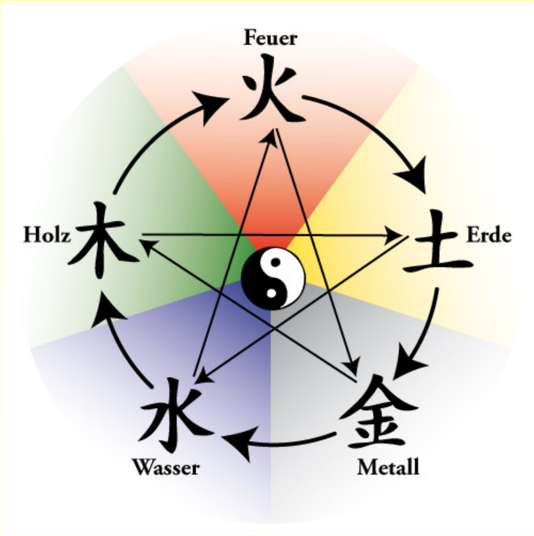
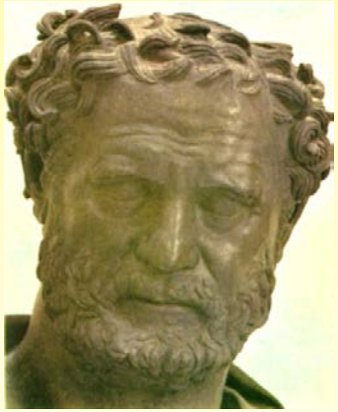
Matter matters!

Early Views of the Atom

Fünf-Element-Lehre

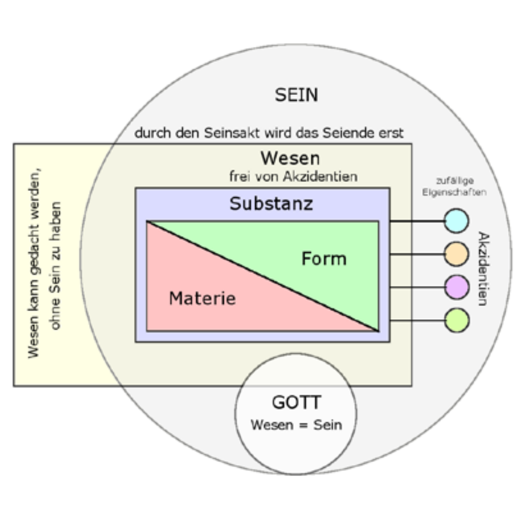


Demokrit/Leukipp 450 BC:



Demokrit

Hyle-Steresis-Eides



‚atomos' - indivisible smallest building block of the Universe

Early Views of the Atom

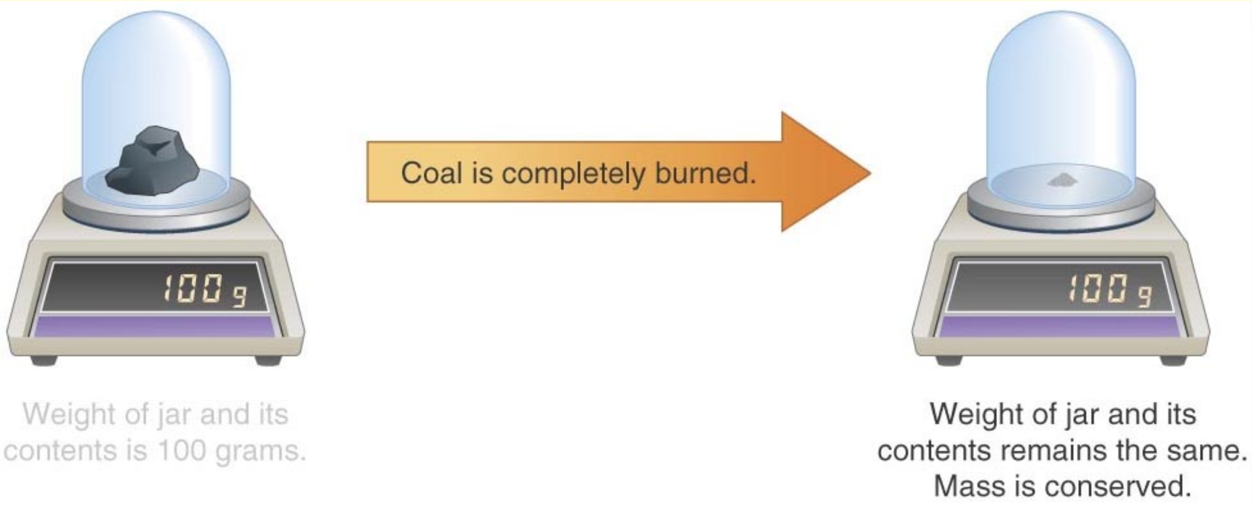
Dalton´s atomic theory of matter (1807)

- All matter consists of atoms – smallest particle of an element that has all the properties of this element

- All atoms of a given element, such as gold, are identical and immutable
- In a chemical reaction, atoms are merely **rearranged** to form new compounds; they are not created or destroyed, or changed into atoms of any other elements
- Atoms of different elements have different masses

Early Views of the Atom

Law of Conservation of Mass - Lavoisier (1743-1794)



In a chemical reaction, matter is neither created nor destroyed

$$CuCO_3(s) \rightarrow CuO(s) + CO_2(g)$$

$$123.6\ g = 79.6\ g + ?$$

Early Views of the Atom

Dalton´s atomic theory of matter (1807)

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Atomic theory - some mysteries

Atomic weights do not always increase with atomic number, i.e. position in Periodic table:

Atomic weight of Argon (Ar) exceeds that of the succeeding element Potassium (K)

Atomic weight of Cobalt (Co) exceeds that of the succeeding element Nickel (Ni)

Pb from different localities has different atomic weights

The Periodic Table of elements

s-block

1 New Designation
IA Original Designation

Non-Metals

Atomic #
Symbol
Atomic Mass

s-block | p-block | d-block | Transition Metals

Period	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 H 1.0094																	2 He 4.00260
2	3 Li 6.941	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 20.179
3	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
4	19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.69	29 Cu 63.546	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
5	37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	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 121.75	52 Te 127.60	53 I 126.91	54 Xe 131.29
6	55 Cs 132.91	56 Ba 137.33	57 to 71	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	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)
7	87 Fr (223)	88 Ra 226.03	89 to 103	104 Unq (261)	105 Unp (262)	106 Unh (263)	107 Uns (262)	108 Uno (265)	109 Une (266)	110 Uun (267)								

Metals

(Mass Numbers in Parentheses are from the most stable of common isotopes.)

