Lecture General Chemistry
Winter Term 2024/25

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- Website (Slides, Excercises):
- http://www.chemie.uni-siegen.de/pc/lehre/nanoscitec/

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Degree programme	**Master *Nanoscience and Nanotechnology***
Course title, Topic	**General chemistry (incl. laboratory course)**
Subtitle (optional)	5
Module ID	GChem
Specialization	
Responsible lecturer	Prof. Dr. Schönherr
Teaching type	Lecture, tutorial, Lab-course
Relation to curriculum	mandatory basic module for students with a B.Sc. in Physics or a B.Sc. in Engineering
Semester	1
Credit points (CP)	6
Workload	Lecture: 30 h, tutorial: 30 h, 60 h Lab course, homework time: 60 h
Prerequisites for participation	None

Learning outcomes / Competences	The students know the fundamental concepts of chemistry (e.g. structure-property relationships, donor-acceptor concept) and possess fundamental knowledge on the constitution of matter and laws of chemistry. They possess fundamental understanding of industrial chemical processes and chemical processes in nature. They are further accustomed to the main models in chemistry, they are able to observe, analyze, interpret and adequately report and summarize in written form dedicated natural phenomena. They possess fundamental competences in the planning, execution, analysis and evaluation of chemical experiments, they master fundamental techniques of chemical and analytical laboratory work. Their handling of chemicals is safe and adequately cautious.
Course description	Principles of general chemistry. Atomic theory, electronic structure and properties of atoms, periodic table, ionic, covalent and metallic bonding, molecular orbitals, structures of molecules, chemical formulas, reaction equations, stoichiometry, energy balance of chemical reactions, chemical kinetics, chemical equilibrium, acids and bases, acid-base equilibria, gasses, liquids and solids, phase equilibria, solutions, electrochemistry,
Interdisciplinary qualifications	Ability to think in terms of abstract concepts, recognition of complex problems, application of advanced knowledge and skills in inter- and trans-disciplinary discussion of complex issues, debating and discussing in English, ability to work in a team, organization of a lab workplace.
Assessment method (Contribution)	Exam credits: Written examination (50%), lab course and tutorial (50%). Both parts must be passed separately.
Literature	Chemistry: The Central Science with Mastering Chemistry, Global Edition, Brown, LeMay, Bursten, Murphy, Woodward

Schedule

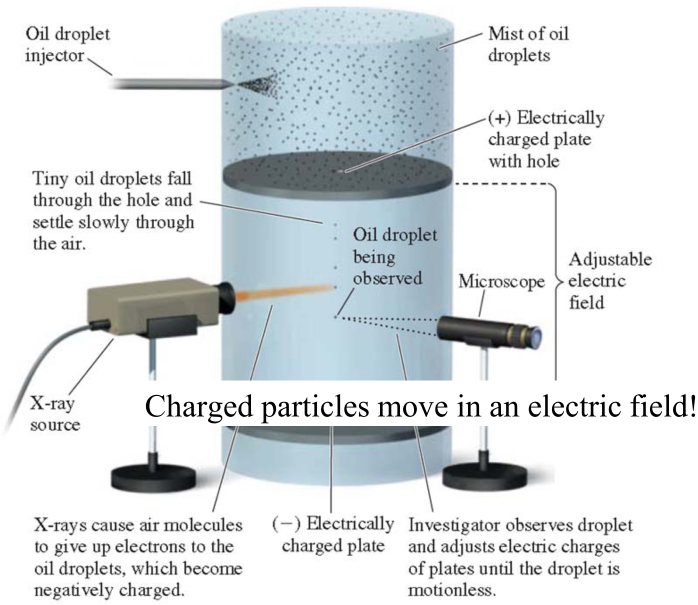
- Lecture: Thursday 14:15 – 15:45
- Tutorial/Exercise: Mo 8:30 – 10:00

- Lab Course: Monday, 13:00 – 18:00
- Start: October 21th or 28th

Atomic Theory

- What does matter consist of?
- What do atoms consist of?
- What properties do atoms have?

