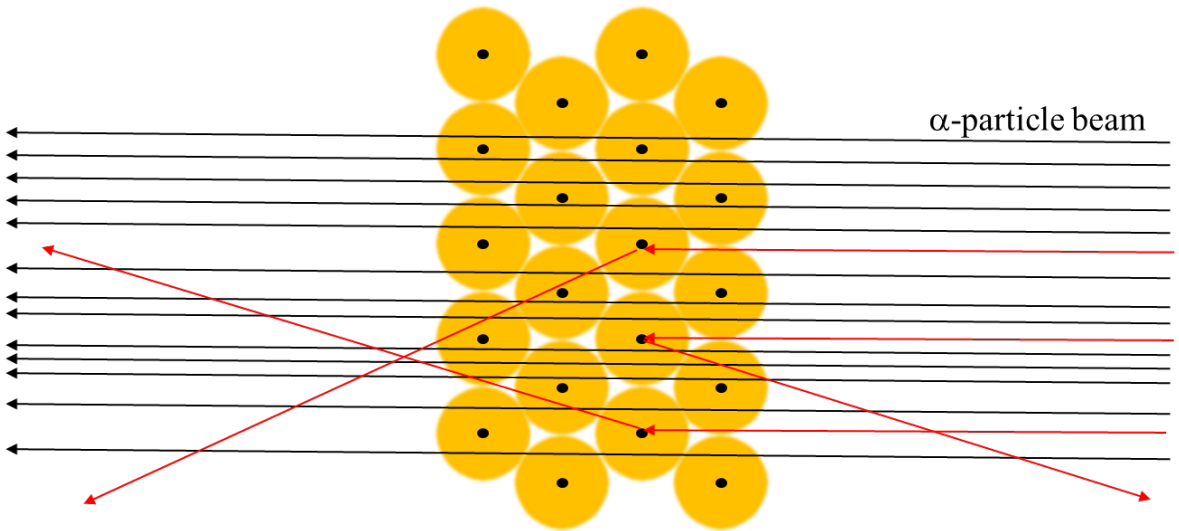
a) The was majority goes straight through

b) **A few gets deflected**

Ernest Rutherford

(1871-1937)

This shows that there is a solid core (nucleus) within the gold



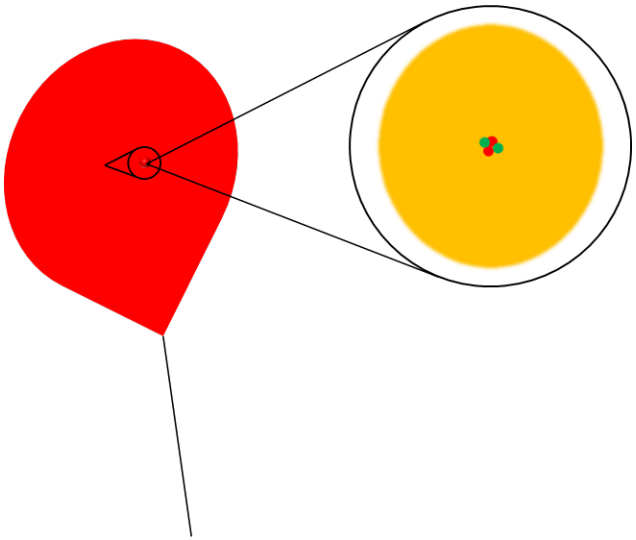
Why did Rutherford use gold for his experiment?

Atomic structure

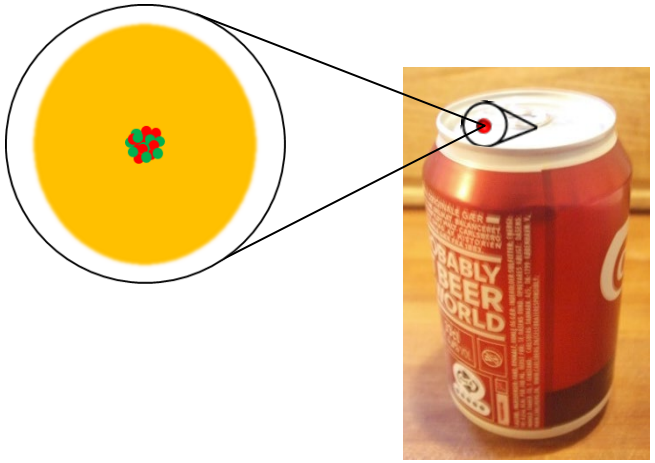
Nucleus consisting of protons (charge +1) and neutrons (neutral)

Electrons (charge -1) circulate around the nucleus in a cloud

Helium:
2 protons
2 neutrons

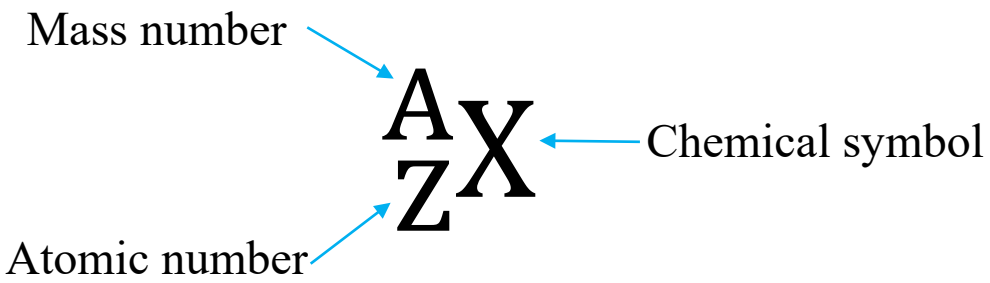


Aluminium:
13 protons
14 neutrons



Mass and Charge

Mass and Charge of subatomic particles			
		Charge	
Particle	**Mass/g**	**Coulomb**	**Charge unit**
Electron	9.10938×10^{-28}	-1.6022×10^{-19}	-1
Proton	1.67262×10^{-24}	-1.6022×10^{-19}	+1
Electron	1.67493×10^{-24}	0	0

