General Chemistry C1020

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General Chemistry C1020

Lecture - lecture hall A11/132

Tue 17 - 19.00
Thu 10 - 12.00

Lecture slides will be posted in IS

Exam = written test

Seminar C1040

General Chemistry C1020

Zumdahl, Steven S.; Zumdahl, Susan A. Chemistry. 6th ed. Boston : Houghton Mifflin Company, 2003. xxiv, 1102 s. ISBN 0-618-22156-5.

Chang, Raymond. Chemistry. 6th ed. Boston : McGraw-Hill, Inc., 1998. xxxviii, 995 s. ISBN 0-07-618-115221-0.

Feigl, Dorothy M.; Hill, John W. General, Organic and Biological Chemistry : Foundations of Life. 2nd ed. New York : Macmillan Publishing Company, 1986. xvi, 589 s. ISBN 0-02-336730-X.

Science and Scientific Method

Science – Quantitative study of Nature and the laws of nature.
Process of acquiring new knowledge.
Empirical approaches to problem solving.

Deals only with **rational** expressions that could be verified or disproved by observations or experiments.

Francis Bacon
(1561-1626)

Science and Scientific Method

Observation (qualitative)
Measurement (quantitative)

Find patterns, trends

A Law of Nature
(describe the behavior of matter, notes that something happens)

Hypothesis

(empirically testable conjecture)

Theory, model
(explains why and how something happens, never 100% proven)

Prediction

Modification of a theory

Experiment, testing of hypothesis

Proper experiment design (e.g. measure one variable, other keep constant).

Support/disprove hypothesis – verify/falsify.

Experiments must be reproducible.

Observation and Explanation

The first explanation of natural phenomenon – **hypothesis successfully tested by a fulfilled prediction** :

Thales of Miletus

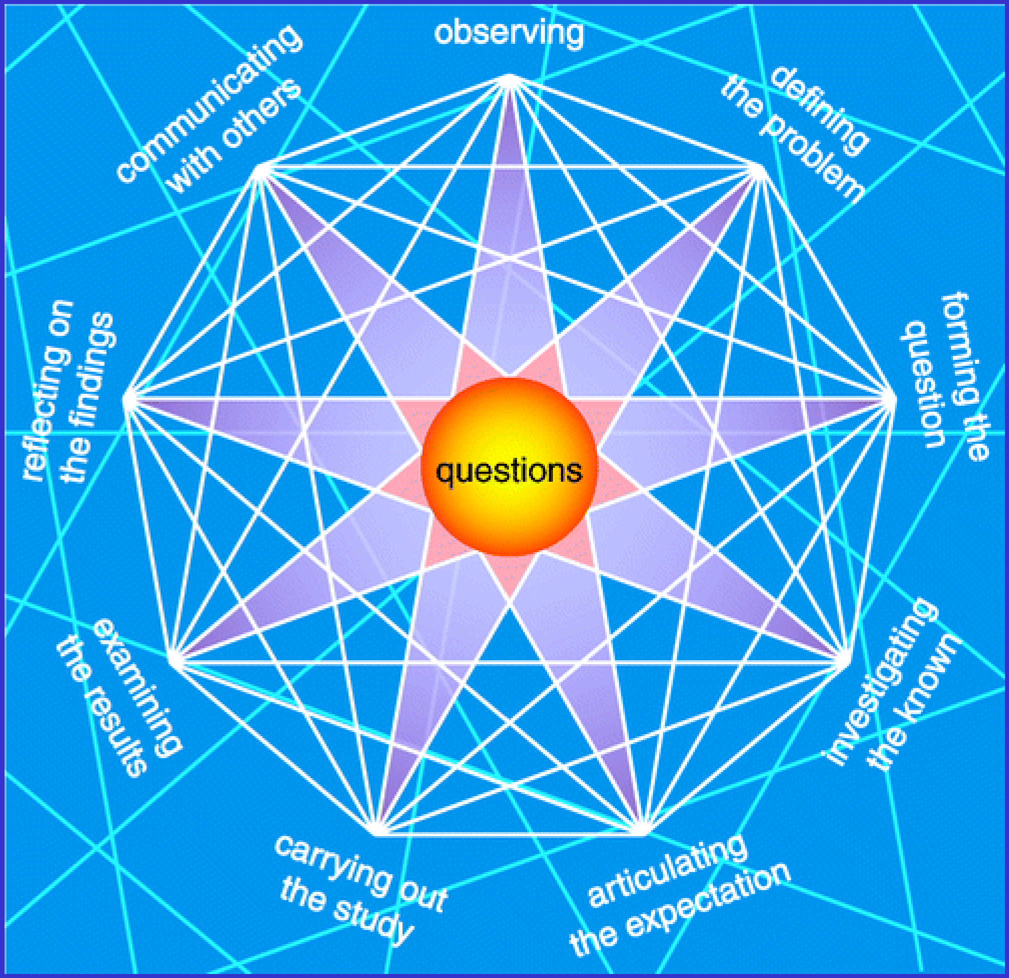
Explained Solar eclipse – new Moon crosses the Sun

Prediction of the next Solar eclipse in 585 BC

Beginning of scientific thinking, rational approach,
no mystics and religion

Primary substance – element = water

Scientific Method



Dawn of Chemistry

The first written note about a chemist
Mezopotamia 1200 BC

Tapputi-Belatekallim – perfume maker

Distillation, filtration

Observation and Explanation

Johann Joachim Becher
(1635 - 1682)

Georg Ernst Stahl
(1660 - 1734)
Phlogiston

The first consistent explanation of several natural phenomenons:

1) Burning of coal = release of **phlogiston**
2) Burning of metals = release of **phlogiston** + formation of oxides
3) Reaction of coal with metal oxides (ores) = reduction to metal
Transfer of **phlogiston** from coal to metal oxide
(metal = oxide + phlogiston)

BUT THERE IS A PROBLEM: Burning metal = oxide + **phlogiston**
Products of metal oxidation have HIGHER mass = phlogiston has negative mass ☹
Beginnings of **quantitative** experiments

Observation and Explanation

Refuting **phlogiston theory** = formation of modern chemistry.
A wrong theory was stepwise refuted based on experiments that supported a new theory.