Phases
Solid
Liquid
Gas

Rare Earth Elements

d-block | f-block

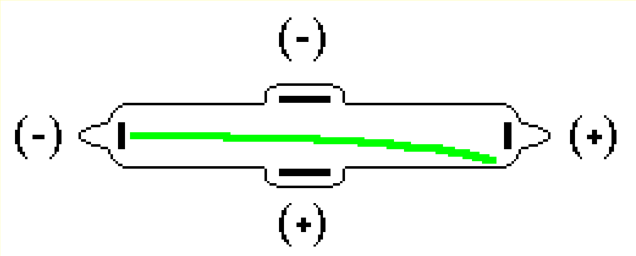
Lanthanide Series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide Series	89 Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu (244)	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 (260)

Discovery of the electron

1897 J.J.Thomsons experiment with cathode rays

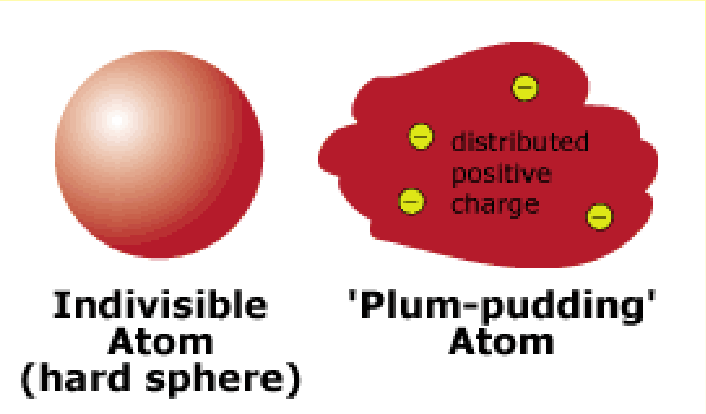
- High voltage applied between two metal contacts (electrodes) in an evacuated glass tube

cathode-ray tube



- Stream of negative charged particles
- This cathode-ray was "bent" towards the positive electrode and repelled by the negative electrode
- All metals emitted the same negative particles - electrons

The Atom



Dalton (~1807)

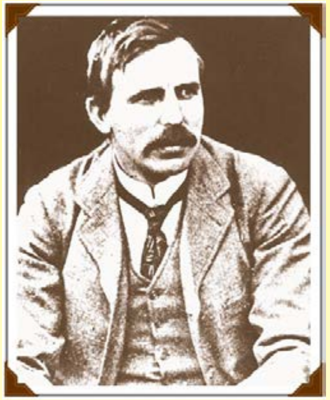
Thomson (~1897)

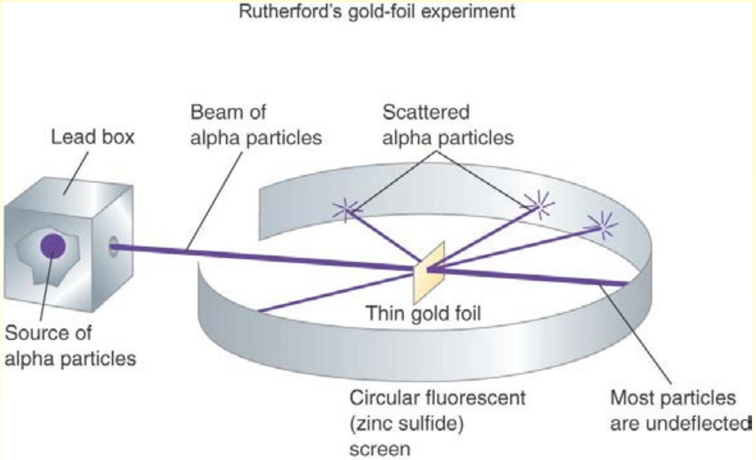
Discovery of the nucleus

- 1909 Rutherford bombarded thin metal foils with **alpha particles** (helium ions)

- Most particles went through - only 1 alpha particle in 10.000 was deflected by the foil

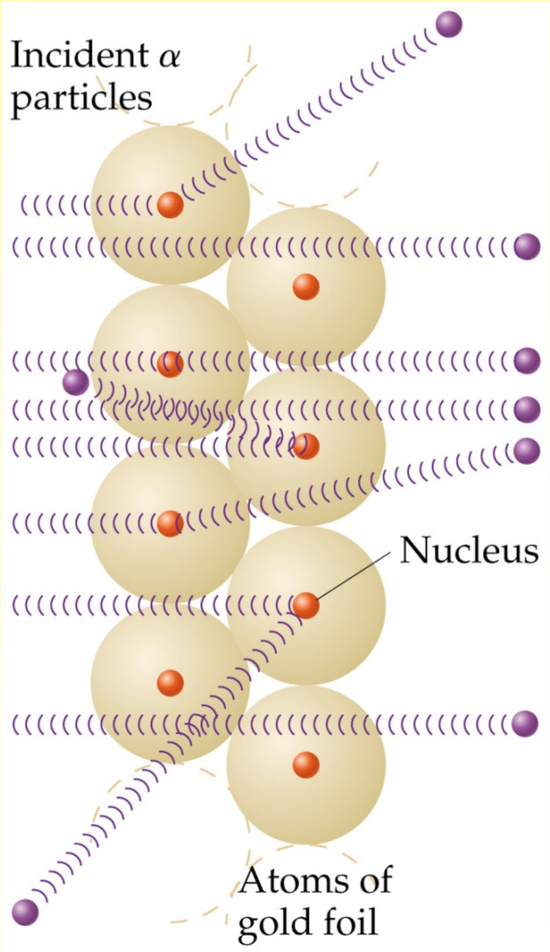
- This deflection indicated the existence of a small, dense, positively charged nucleus





gold can be made into foil that is only 0.00004 cm thick!