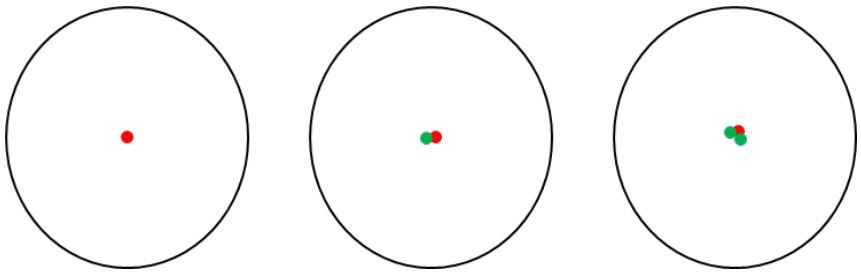


Classification of atoms: The atomic number Z

- Every element has a **different number of protons Z**:
  Example: hydrogen (1), helium (2), carbon (6), gold (79)

- There may be different isotopes of the same element (with different number of neutrons)
  - hydrogen, ^{1}H, deuterium ^{2}H, tritium ^{3}H
  - uranium: ^{235}U og ^{238}U.

- Chemical reactivity is almost the same for different isotopes
  The electrons - responsible for the chemistry –
  interact with the nucleus through electrostatics not gravity



$^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$

The periodic Table

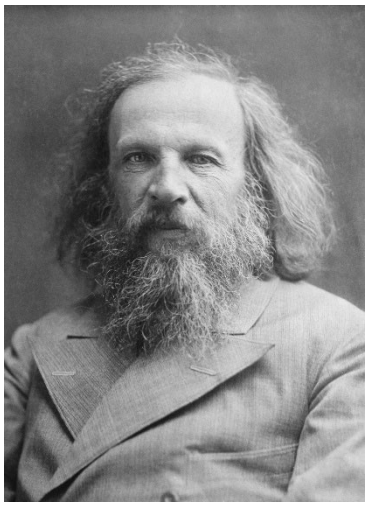
- Categorization of matter has historically been pursued.
- Ancient Greek system:
  - earth
  - wind
  - fire
  - water
  - (cosmos)

The Periodic Table

- In 1869 Siberian born chemist Dmitri Mendeleev arranged the then known 63 elements in a table according to atomic weight.
  - This arrangement grouped elements with similar physical and chemical properties.
  - Empty slots in Mendeleev's table were needed to achieve this.
  - In every main group the elements resemble each other there will be trends when moving strictly in one direction.
  - 4 relatively light unknown elements were correctly predicted:
    - Scandium (eka-boron)
    - Gallium (eka-aluminium)
    - Technetium (eka-manganese)
    - Germanium (eka-silicon)
  - A number of heavier elements including Hafnium were also predicted.

Mendeleev periodic table

Reihen	Gruppo I. — R^1O	Gruppo II. — RO	Gruppo III. — R^2O^3	Gruppo IV. RH^4 RO^2	Gruppo V. RH^3 R^2O^5	Gruppo VI. RH^2 RO^3	Gruppo VII. RH R^2O^7	Gruppo VIII. — RO^4
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —



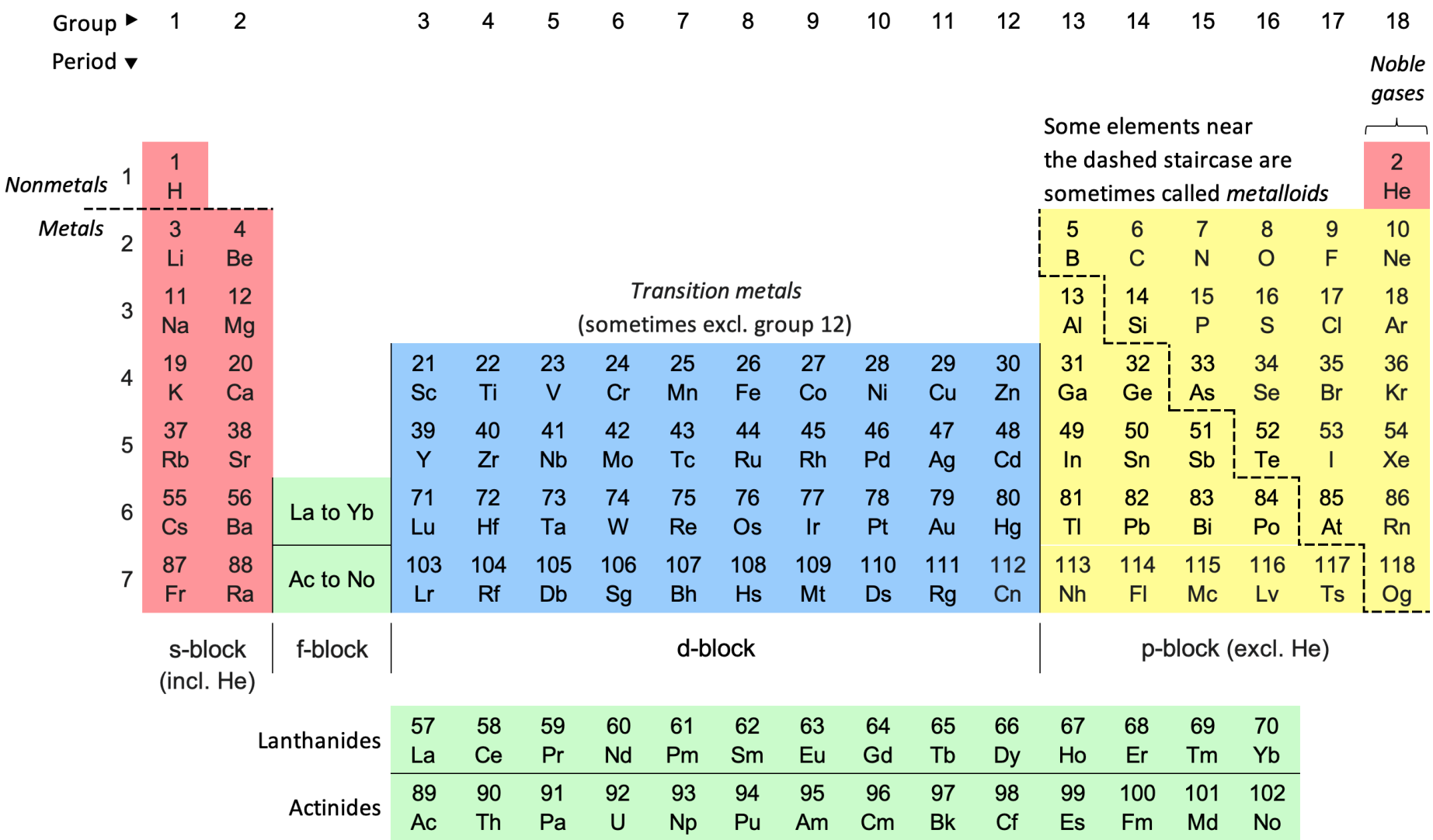
Dmitri Mendeleev

(1834-1907)

4 relatively light unknown elements were correctly predicted:

Scandium (eka-boron)	(1879)
Gallium (eka-aluminium)	(1875)
Technetium (eka-manganese)	(1937)
Germanium (eka-silicon)	(1869)

The periodic Table



The periodic table

1																	18
1 **H** 1.008	2											13	14	15	16	17	2 **He** 4.0026
3 **Li** 6.94	4 **Be** 9.0122											5 **B** 10.81	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
11 **Na** 22.990	12 **Mg** 24.305	3	4	5	6	7	8	9	10	11	12	13 **Al** 26.982	14 **Si** 28.085	15 **P** 30.974	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.948
19 **K** 39.098	20 **Ca** 40.078	21 **Sc** 44.956	22 **Ti** 47.867	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.845	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.546	30 **Zn** 65.38	31 **Ga** 69.723	32 **Ge** 72.630	33 **As** 74.922	34 **Se** 78.97	35 **Br** 79.904	36 **Kr** 83.798
37 **Rb** 85.468	38 **Sr** 87.62	39 **Y** 88.906	40 **Zr** 91.224	41 **Nb** 92.906	42 **Mo** 95.95	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
55 **Cs** 132.91	56 **Ba** 137.33	57-71 *	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	89-103 #	104 **Rf** (265)	105 **Db** (268)	106 **Sg** (271)	107 **Bh** (270)	108 **Hs** (277)	109 **Mt** (276)	110 **Ds** (281)	111 **Rg** (280)	112 **Cn** (285)	113 **Nh** (286)	114 **Fl** (289)	115 **Mc** (289)	116 **Lv** (293)	117 **Ts** (294)	118 **Og** (294)

* Lanthanide series	57 **La** 138.91	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97
# Actinide series	89 **Ac** (227)	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)

https://iupac.qmul.ac.uk/AtWt/table.html
World Wide Web version prepared by G. P. Moss

The periodic Table

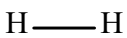
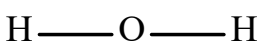
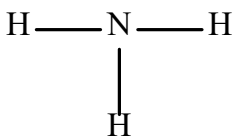
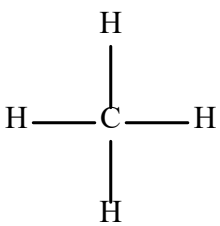
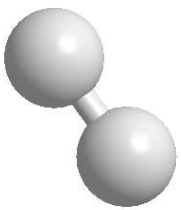
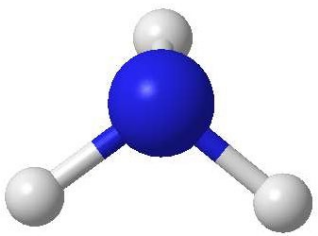
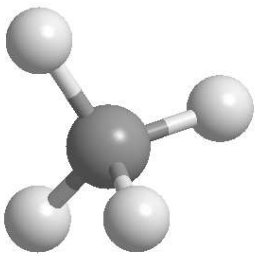
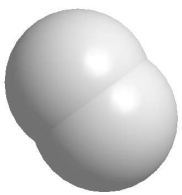
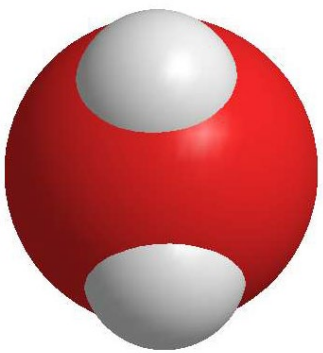
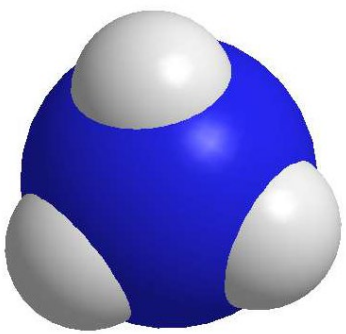
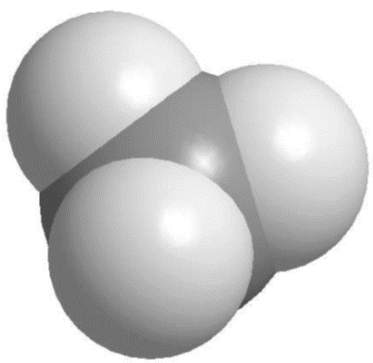
- Manny form available on the WEB:
- Crystal structures:
  https://en.wikipedia.org/wiki/Periodic_table_(crystal_structure)
- Interactive Royal Society version:
  https://www.rsc.org/periodic-table
- ACS downloads in different formats (free):
  https://www.acs.org/education/whatischemistry/periodictable.html
- And many more

Break

Until …

Molecular formula

Many ways to describe the structure of a molecule:

	H_2	H_2O	NH_3	CH_4
molecular formula				
structural formula				
ball-and-stick model				
space-filling model				

What is 1 mol?