Burning = combination with O_2,
higher mass of products - **weighing**

Antoine Laurent Lavoisier
(1743 – 1794)

The law of conservation of mass

phlogiston = $-O_2$

Heating HgO
(reduction to metal without phlogiston from coal)

Three Discoveres of Oxygen

Carl Wilhelm Schelle
(1742 – 1786)
Prepared O_2 in 1771
Published in 1777
(tasted chemicals)

Joseph Priestley
(1733 – 1804)
Published prep in 1774,
named it
Dephlogisticated air

Antoine Lavoisier
(1743 – 1794)
1783
Oxygen = **Element**

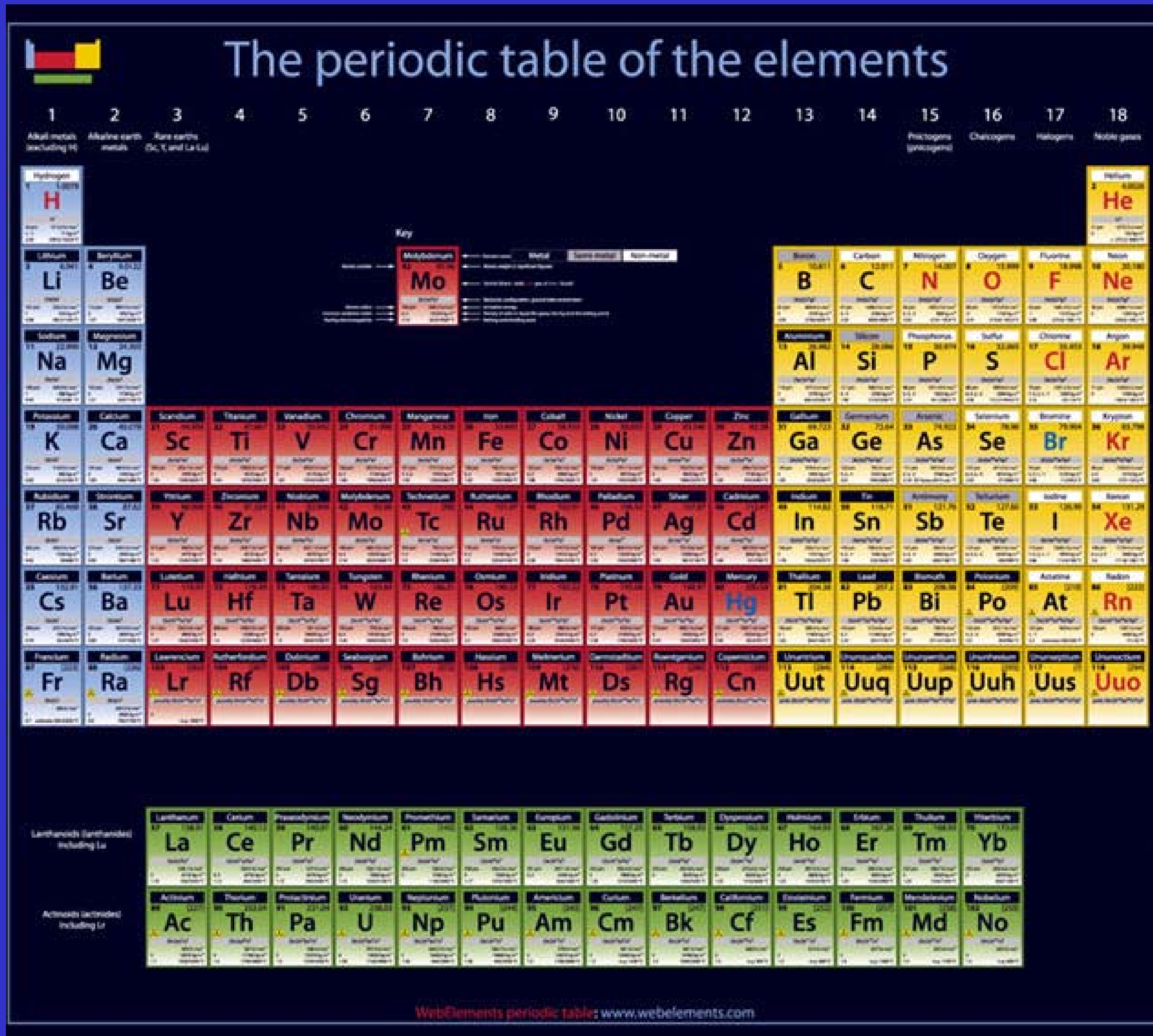
Heating HgO, Ag_2CO_3, $Mg(NO_3)_2$, $NaNO_3$

The Laws of Nature and Theories

The Law of Nature
– principles that summarises repeated observations of natural phenomenons, does not change (Coulomb law, Periodic law, Newton's law of gravitation, laws of motion, the ideal gas laws)
True, universal, absolute, stable, reversible, simple, omnipotent.

Theory
– coherently explains some aspect of reality, known facts, empirically supported, may change, may be falsified and rejected based on new experimental methods and more precise measurements

Objectivity – holds true under necessary conditions
Power of prediction – predicts new and unknown


The periodic table of the elements
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Key
Mo
H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Lr Rf Db Sg Bh Hs Mt Ds Rg Cn Uut Uuq Uup Uuh Uus Uuo
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No
WebElements periodic table: www.webelements.com

Joachim Jungius
(1587 - 1657)

Scientific Language

Founder of scientific language

Precise definitions of terms

The base of science is experiment and its results

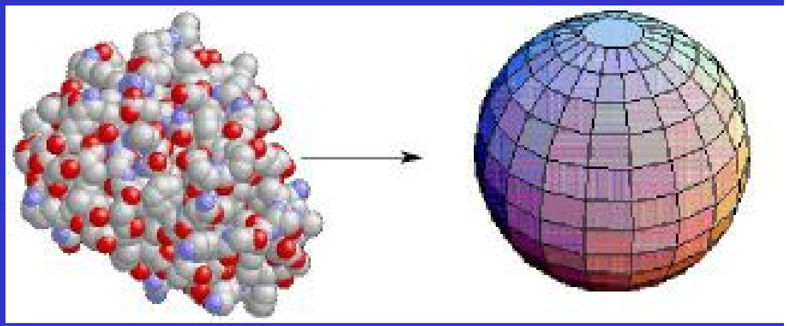
• Chemical nomenclature (names of elements, compounds, IUPAC Red Book, Blue Book)

• Names of lab equipment and instruments (Bunsen burner, Erlenmeyer flask, Soxlet extractor)

• Name reactions (Grignard, Wittig, Heck, Suzuki)

• Laws, equations and principles (Boyle, Schroedinger, Boltzman, Avogadro, Arrhenius)