Discovery of the nucleus

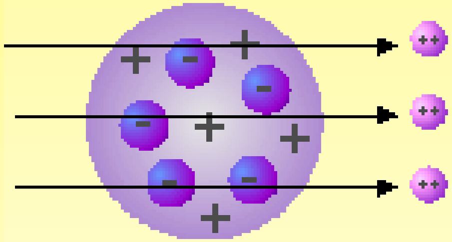


- The nucleus, being positive in charge, is composed of positively charged subnuclear particles known as *protons*
- The protons have a positive charge equal in magnitude to the negative charge of an electron

The Atom

- **Thomson's Atom:**

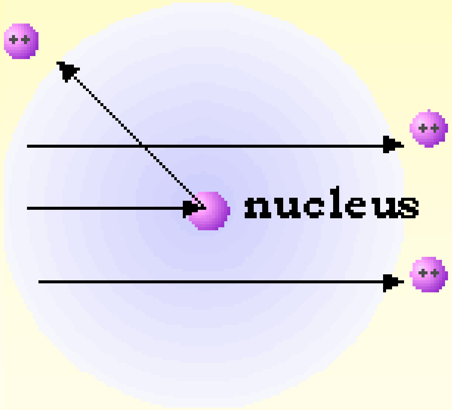
  Diffusive mass and charge



- **Rutherford's Atom**

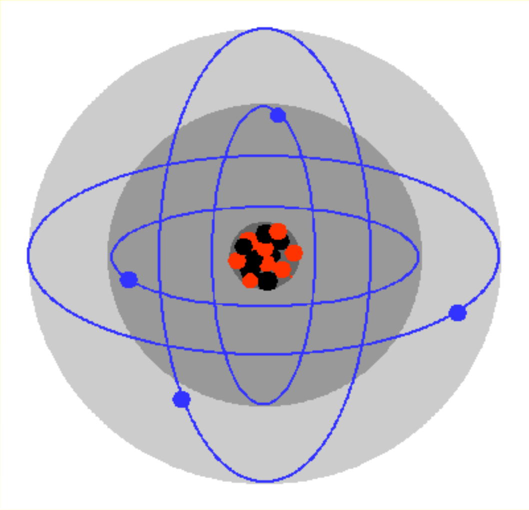
  Concentrated mass and positive charge at the nucleus

  Electrons roam through empty space around nucleus



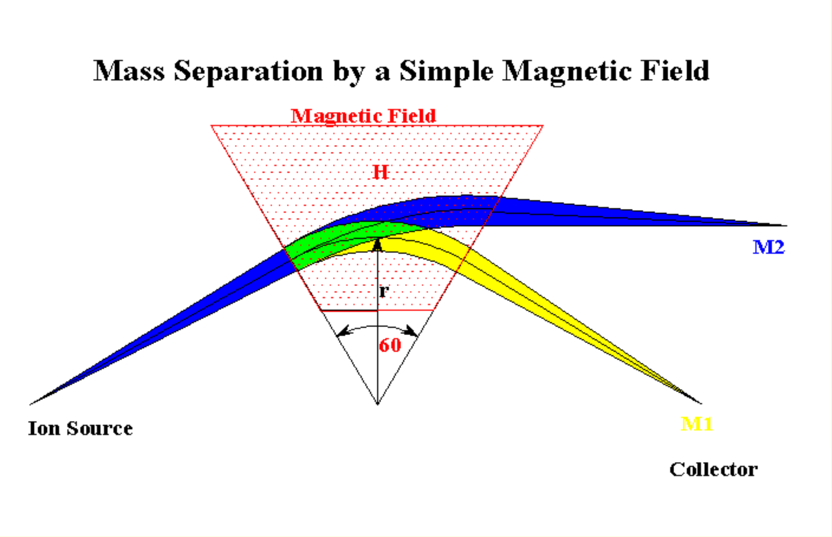
Bohr model of the atom, 1915

- Bohr proposed a model of how electrons moved around the nucleus
- Electrons occupy only certain orbits around the nucleus
- Each orbit has an energy associated with it. For example the orbit closest to the nucleus has an energy E1, the next closest E2 and so on (i.e. energy of the electron is quantized – only occurs at specific energy levels)
- Light is emitted when an electron jumps from a higher orbit to a lower orbit and absorbed when it jumps from a lower to higher orbit



Massenspektrometrie

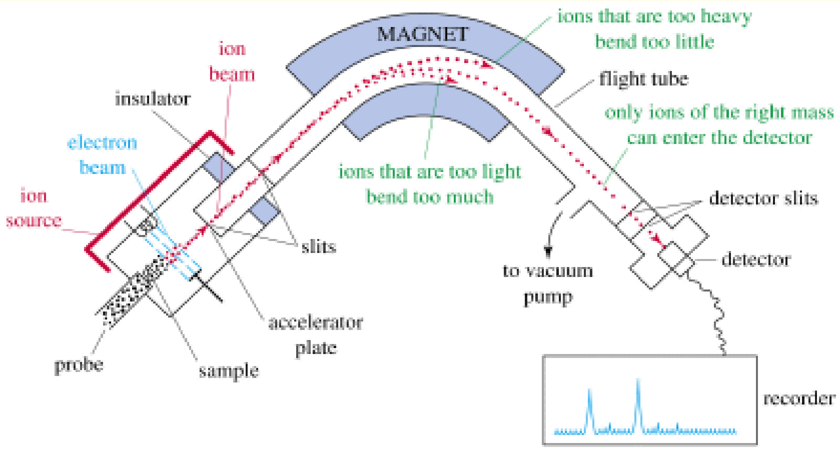
Device used to measure the mass of a given type of atom



Mass spectrum:

Position of peaks give the mass of the atoms

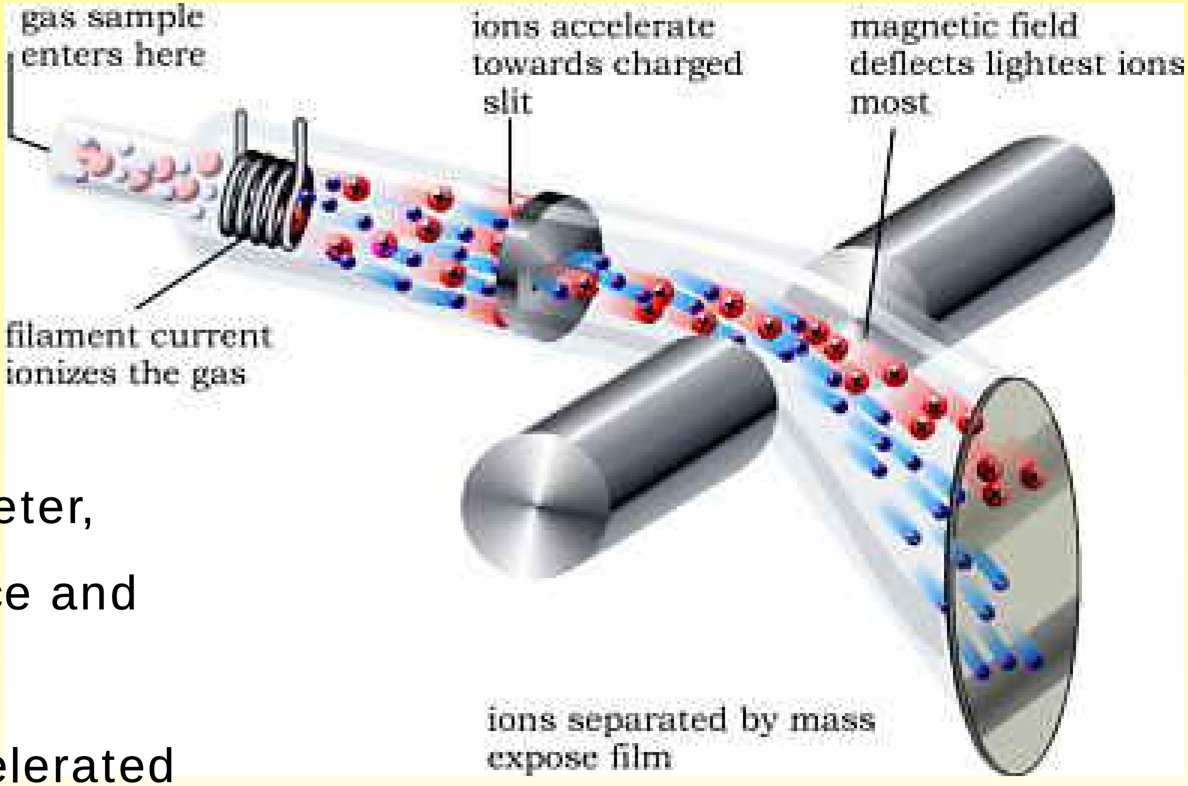
Relative heights of the peaks indicate the relative number of atoms with each mass



Massenspektrometrie

<u>Great names of MS:</u>

Thomson
Aston
Dempster
Nier



- In the mass spectrometer, atoms enter the device and are ionized.
- The ions are then accelerated through a magnetic field which bends the ion paths into a semicircular shape.
- The radius of this path is dependent upon the mass of the particle (with all other factors such as speed and charge being equal). Thus ions of different masses can be separated.

Ionentrennung im Magnetfeld

Wenn ein Ion der Masse m, das mit einer Spannung V beschleunigt wird, in ein magnetisches Feld eintritt, wird es auf eine kreisförmige Flugbahn gelenkt. Der Bahnradius des Ions berechnet sich aus der Gleichung der **Zentrifugalkraft:**

$$F = \frac{mv^2}{r}$$

und der **Lorenzkraft:**

$$F = Bqv$$

F	=	Kraft,
v	=	Geschwindigkeit des Ions,
q	=	elektrische Ladung,
r	=	Radius der Flugbahn,
B	=	magnetische Feldstärke

Bei Gleichheit der Kräfte ergibt sich also:

$$\frac{mv^2}{r} = Bqv, \quad \text{oder} \quad mv = Bqr \qquad (1.1)$$

Das magnetische Feld wirkt somit als Impuls (mv) – Analysator für Partikel einer bestimmten Ladung q und magnetische Feldstärke B.

Da ein Ion durch die elektrische Energie qV (Ladung x Beschleunigungs-potential) die kinetische Energie ($mv^2/2$) erhält gilt die Gleichung:

$$qV = \frac{1}{2}mv^2 \quad \text{oder} \quad v = \sqrt{\frac{2qV}{m}}$$

substituiert man v in Gl. (1.1) so erhält man:

$$m\sqrt{\frac{2qV}{m}} = Bqr, \quad \text{oder} \quad r = \sqrt{\frac{2mV}{qB^2}} \quad \text{bzw.} \quad \mathrm{B} = \frac{1}{r} \times \sqrt{\frac{2mV}{q}}$$

Die Ionen werden also auf gekrümmte Bahnen gezwungen, entsprechend ihrem Verhältnis von Masse m zu Ladung q, mit anderen Worten, die Ablenkung von der geraden Flugrichtung ist umso größer, je kleiner die Masse oder je größer die Ladung ist.

Massenspektrometrie

Isotopenanalysen mittels ICP-MS

z.B. Agilent 8800 Triple Quad (ICP-QQQ)