- 1 mol equals 6.022×10^{23}
- Definition: the number of C atoms in 12 grams of the isotope ${}^{6}_{12}\mathrm{C}$.
- C has atomic mass 12.01
  H has 1.0008
  O has 15.999
  N has 14.007
- How many moles are there approximately in a 1-kg package of sugar?

- A: ~0.03 moles; B: ~0.3 moles; C: ~3 moles; D: ~30 moles; E: ~300 moles

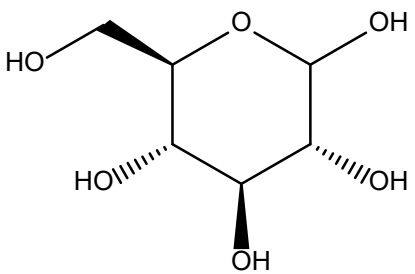
1 mol = 6.022 x 10^{23}: Two more examples

A 623 g heat deflector
M_{Cu}=63.5g
~10 mol

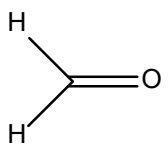
½ l water (500g)
M_{water}=18g
~28 mol

Empirical Formula

- Only provides the ratio between elements in the molecule (not total count)
- Thus, there will be molecules with the same ratio but different number of atoms in total.
- Both glucose and formaldehyde have the empirical formula CH_2O:



glucose
$C_6H_{12}O_6$

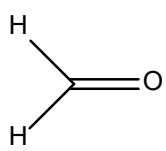


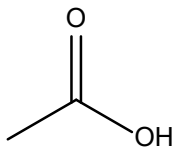
formaldehyde
CH_2O

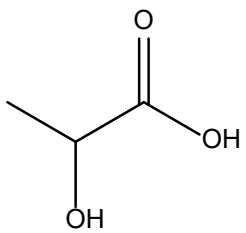
More compounds with same empirical formula

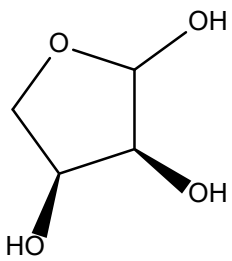
Examples of compounds with empirical formula CH_2O (composition by mass 40.0% C, 6.71% H, 53.3% O

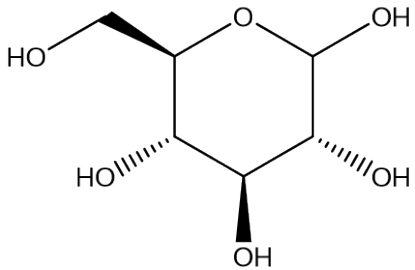
Name	Molecular formula	Whole-number multiple	M/(g/mol)	use or function
Formaldehyde	CH_2O	1	30.03	Disinfectant; biological preservative
Acetic acid	$C_2H_4O_2$	2	60.06	Acetate polymers, vinegar (5% solution); cleaning
lactic acid	$C_3H_6O_3$	3	90.08	causes milk to sour, forms in muscles during anaerobic work; polymers
erythrose	$C_4H_8O_4$	4	120.10	forms during sugar metabolismpart of RNA and DNA
ribose	$C_5H_{10}O_5$	5	150.13	part of RNA and DNA and vitamin B_2
glucose	$C_6H_{12}O_6$	6	180.16	Major sugar in carbohydrate metabolism, the sweetener in some fruits