Model



Simplified picture of reality

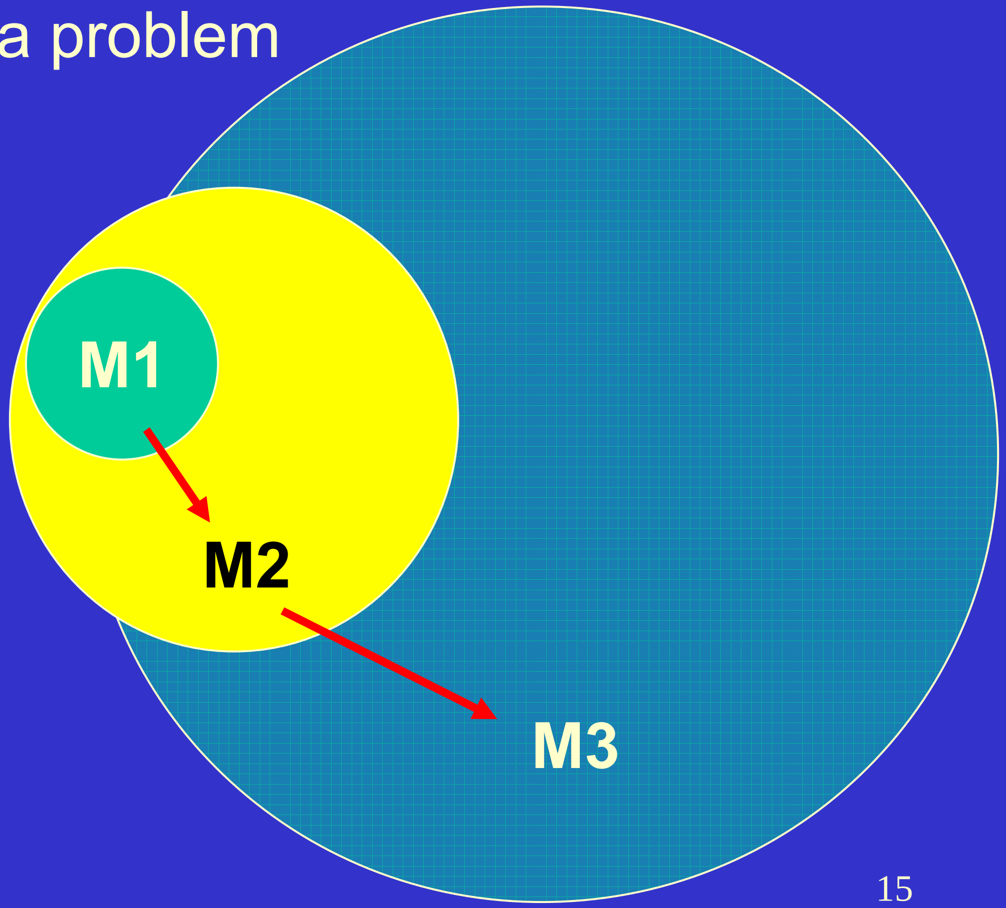
Facilitates explanation of a problem

Idealisation

Approximation

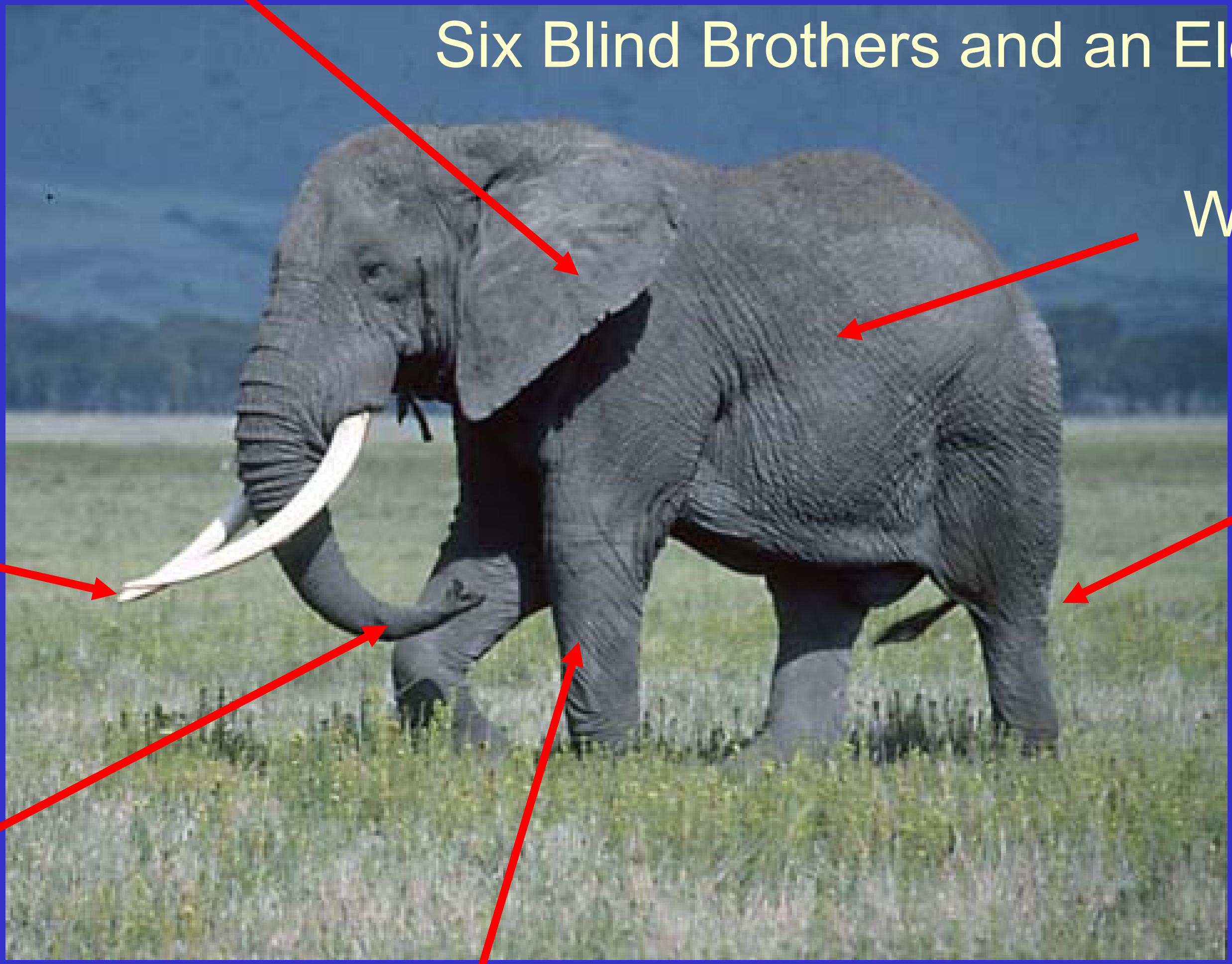
Restriction

New more precise models are proposed with development of more advanced methods of measurement