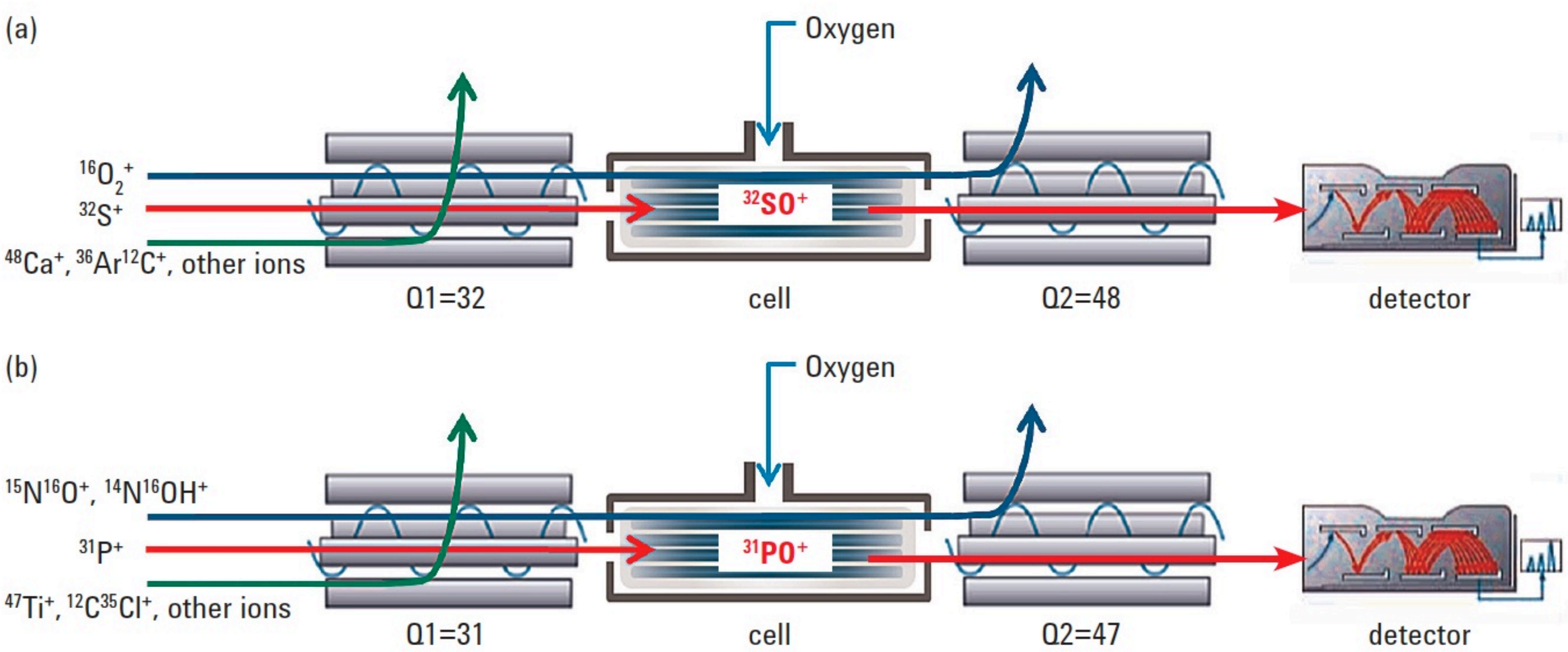
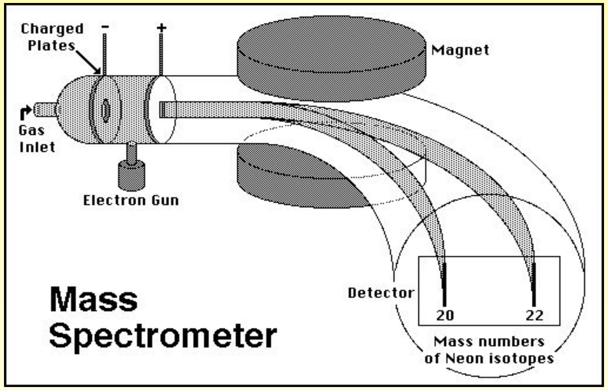


Figure 1. 8800 ICP-QQQ MS/MS operation in mass-shift mode to remove interferences on S (a) and P (b)

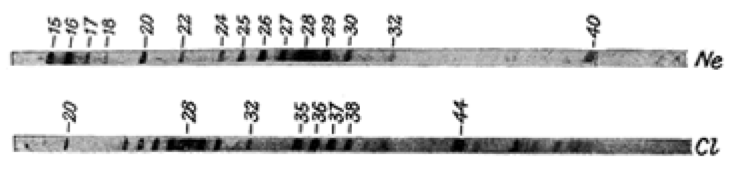
Massenspektrum von Neon

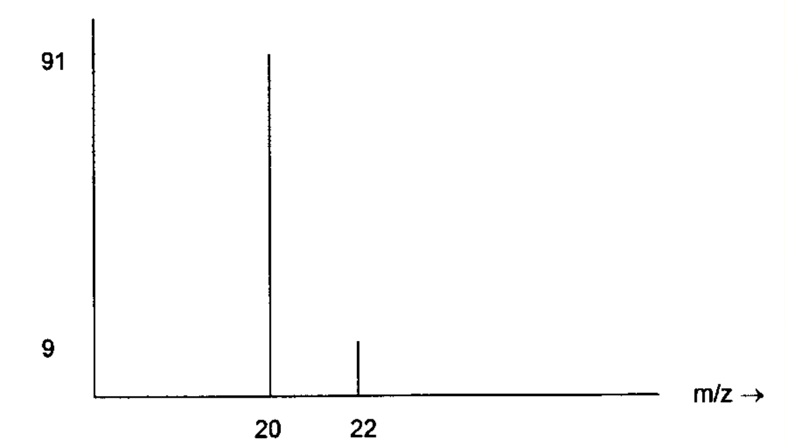
Neon was the first non-radioactive element proven to be isotopic

- Most atoms of Neon had a mass of 20, some 21 and some 22



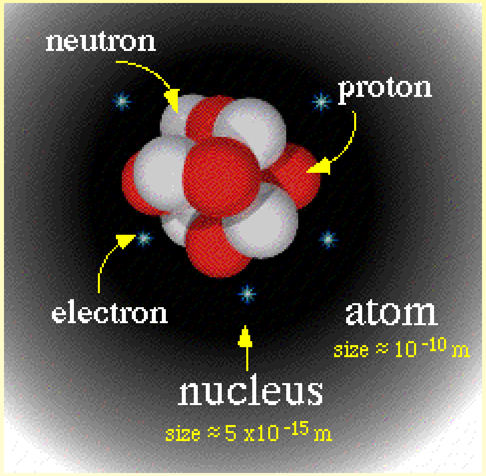
Aston's Massenspektren von 1920:



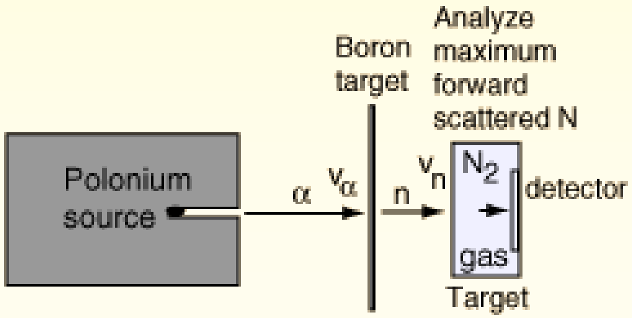


Das Neutron

- The difference in mass is due to a third subatomic particle in the nucleus called neutron (no charge)
- Discovered 1932 (Chadwick)
- Neutrons contribute to the force that holds the nucleus together and reduce the repulsive force between positively charged protons



$$^{9}_{4}\mathrm{Be} + ^{4}_{2}\alpha \rightarrow ^{12}_{6}\mathrm{C} + ^{1}_{0}\mathrm{n}$$