Calculating the empirical formula

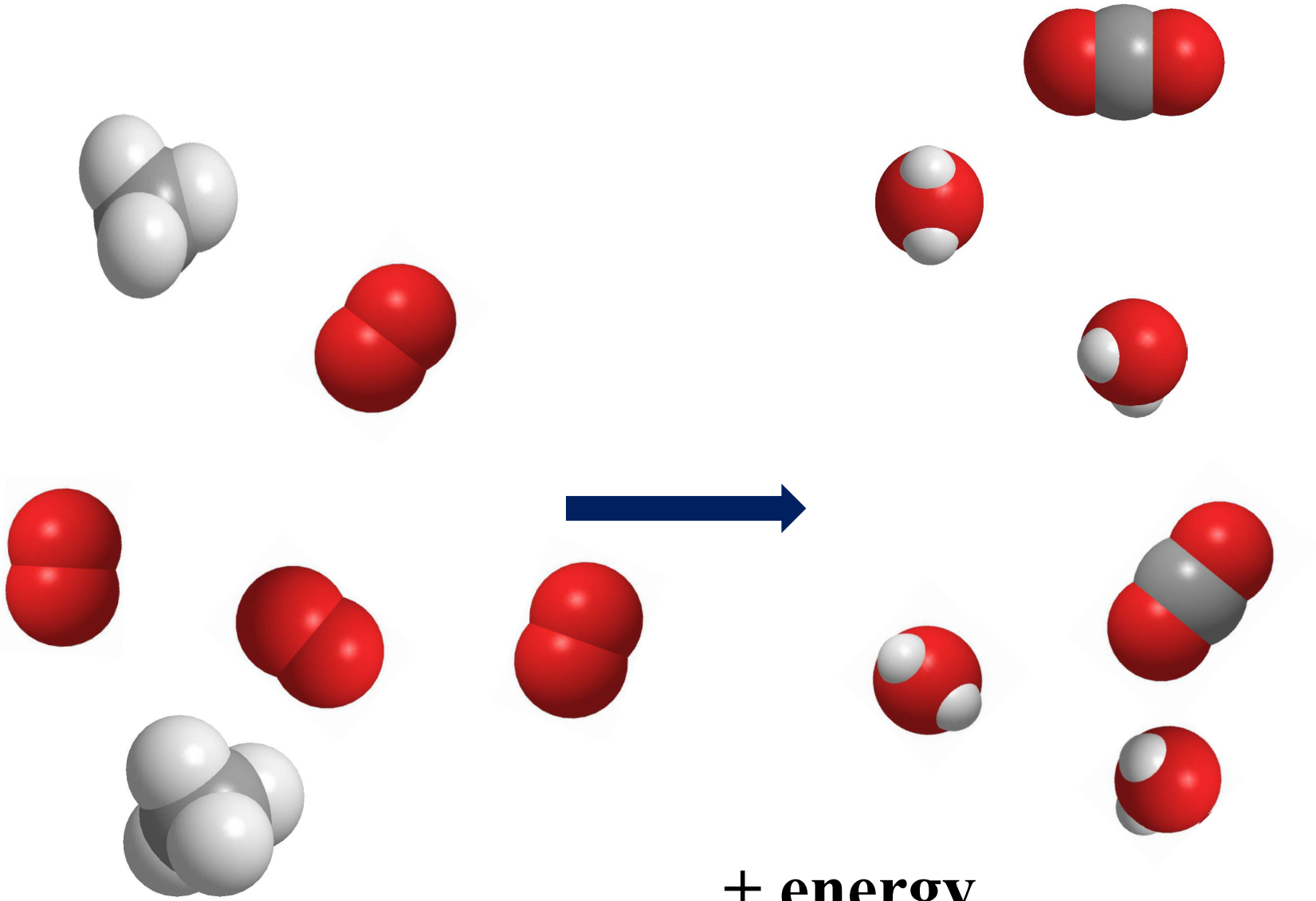
Mass %

Mol of each element %

Mol ration of elements

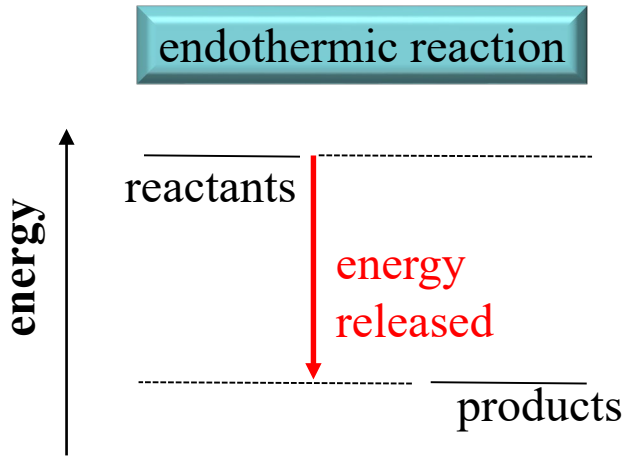
Empirical formula

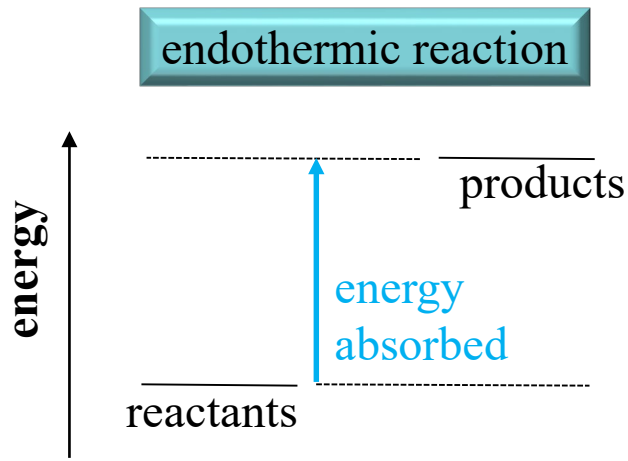
An example of a reaction: What is this?



Endothermic & exothermic

Reactions can be classified as either **endothermic** (take up heat/energy) or **exothermic** (release heat/energy).





Units of energy

Energy conversion tables

1 calorie (cal)	=	4.184 joule (J)
1 Calorie (Cal)	=	1000 calories (cal)
1 kilowatt hour (kWh)	=	3.6×10^{6} joule (J)

Energy use in various units

unit	energy to raise temperature of 1 g of water by 1°C	Energy to run a 1000 lumen light-bulb for 1 hour	total daily energy use of a Danish citizen
joule (J)	4.18	4.68×10^{4}	3.26×10^{8}
calorie (cal)	1	1.12×10^{4}	7.78×10^{7}
Calorie (Cal)	0.001	11.2	7.78×10^{4}
kilowatt-hour (kWh)	1.16×10^{-6}	0.013	90.5

Salts: Nomenclature

Positive ions – the cation - first

sodium Na^+

potassium K^+

magnesium Mg^{2+}

ammonium NH_4^+

Negative ions – the anion – last:

oxide, O^{2-}

sulfide, S^{2-}

fluoride, F^-

bromide, Br^-

carbonate, CO_3^{2-}

dihydrogen phosphate, $H_2PO_4^-$

e.g. NaBr: sodiumbromide

Some common anions

nonmetal	symbol for ion	base name	anion name
fluorine	F^-	fluor-	fluoride
chlorine	Cl^-	chlor-	chloride
bromine	Br^-	brom-	bromide
iodine	I^-	iod-	iodide
oxygen	O^{2-}	ox-	oxide
sulfur	S^{2-}	sulf-	sulfide
nitrogen	N^{3-}	nitr-	nitride