Experiment

Six Blind Brothers and an Elephant



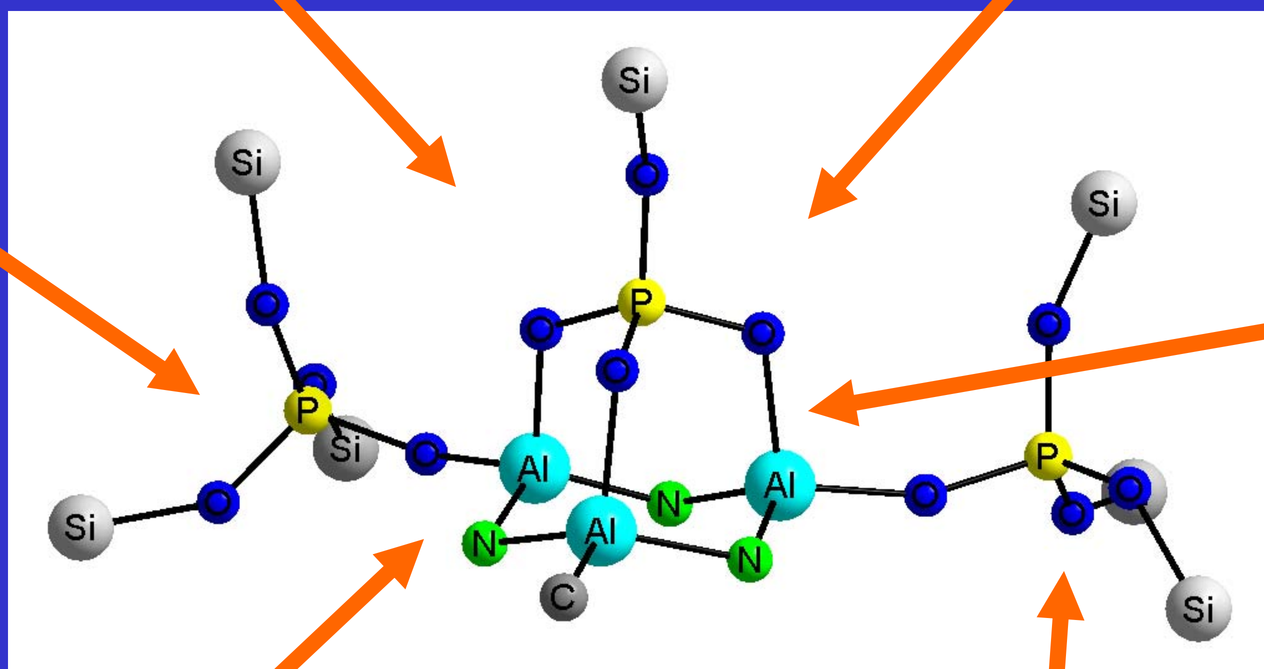
Experiment

Elemental analysis

X-ray diffraction analysis

NMR

UV-vis



Mass spectrometry, MS

Vibrational spectroscopy, IR, RA

Quantitative experiments

Johann Baptista van Helmont
(1579 - 1644)

Robert Boyle
(1627 - 1691)

Joseph Black
(1728 - 1799)

Henry Cavendish
(1731 - 1810)

Measurements

↓

Gas volumes

Mass of reactants and products

Quantitative experiments

Messen heist Wissen

"When you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind. It may be the beginning of knowledge, but you have scarcely, in your thoughts, advanced to the stage of science."

Lord Kelvin
(William Thomson)
(1824 - 1907)

Physical Quantities, Dimensions, Units

Quantity Kind: *E*, energy

http://www.labo.cz/mftabulky.htm

Quantity Magnitude: 100

Dimension: kg m^2 s^{-2}

Units: J, eV, calorie,.....

Base Quantity Kinds: length, mass, time, force, energy,…

Derived Quantity : speed = length $\times$ $(\text{time})^{-1}$

Frequency?

Dimensionless Quantities:

Ratio of two same quantities (molar fraction)

Arguments of ln, exp, sin, cos, tan

Base SI Units

Quantity	Unit	Unit symbol
Mass	**Kilogram**	**kg**
Length	**Meter**	**m**
Time	**Second**	**s**
Temperature	**Kelvin**	**K**
Electric current	**Amper**	**A**
Amount of substance	**Mol**	**mol**
Luminous intensity	**Candela**	**cd**

Base SI Units

1 m = The meter is the length of the path travelled by light in vacuum during a time interval of 1/299 792 458 of a second

1 kg = The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram. Sévres near Paris

1 s = The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 atom.

Base SI Units

1 A = The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 meter apart in vacuum, would produce between these conductors a force equal to 2×10^{-7} newton per meter of length.

1 K = The kelvin, unit of thermodynamic temperature, is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.

Base SI Units

1 mol = The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12.

1 cd = The candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency 540 x 10^{12} hertz and that has a radiant intensity in that direction of 1/683 watt per steradian.

Multiples – prefixes

Y	Yotta	10^{24}
Z	Zetta	10^{21}
E	Exa	10^{18}
P	Peta	10^{15}
T	Tera	10^{12}
G	Giga	10^{9}
M	Mega	10^{6}
k	kilo	10^{3}
1		10^{0}

Multiples – prefixes

1		10^0
m	mili	10^{-3}
μ	micro	10^{-6}
n	nano	10^{-9}
p	pico	10^{-12}
f	femto	10^{-15}
a	atto	10^{-18}
z	zepto	10^{-21}
y	yocto	10^{-24}