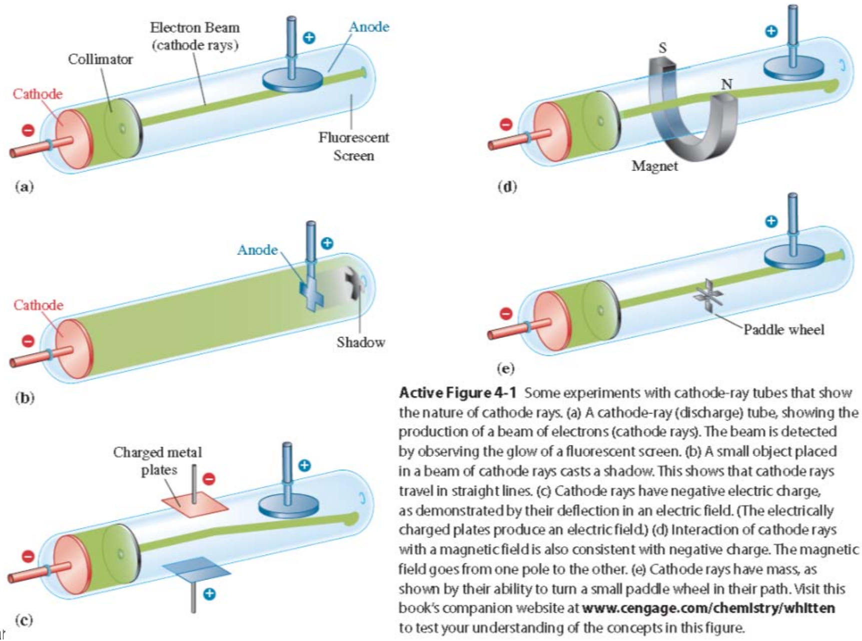
Structure of atoms: Millikan's experiment



Charged particles move in an electric field!

Abbildung aus: Brown-LeMay, Chemie siehe www.pearson-studium.de

Cathode ray tube



Active Figure 4-1 Some experiments with cathode-ray tubes that show the nature of cathode rays. (a) A cathode-ray (discharge) tube, showing the production of a beam of electrons (cathode rays). The beam is detected by observing the glow of a fluorescent screen. (b) A small object placed in a beam of cathode rays casts a shadow. This shows that cathode rays travel in straight lines. (c) Cathode rays have negative electric charge, as demonstrated by their deflection in an electric field. (The electrically charged plates produce an electric field.) (d) Interaction of cathode rays with a magnetic field is also consistent with negative charge. The magnetic field goes from one pole to the other. (e) Cathode rays have mass, as shown by their ability to turn a small paddle wheel in their path. Visit this book's companion website at **www.cengage.com/chemistry/whitten** to test your understanding of the concepts in this figure.

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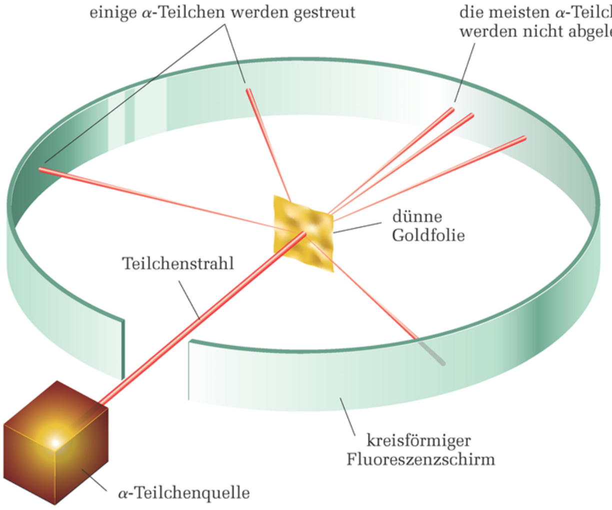
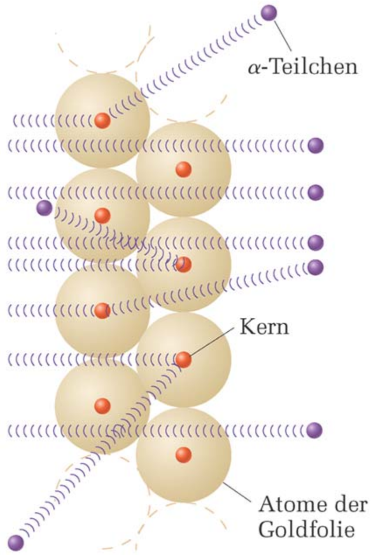
Rutherfords Experiment