More anion names

Some common polyatomic ions			
name	**formula**	**name**	**formula**
acetate	$C_2H_3O_2^-$	hypochlorite	ClO^-
carbonate	CO_3^{2-}	chlorite	ClO_2^-
hydrogen carbonate (bicarbonate)	HCO_3^-	chlorate	ClO_3^-
hydroxide	OH^-	perchlorate	ClO_4^-
nitrite	NO_2^-	permanganate	MnO_4^-
nitrate	NO_3^-	sulfite	SO_3^{2-}
chromate	CrO_4^{2-}	hydrogen sulfite (bisulfite)	HSO_3^-
dichromate	$Cr_2O_7^{2-}$	sulfate	SO_4^{2-}
phosphate	PO_4^{3-}	hydrogen sulfate (bisulfate)	HSO_4^-
hydrogen phosphate	HPO_4^{2-}	oxide	O_2^{2-}
ammonium	NH_4^+	cyanide	CN^-

Increasing oxidation state: hypo-; -ite;- ate; per-

Names of oxyanions

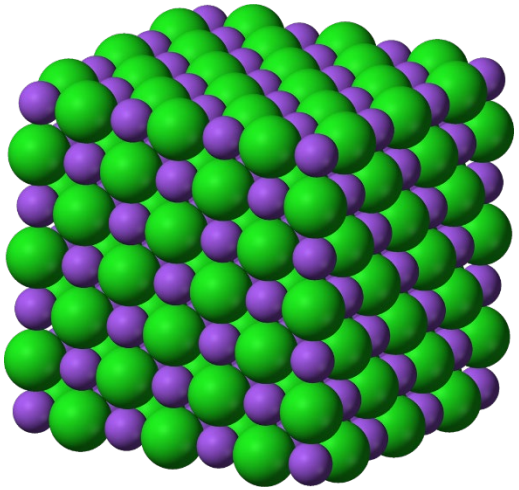
Some common oxyacids and the corresponding oxyanions

acid	formula	oxyanion	formula
nitrous acid	HNO_2	nitrite	NO_2^-
nitric acid	HNO_3	nitrate	NO_3^-
sulfurous	H_2SO_3	sulfite	SO_3^{2-}
sulfuric	H_2SO_4	sulfate	SO_4^{2-}
chlorous	$HClO_2$	chlorite	ClO_2^-
chloric	$HClO_3$	chlorate	ClO_3^-
perchloric acid	$HClO_4$	perchlorate	ClO_4^-
acetate	C_2H_4O	acetate	$C_2H_3O^{2-}$
carbonic acid	H_2CO_3	carbonate	CO_3^{2-}

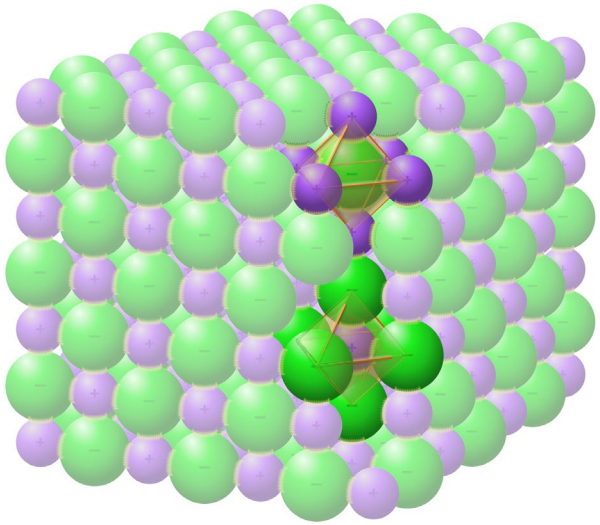
Increasing oxidation state: hypo-; ous;- ic; per-

Structure of solids: NaCl

- NaCl is crystalline with Na^+ and Cl^- arranged in a periodic lattice structure
- This enables electrostatic stabilization of the structure



Goran tek-en CC BY-SA 4.0
https://commons.wikimedia.org/wiki/File:NaCl_bonds.svg



Goran tek-en CC BY-SA 4.0
https://commons.wikimedia.org/wiki/File:NaCl_bonds.svg

Halite Location: Wieliczka Salt Mine, UNESCO World Heritage Site, Wieliczka, Małopolskie, Poland Size 16×15×13 cm CC BY-SA 4.0
https://commons.wikimedia.org/wiki/File:Selpologne.jpg#/media/File:Selpologne.jpg