Multiples – prefixes

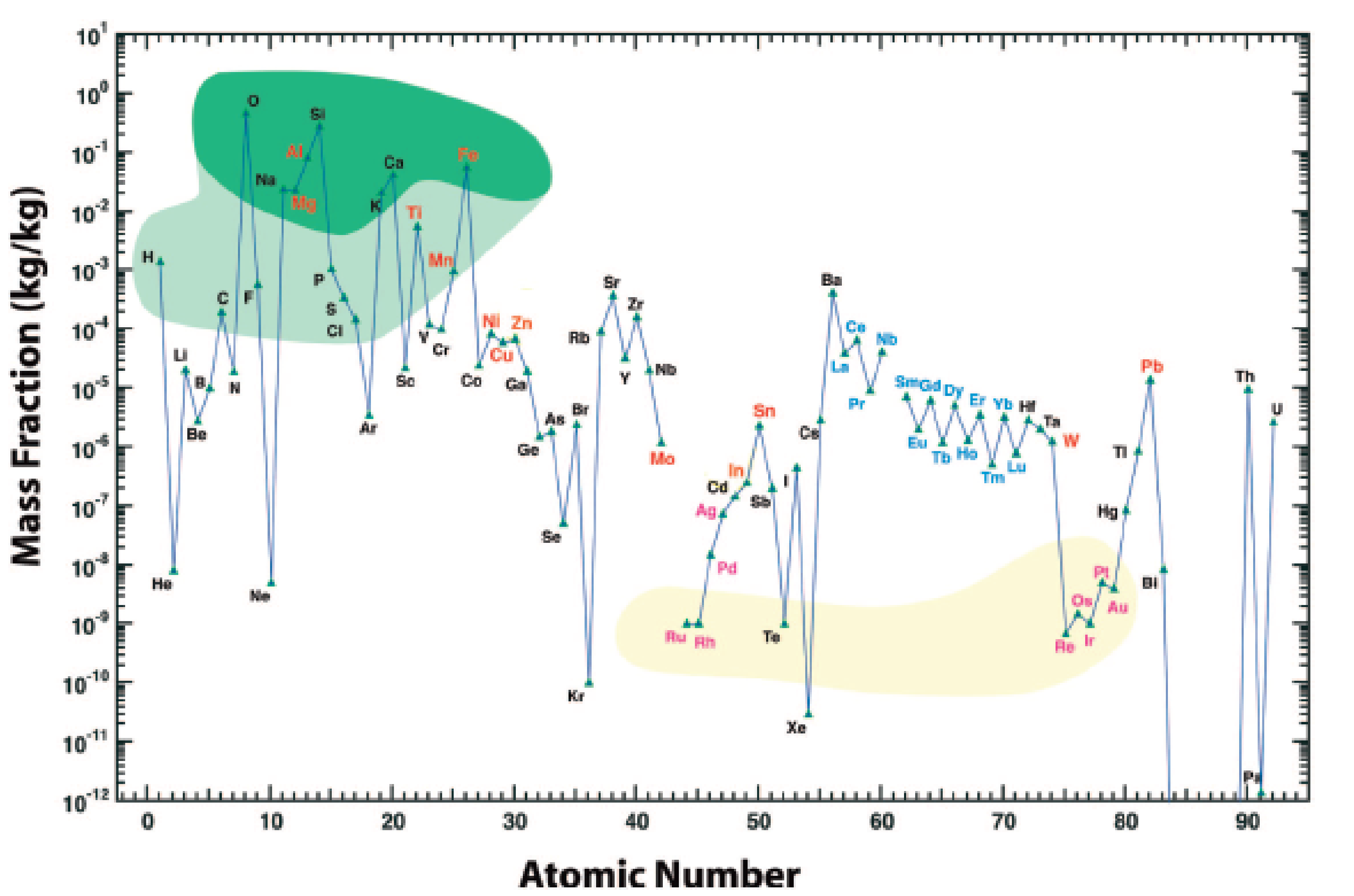
% = 0,01 = 1 v 10^2

‰ = 0,001 = 1 v 10^3

ppm = 1 g in 1 t or 1 atom in 10^6 atoms (part per million)

ppb = 1 mg in 1 t or 1 atom in 10^9 atoms

ppt = 1 mg in 1 t or 1 atom v 10^{12} atoms


Mass Fraction (kg/kg)
Atomic Number
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
La
Ce
Pr
Nb
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Hf
Ta
W
Re
Os
Ir
Pt
Au
Hg
Tl
Pb
Bi
Th
Pa
U

Mass m / kg

Atomic mass unit (Dalton)

1/12 of the rest mass of an unbound neutral atom of ^{12}C in its nuclear and electronic ground state

1 u = (1 amu) = 1 Da = 1.660538921 10^{-27} kg

A. Einstein: relativistic mass > rest mass

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Velocity v

rest mass m_0

Speed of light c = 2.9979 10^8 m s^{-1}

Amount of Substance *n* / mol

Avogadro's number = number of carbon atoms in 0.012 kg (12 g) of nuclide ^{12}C

$$N_A = 6.022\ 140\ 78(18)\ 10^{23}\ \text{mol}^{-1}$$

Amount of Substance *n*, unit mol
n = ratio of number of entities N (atoms, molecules, electrons,....) and N_A

$$n = \frac{N}{N_A}$$

$$n = \frac{m}{M_r}$$

Atomic and Molar Mass

Atomic A_m and molar mass M_m

Mass of 1 mol of a substance, kg mol^{-1}

$A_m(^{12}C) = 12 \times u \times N_A =$

$= 12 \times 1.6606\ 10^{-27}$ kg $\times\ 6.022\ 10^{23}$ mol^{-1} =

$= 0.01200$ kg mol^{-1} = 12.00 g mol^{-1}

Length *l* / m

1 Ångström = 10^{-10} m

1 Å = 100 pm = 0.1 nm

Bohr radius
a_0 = 5.3 10^{-11} m = 0.53 Å

Bond lengths in molecules 1 - 4 Å

Diameter of Cu atom is 2.55 Å

Diameter of Universe: 17 G ly = 1.6 10^{26} m

Diameter of atomic nucleus = 10^{-15} m

Anders Jonas Ångström
(1814 - 1874)

Atomoic radii (pm)

1 Å = 100 pm

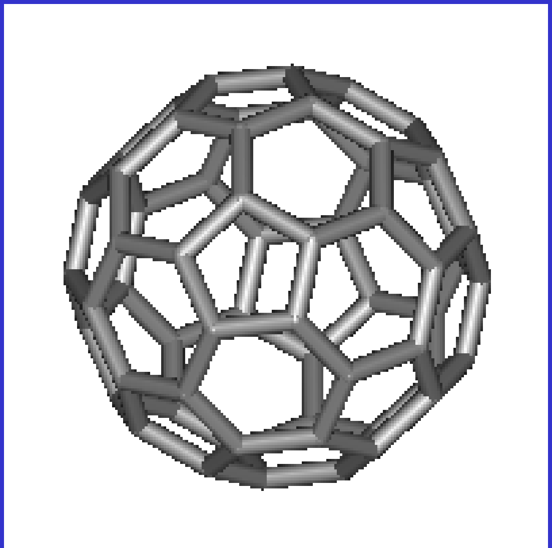
Bond Lengths

(in Å)

Bond	**CC**	**CN**	**CO**	**CH**	**NH**	**OH**
Single	1.53	1.47	1.42	1.09	1.00	0.96
Double		1.34	1.27	1.21		
Triple	1.20	1.15				

How long in pm?

Volume, *V* / m³



1 $pm^3 = 10^{-6}$ $Å^3$

Volume of fullerene C_{60} molecule about 500 $Å^3$

Molar volume of ideal gas = Volume of 1 mol of gas

At temperature 0 °C and pressure 101 325 Pa (STP)
V_M = **22.414** l mol^{-1}

At temperature 0 °C and pressure 100 000 Pa (1 bar)
V_M = **22.71** l mol^{-1}

$$\rho = \frac{m}{V}$$

g cm^{-3}

Density depends on temperature and pressure

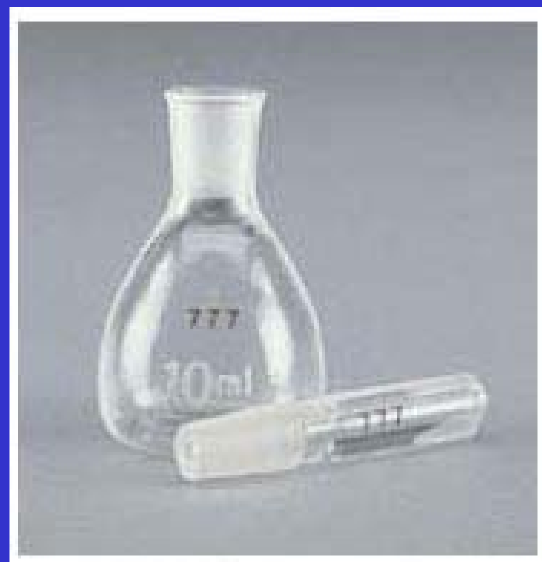
Density, ρ

Substance	Density at 20 °C / g cm^{-3}	State
Oxygen	0.00133	g
Benzene	0.880	l
Lithium	0.535	s
Water	0.9982 (1.00 for calculations)	l
Al	2.70	s
Fe	7.87	s
Pb	11.34	s
Hg	13.6	l
Au	19.32	s
Ir	22.65	s