Rutherfords Experiment



Mass and charge of subatomic particles

particle	**mass** in kg	**charge** in Coulomb
Elektron	$9{,}10938 \cdot 10^{-31}$	$-1{,}6022 \cdot 10^{-19}$
Proton	$1{,}67262 \cdot 10^{-27}$	$1{,}6022 \cdot 10^{-19}$
Neutron	$1{,}67493 \cdot 10^{-27}$	0

How to get to masses which can be used in the lab?

Definition of a useful conversion factor

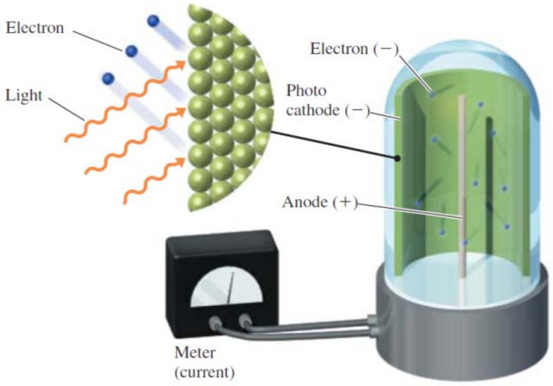
- Molar amount *n*: Number of particles, unit Mol

  $1\,\text{Mol} = 6{,}022 \cdot 10^{23}$ particles
- 1 Mol has as many particles as12 g of $^{12}_{6}C$ (defined)
- Molar Mass *M*: Mass of 1 Mol of particles, unit g/mol

Properties of electrons

- So, what do we know of electrons?

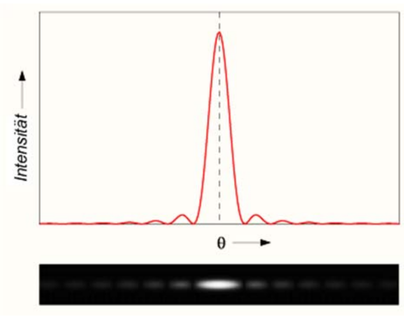
Electrons behave as particles



Active Figure 4-15 The photoelectric effect. When electromagnetic radiation of sufficient minimum energy strikes the surface of a metal (negative electrode or cathode) inside an evacuated tube, electrons are stripped off the metal to create an electric current. The current increases with increasing radiation intensity. Visit this book's companion website at **www.cengage.com/chemistry/whitten** to test your understanding of the concepts in this figure.