Isotope

- If we compare different isotopes of the same element:

The number of protons and electrons are the same, i.e. atomic number, Z, is the same

The number of neutrons are different

The number of nucleons (protons and neutrons) are different, i.e. mass number, A, is different

Isotope

- isotopes: same Z, different M

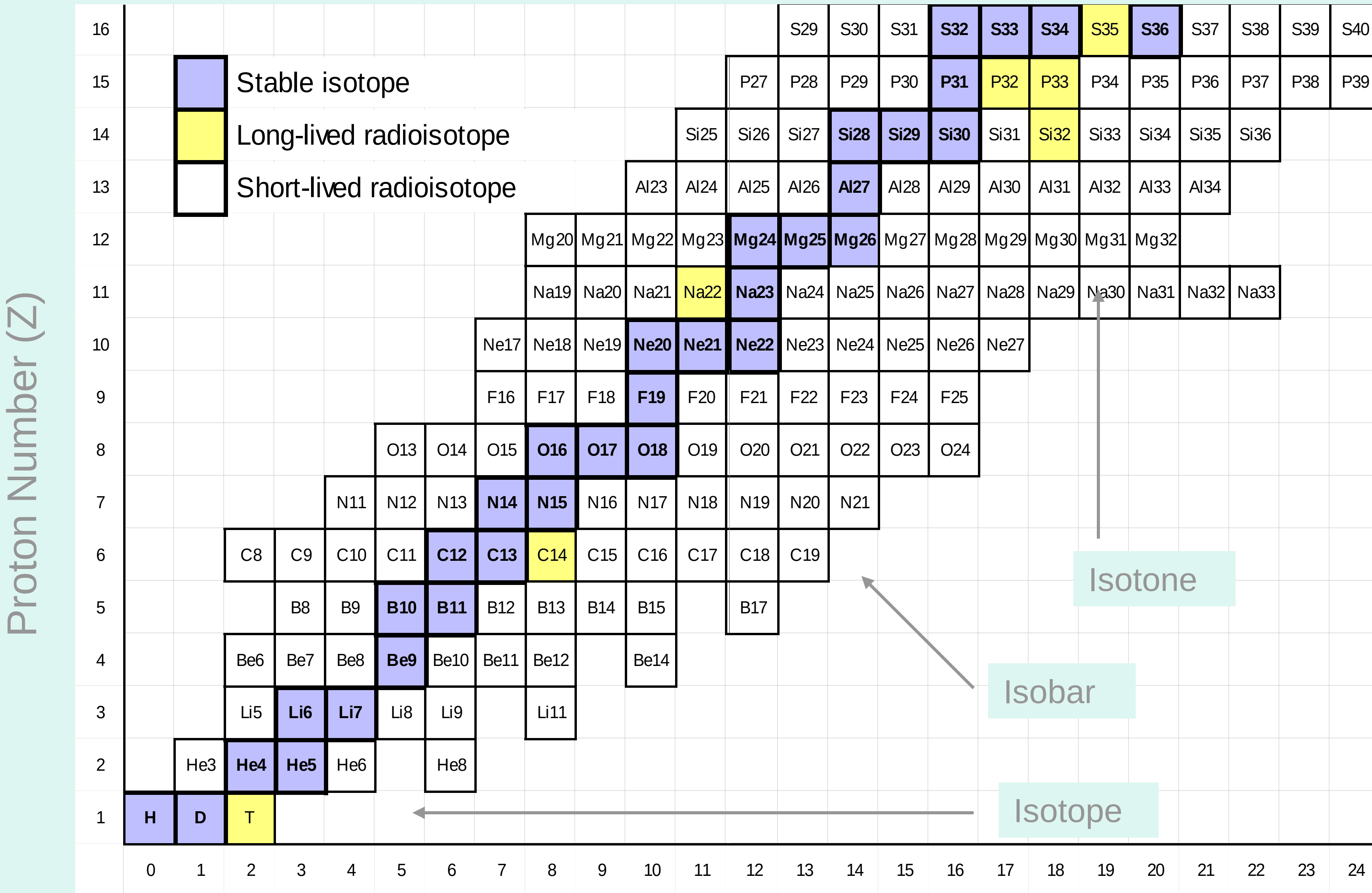
$^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$ $^{12}_{6}C$ $^{13}_{6}C$ $^{14}_{6}C$ $^{235}_{92}U$ $^{238}_{92}U$

- isotopic abundance: $\frac{\text{\# atoms of isotope present}}{\text{\# atoms of element present}}$

isotope	natural abundance	mass (amu)
carbon-12	98.89 %	12.000000
carbon-13	1.11 %	13.003354