Density Measurement

$$\rho = \frac{m}{V}$$

g cm^{-3}



Density depends on temperature

Pycnometer

At 20 °C

Vessel contains volume IN

Vessel delivers volume EX

Time, *t* / s

Kinetics of chemical reactions

t / s	Event
10^{-21}	Nuclear collisions
10^{-15}	Excitation of electron by photon, fs
10^{-12}	Radical reactions, energy transfer, valence vibrations
10^{-9}	Fluorescence, rotations, proton transfer
10^{-6}	Phosphorescence, diffusion, conformation
10^{-3}	Fast bimolecular reactions
10^{0}	Heart beat, slow bimolecular reactions

Velocity, *v*

The speed of light in vacuun

$c = 2.99792458 \; 10^{8} \; \text{m s}^{-1}$
(exact)

$3 \; 10^{8} \; \text{m s}^{-1}$
$300\,000 \; \text{km s}^{-1}$

$$E = m c^2 \qquad \nu \; \lambda = c$$

Albert Abraham Michelson
(1852 - 1931)
NP in physics 1907

Frequency, wavelength, wavenumber

Frequency ν = 1/ t ,   Hz = s^{-1}

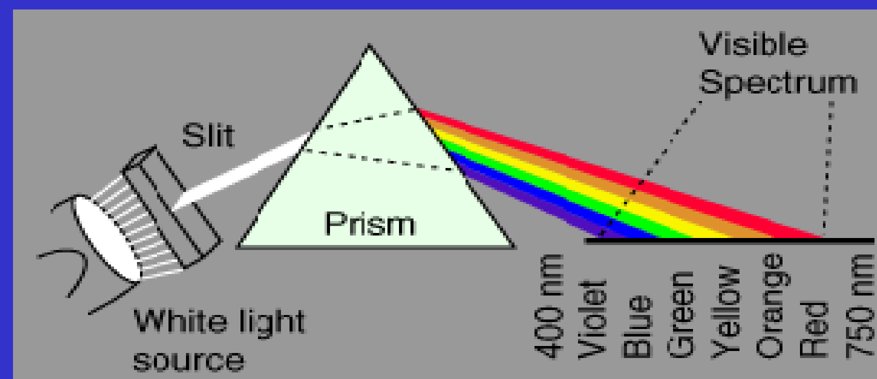
Number of periodical events in a time interval:

Oscillations

Vibrations

Rotations

Collisions of molecules



Wavelength λ , m

Distance between two maxima

$$\nu \lambda = c$$

c = 2.998 10^8 m s^{-1}

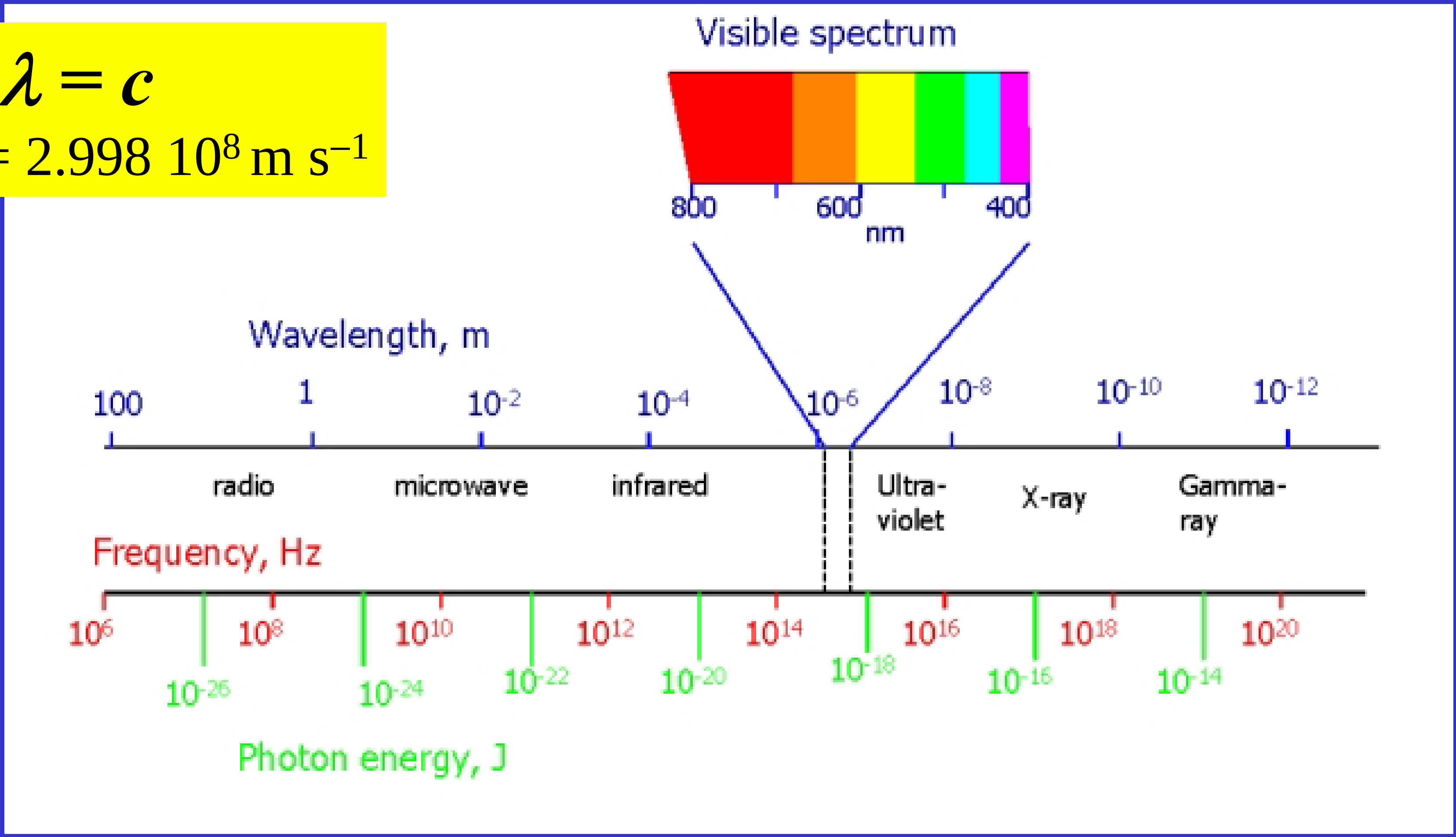
Wavenumber $\tilde{\nu}$ **= 1 /** λ , cm^{-1}

Number of waves per unit of length

Frequency, wavelength, wavenumber

$$\nu\lambda = c$$

$c = 2.998\ 10^8\ \mathrm{m\ s^{-1}}$



Four Basic Forces - Interactions

Gravitational

Electromagnetic (e-e repulsion, p-e attraction)