•aus:**Chemistry, 9th Edition** KW Whitten,
•RE Davis, ML Peck, GG Stanley

Electron diffraction at single slit



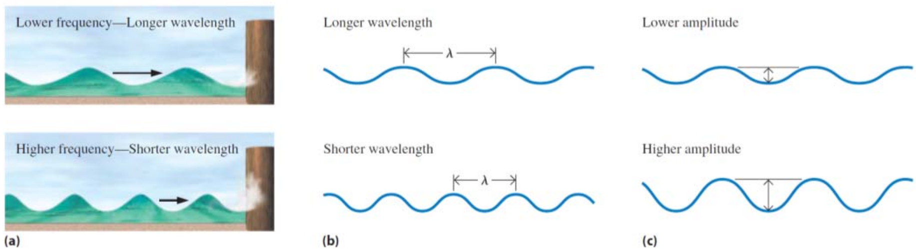
Bildquelle: Wikepedia

Electrons behave as waves

Properties of waves

$$\lambda \cdot \nu = c$$

$$E = h \cdot \nu = h \cdot \frac{c}{\lambda}$$



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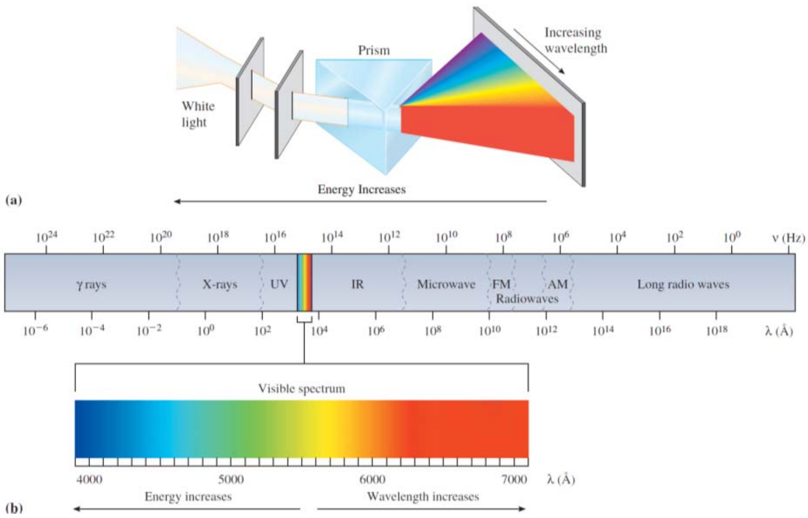

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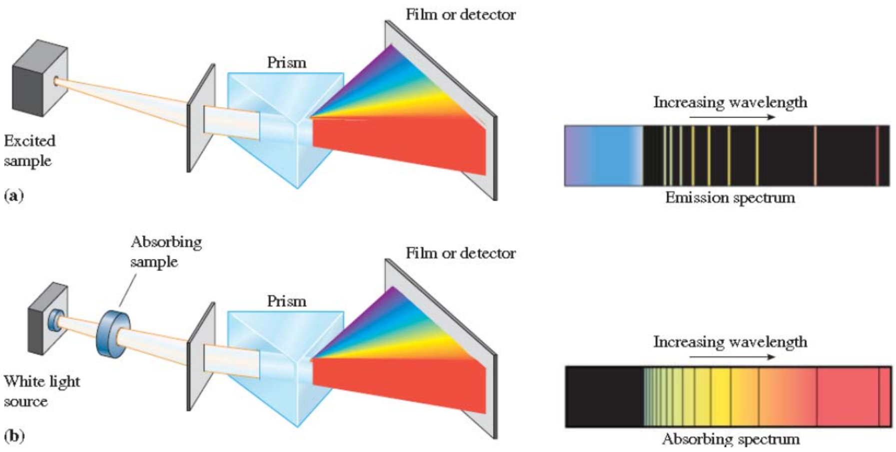