average mass: 12.01_{11} amu

Die Nuklidkarte

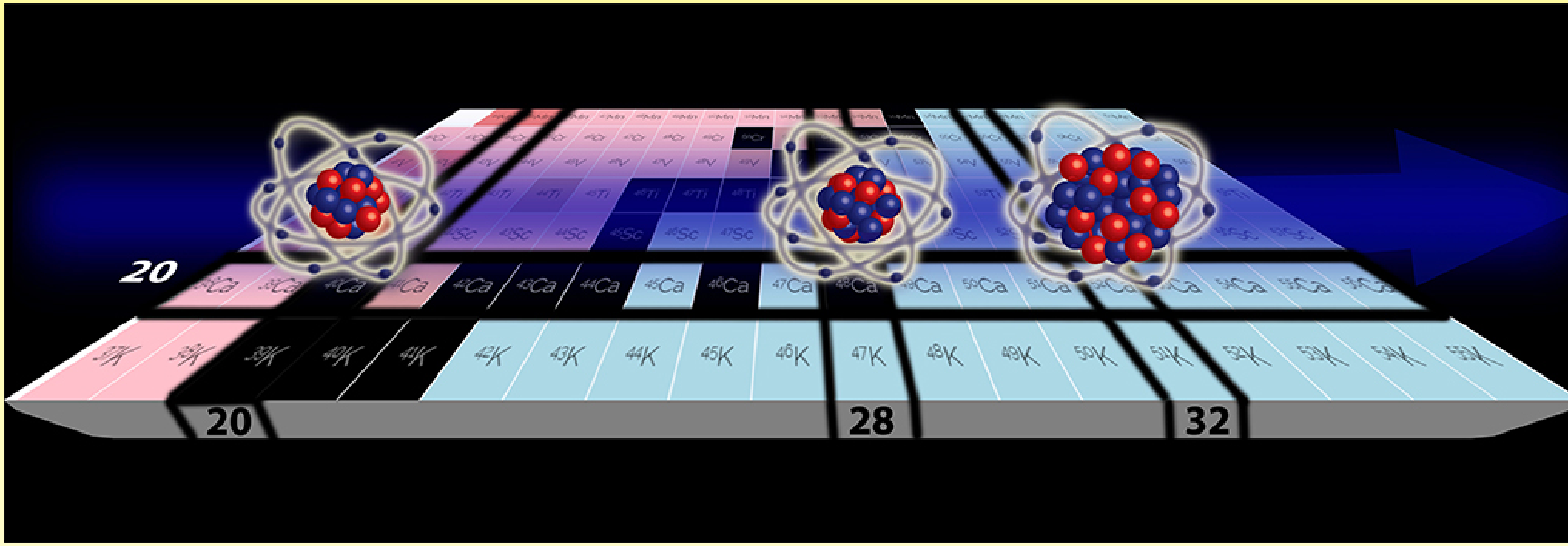


He5 not stable!

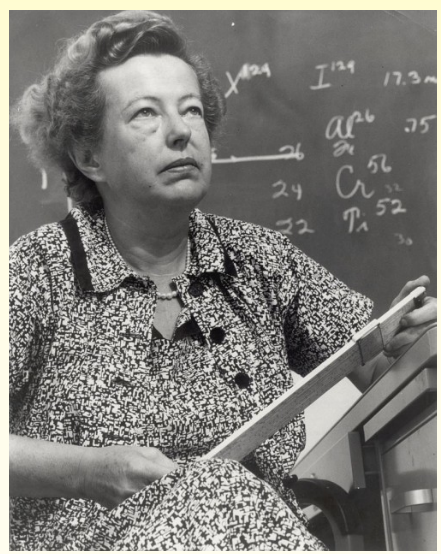
Neutron Number (N)

http://www2.bnl.gov/CoN/

Magische Zahlen



${}^{4}_{2}He$ ${}^{16}_{8}O$ ${}^{40}_{20}Ca$ ${}^{48}_{20}Ca$ ${}^{208}_{82}Pb$



2, 8, 20, 28, 50, 82, 126

Maria Goeppert-Mayer
Schalenmodell der Kernphysik
Nobelpreis 1963

Klassifikation der Elemente

FeNi-rich core

SiMg-rich mantle

SiAl-rich crust

V.M.Goldschmidt scheme:

Atmophile (gas loving)

H, N, noble gases….

Lithophile (silicate loving)

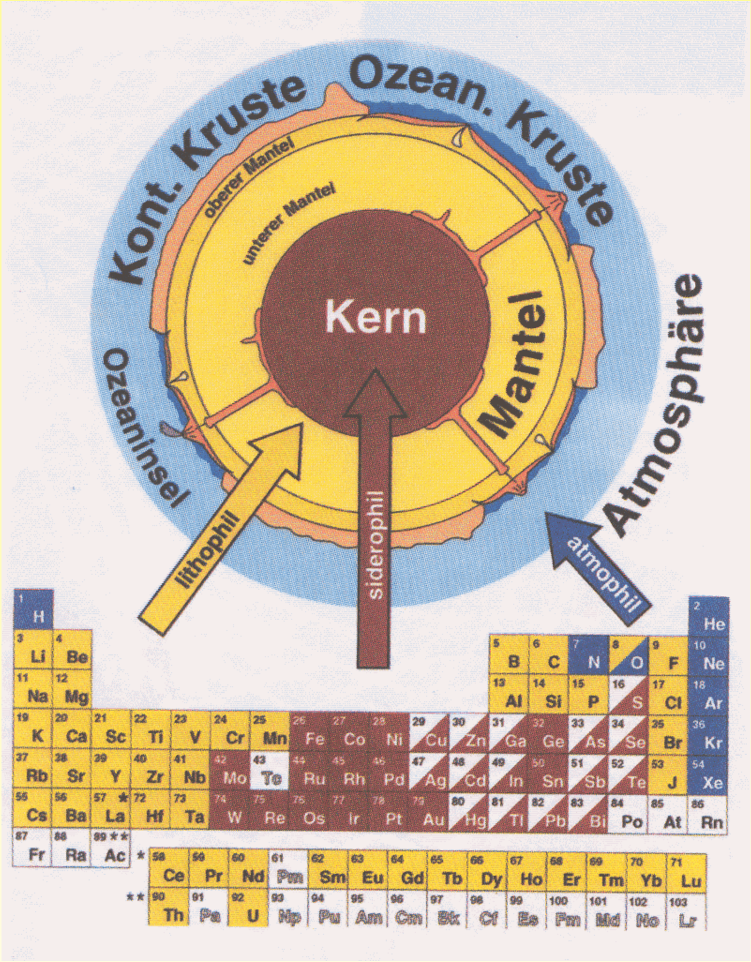
Si, Al, Mg, Na, K, Ca, Ti...

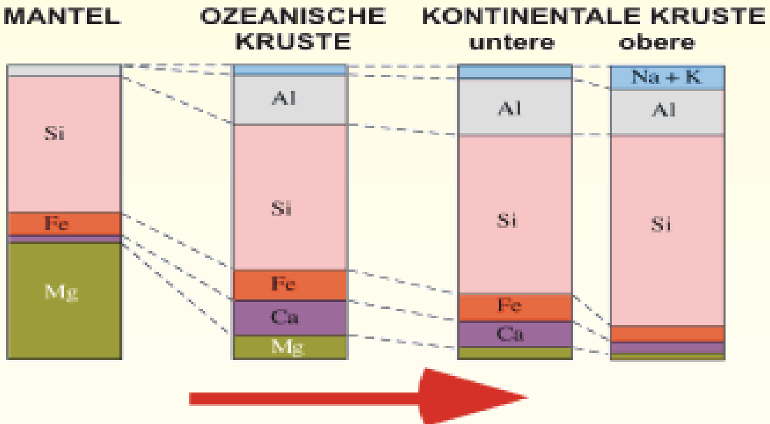
Chalcophile (sulfur loving)

Cu, Se, Cd….

Siderophile (iron loving)

Fe, Ni, Co, Pt, Au, W, PGE….