Strong interactions (nuclear, holds protons bound in nucleus)

Weak interactions (holds p and e bound together in a neutron)

Force, *F* / N

1 Newton = gravitational force acting on an apple

$F = m\,g$

$g = 9.80665\ \text{m s}^{-2}$

Isaac Newton
(1642 - 1727)

Electric charge, *q*

Elementary charge, *e*

$e = 1.602\ 10^{-19}$ C 1 C = 1 A s

All charges all multiples of e

$\boldsymbol{q = Z e}$

Charles Augustin Coulomb (1736 - 1806)

Coulomb's Law

The electrical force *F* between two charged objects is directly proportional to the product of the quantity of charge on the objects and inversely proportional to the square of the separation distance *r* between them.

$$F = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}$$

Pressure, *p*

1 Pascal = pressure, by which an apple acts on 1 m^2

1 Pa = 1 N m^{-2}

1 atm = 101 325 Pa = 760 mm Hg (Torr) = 1.01325 bar

1 bar = 10^5 Pa = 100 kPa

Standard pressure = 1 bar = 100 000 Pa

Temperature, *T*

Kelvin, K
Absolute zero 0 K (cannot be reached
entropy reaches its minimum)

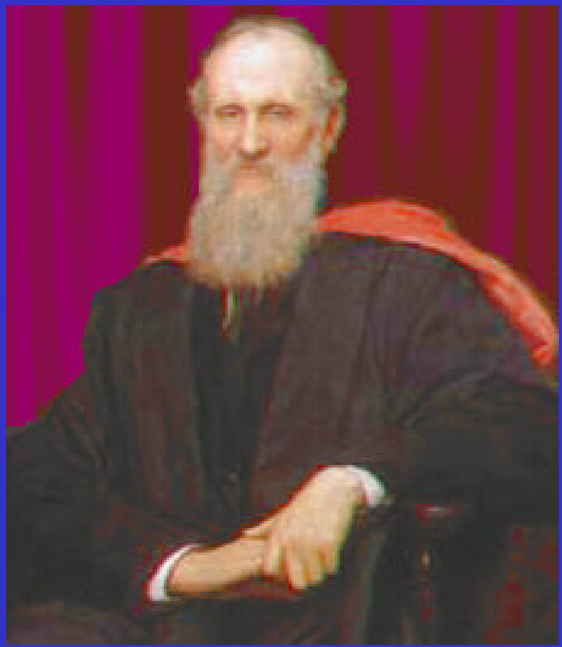
– 273.15 °C

Current record: ~100 pK
(superconductivity and superfluidity)

Celsius, °C
0 °C = 273.15 K

T[°C] = T[K] – 273.15

Standard temperature = 25 °C = 298 K



Lord Kelvin
(William Thomson)
(1824 - 1907)

1592 Galileo

Themometer

1629 Themometer filled with brandy
Joseph Solomon Delmedigo
medial doctor and rabi

Change of physical properties with temp:

- Volume expansion, Hg, Ga, ethanol
- Length expansion of metals
- Electrical resistance of metals
- Liquid crystals

Celsius scale
Melting of ice at 1 atm = 0 °C
Boiling of water at 1 atm = 100 °C
Divide into 100 divisions

ITS-90 International temperature scale
Triple point of water = 273.16 K

ITS-90

International temperature scale

Triple point of water = 273.16 K

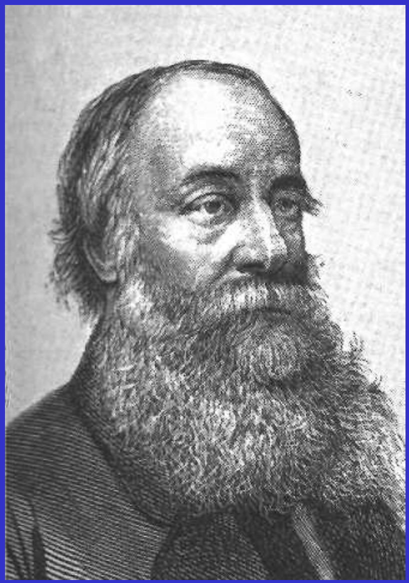
Interpolation

Calibration

	T, K
e-Hydrogen (T)	13,8033
Neon (T)	24,5561
Oxygen (T)	54,3584
Argon (T)	83,8058
Mercury (T)	234,3156
Water (T)	273,16
Gallium	302,9146
Indium	429,7485
Tin	505,078
Zinc	692,677
Aluminium	933,473
Silver	1234,93
Gold	1337,33
Copper	1357,77

Energy, *E*

1 Joule = energy of a heart beat



James Prescott Joule
(1818 - 1889)

1 cal = 4.184 J

1 eV = kinetic energy of an electron, accelerated by a potential of 1 V

$E = e\,U = 1.60210\ 10^{-19}\ \mathrm{C} \times 1\ \mathrm{V} =$
$= 1\ \mathrm{eV} = 1.60210\ 10^{-19}\ \mathrm{J}$

$1\ \mathrm{eV\ (molecule)^{-1}} = 1\ \mathrm{eV} \times N_A = 96\ 485\ \mathrm{J\ mol^{-1}}$

Energy E

$\boldsymbol{E = m\,c^2}$ = 1.66 10^{-27} kg × (3.00 10^{8} m s $^{-1})^2$ = 1.49 10^{-10} J

1 amu = 931.4 MeV

$\boldsymbol{E_{kin} = \frac{1}{2}\, m\, v^2}$

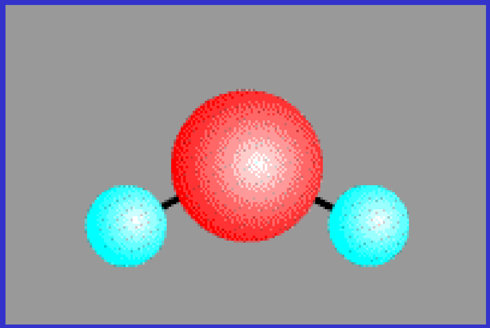
$E_{kin} = 3/2\; k\; T$
k = 1.380662 10^{-23} J K^{-1} Boltzmann constant
kT = 1 zJ at laboratory temperature

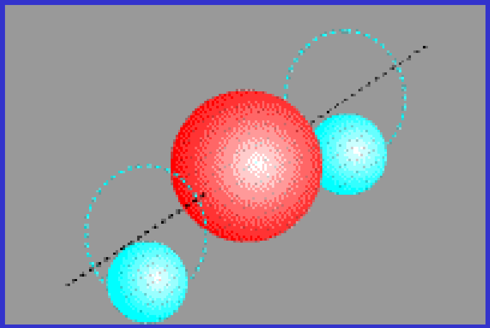
$\boldsymbol{E = h\,\nu}$
h = 6.626176 10^{-34} J s Planck constant