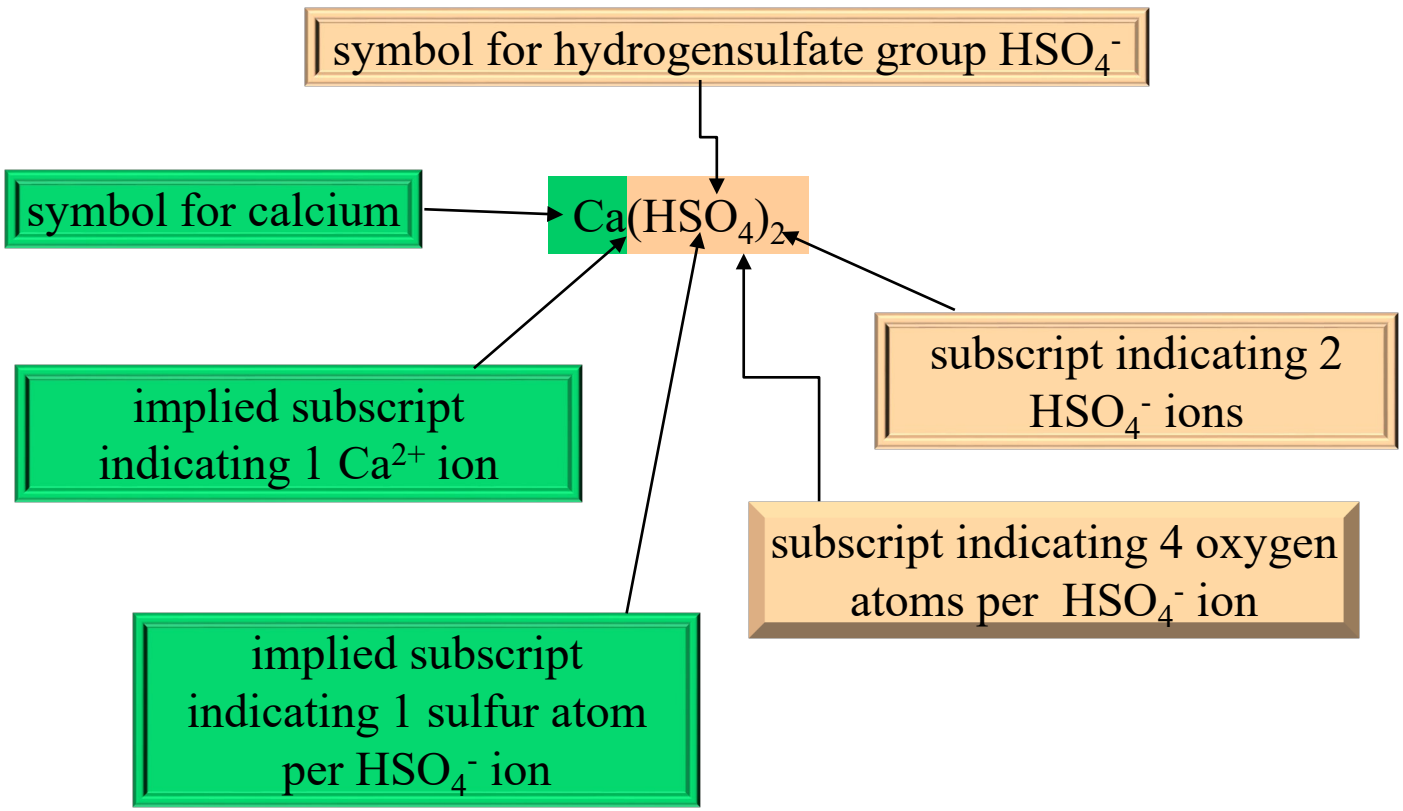
What happens when NaCl get in contact with water?

Nomenclature in general

write up the structures with element symbols and charge

let the charges cancel

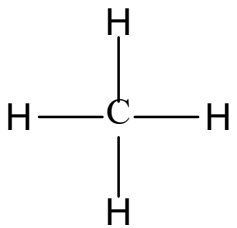
(molecular formula):

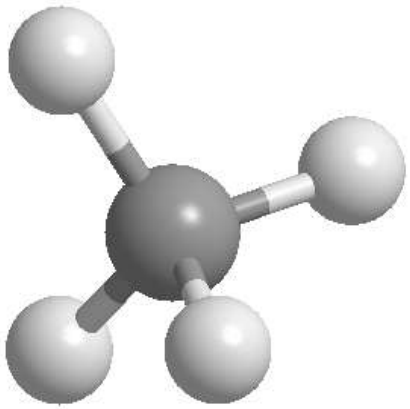


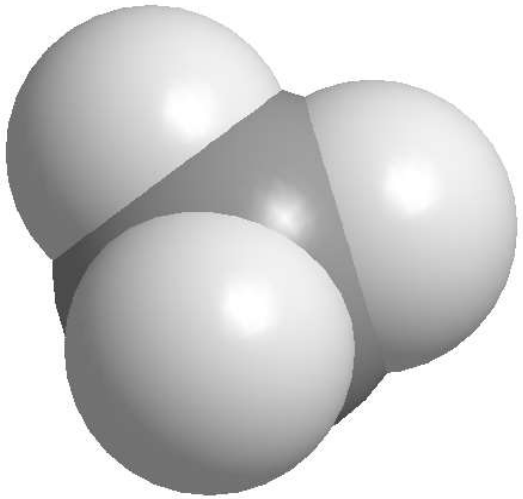
How to visualize molecules

Most important examples:

CH_4







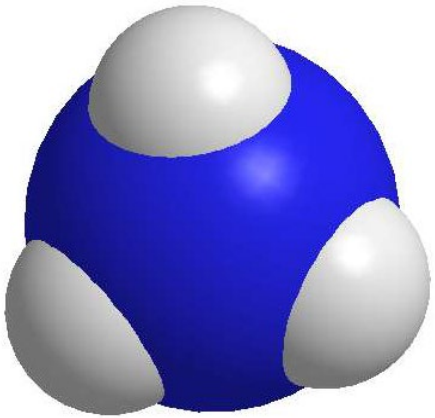
molecular formula

structural formula

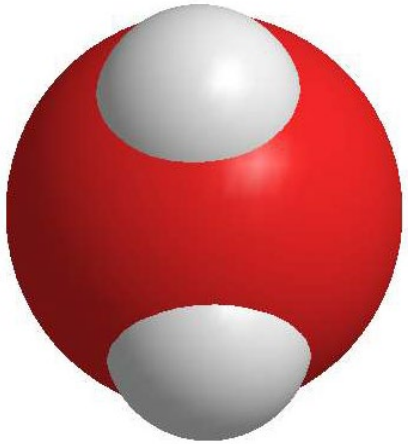
ball-and-stick model

space-filling model

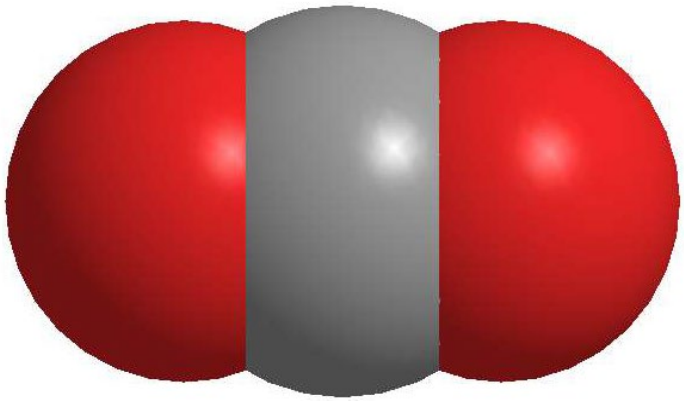
Sizes of molecules



|NH|=0.101 nm
HNH-angle=107°

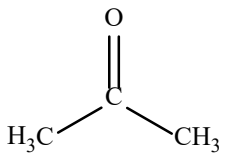


|OH|=0.0958nm
HOH-angle 104.5°

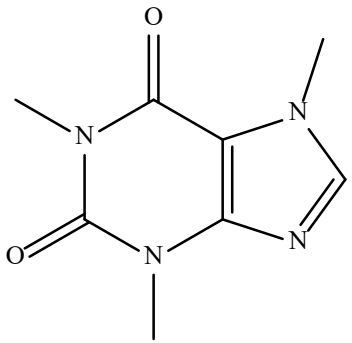


|CO|=0.116nm

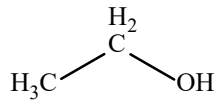
Some structural formulas



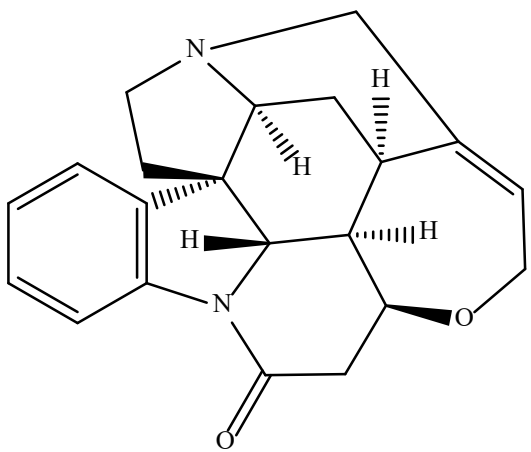
acetone



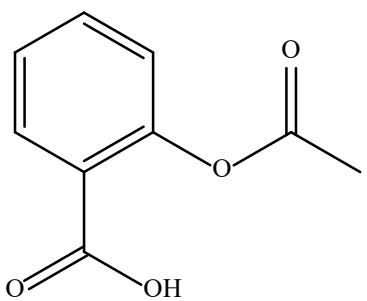
caffeine



ethanol

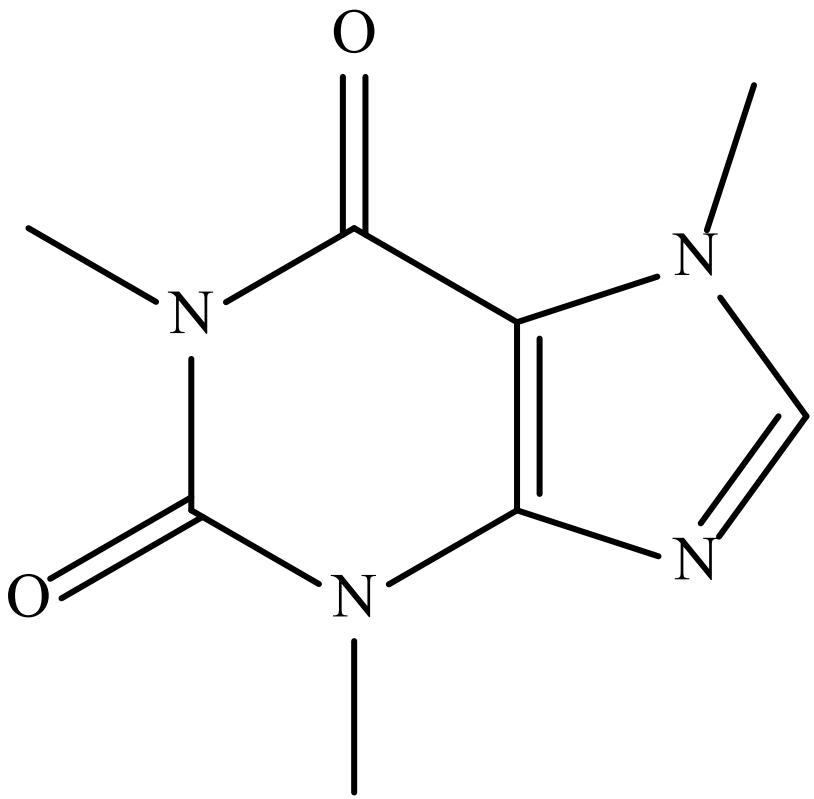


strychnine



aspirine

Test: Molar mass: Calculate for caffeine



caffeine

Summary

- On the perception of chemistry
- Structure of atoms and molecules
- Conversion between # of molecules and mass
- Representation of chemical structures in drawings
- The organization of the elements in the periodic table
- Introductory nomenclature – naming of compounds
- Relating to molecular size

Questions and comments

- Question are nice –
  - Tough with 300 – 400 students in the audience but we try
  - Whoever speaks learns the most

  - Se you next week