Gemäß ihrer Häufigkeit werden Elemente unterteilt in *Hauptelemente, Nebenelemente,* und *Spurenelemente*

Hauptelemente (>0.1%):
O,
Si,
Al,
Mg,
Fe,
Na,
K,
Ca

Diese 8 Elemente bauen zu mehr als 98% der Erdkruste auf

Spurenelemente (<0.1%)*:
Rb,
Sr,
Zn,
Zr
etc.

* in ppm bzw. µg/g (0.1% = 1000 ppm)

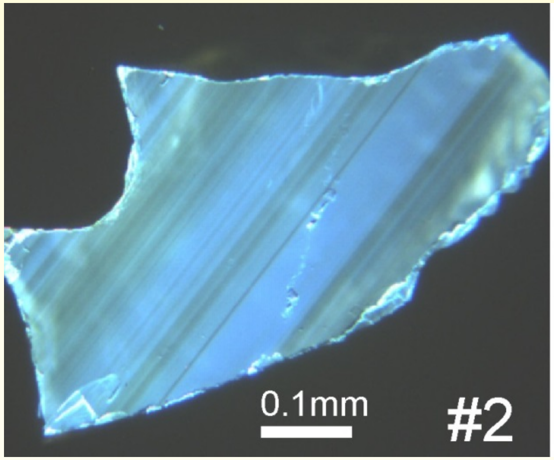
Ausnahmen, Beispiel Kalium (K)
Hauptelement in Granit
aber *Spurenelement* in Peridotit

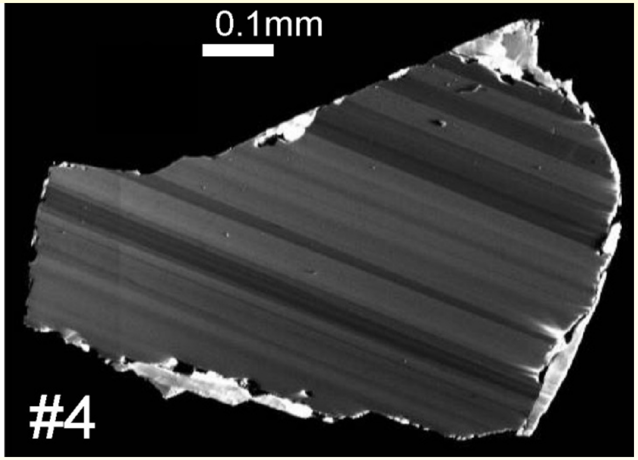
Substitutionen sind allgegenwärtig

Minerale zeigen *chemische Variation* oder sind *zoniert*

Beispiel Zirkon ($ZrSiO_4$)
SEE (La-Lu) substituieren Zr:
$(Y, SEE)^{3+} + (Nb, Ta)^{5+} = 2Zr$

verschiedenen Farben durch Einbau unterschiedlicher Mengen an SEE



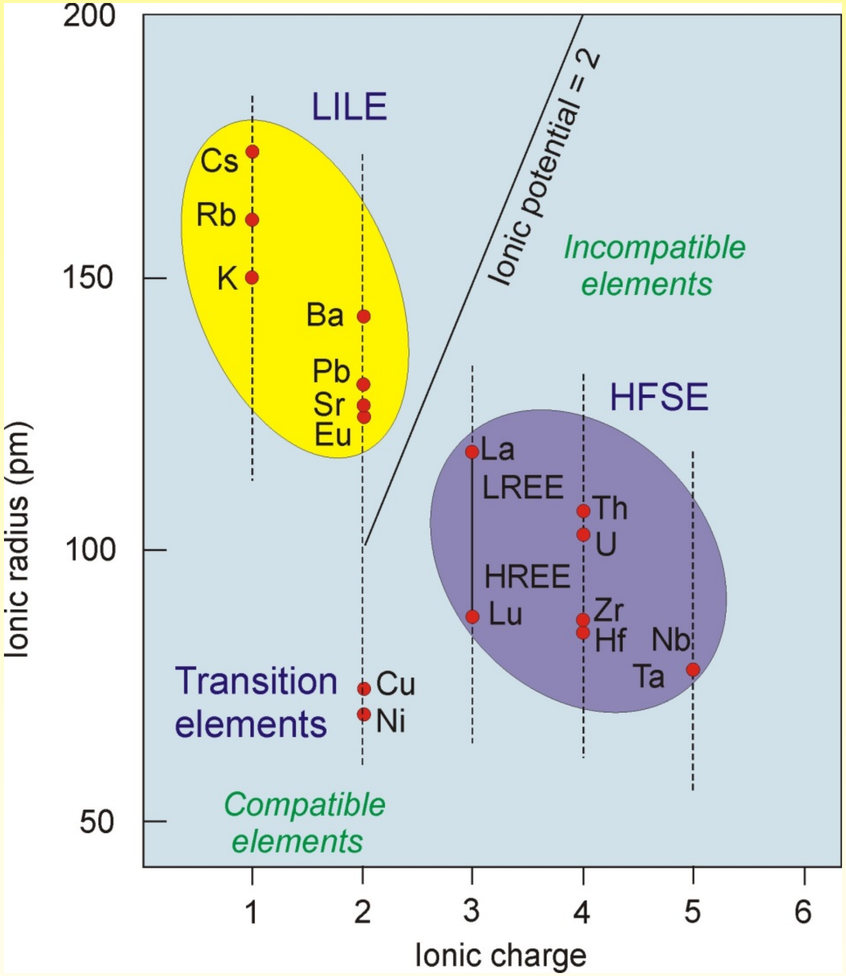


Ionenpotential

Ionenpotential = Ladung/Radius (Å)

- Maß für die Dichte der elektrischen Ladung an der Oberfläche eines Ions (und damit Maß für die Kraft, ein Anion zu polarisieren)
- Beispiele:
  - K^+ = 1/1.46 Å = 0.68
  - Rb^+ = 1/1.57 Å = 0.64
  - Sr^{2+} = 2/1.21 Å = 1.65
  - Nb^{5+} = 5/0.7 Å = 7.14

Das Ionenpotential eines Kations gibt einen wichtigen Hinweis auf sein Verhalten in magmatischen und wässrigen Systemen



LILE: large ion lithophile elements: Großionige lithophile Elemente
HFSE: high field strenght elements: Elemente mit hoher Feldstärke

mobile Elemente - immobile Elemente