Energy E

$$E_{Total} = E(\text{electronic}) + E(\text{vibrational}) + E(\text{rotational}) + E_{other}$$

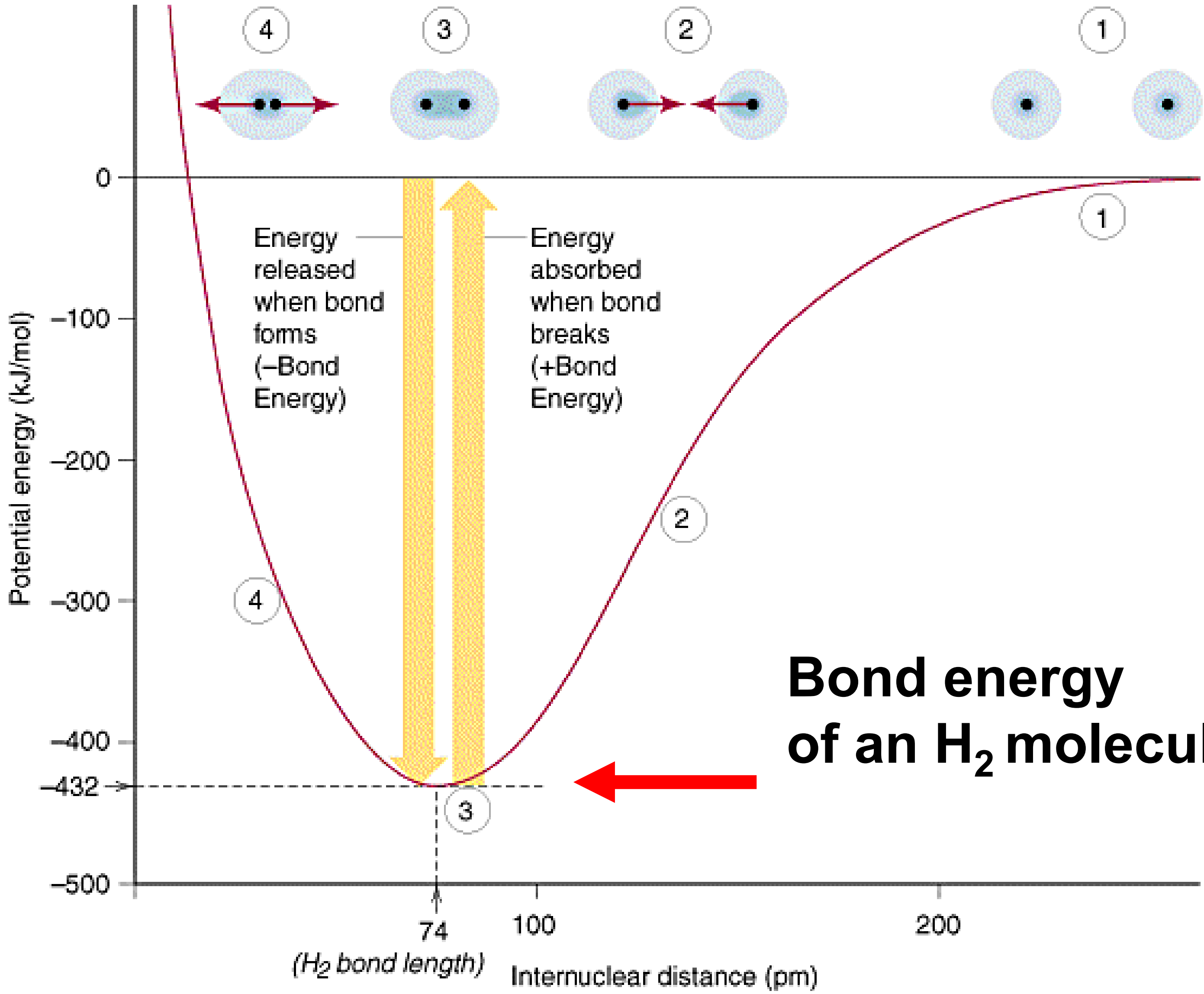
E(electronic)	100 kJ mol^{-1}
E(vibrational)	1.5 – 50 kJ mol^{-1}
E(rotational)	0.1 – 1.5 kJ mol^{-1}





Bond energies, kJ mol^{-1}
(single bonds)

	H	C	N	O	S	F	Cl	Br	I
H	432								
C	411	346							
N	386	305	167						
O	459	358	201	142					
S	363	272	---	---	226				
F	565	485	283	190	284	155			
Cl	428	327	313	218	255	249	240		
Br	362	285	---	201	217	249	216	190	
I	295	213	---	201	---	278	208	175	149



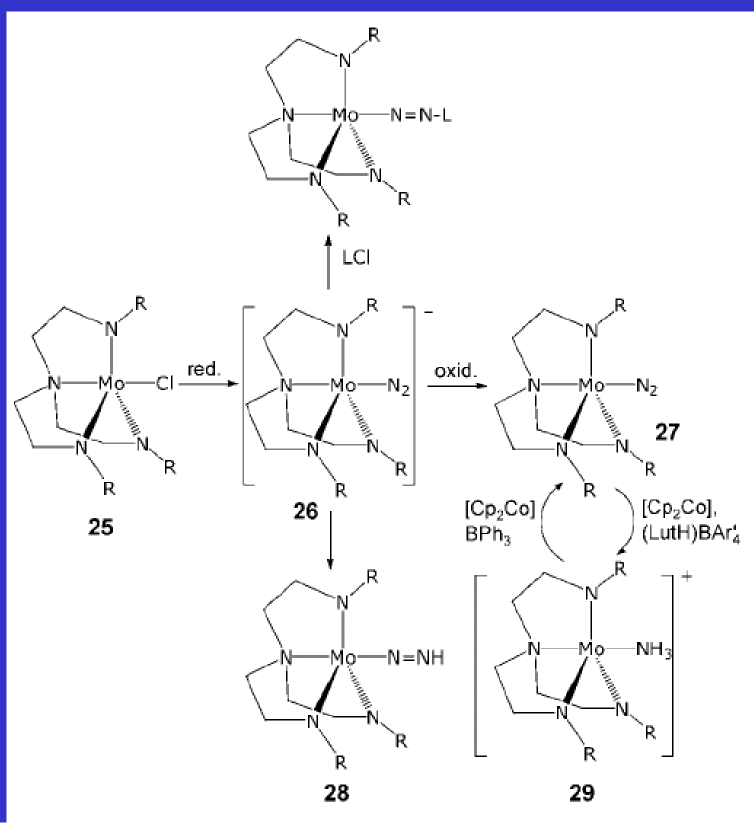
Bond energy of an H_2 molecule

Bond Energy of N_2

E_{vaz} = 942 kJ mol^{-1}

| N≡N | → NH_3

Use
80% fertilizer
10% plastics
5% explosives



1909 Fritz Haber

$N_2(g) + H_2(g)$

500 °C, 250 atm, Fe catalyst, yield 20%