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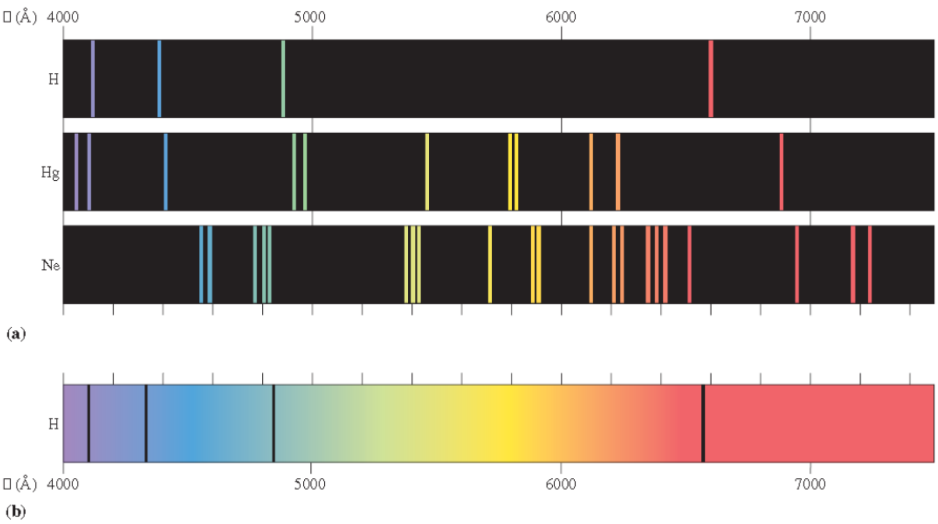
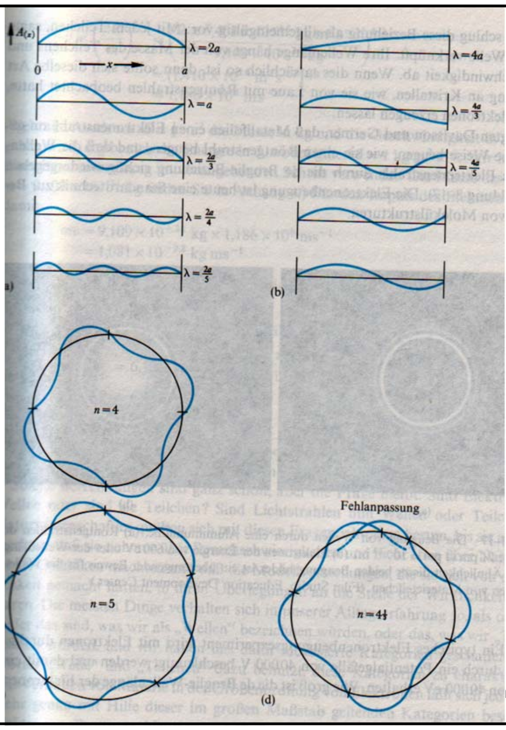
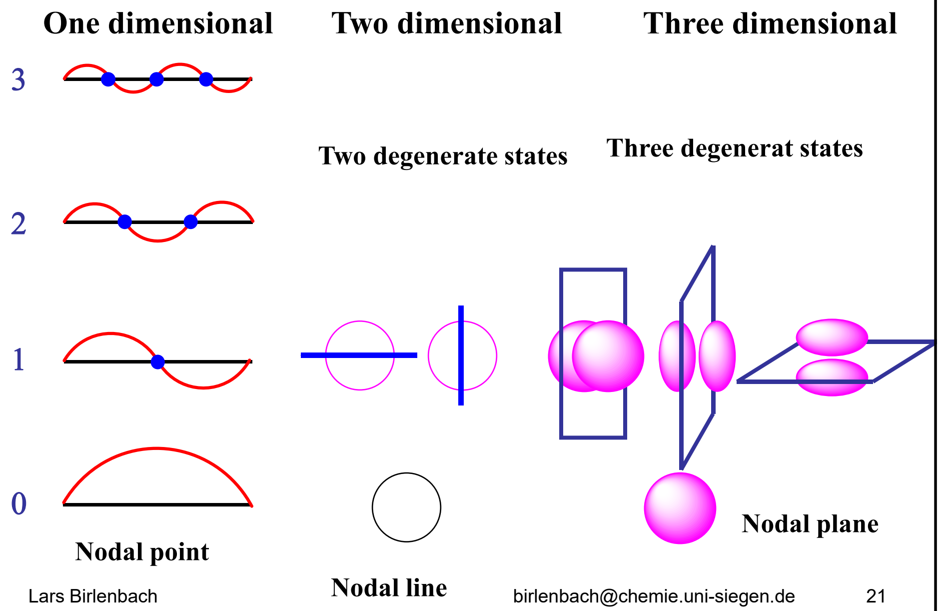
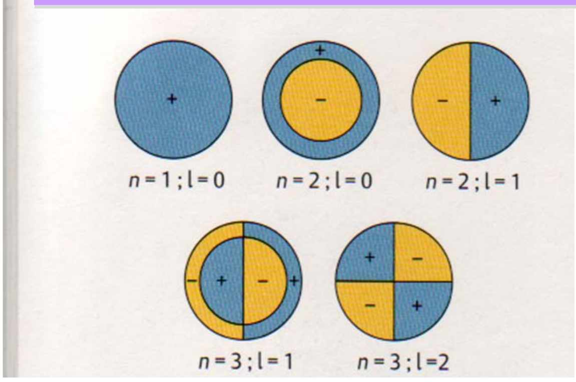

(Å) 4000
5000
6000
7000
H
Hg
Ne
(a)
H
(Å) 4000
5000
6000
7000
(b)


λ = 2a
λ = a
λ = 4a
(b)
n=4
n=5
Fehlanpassung
(d)

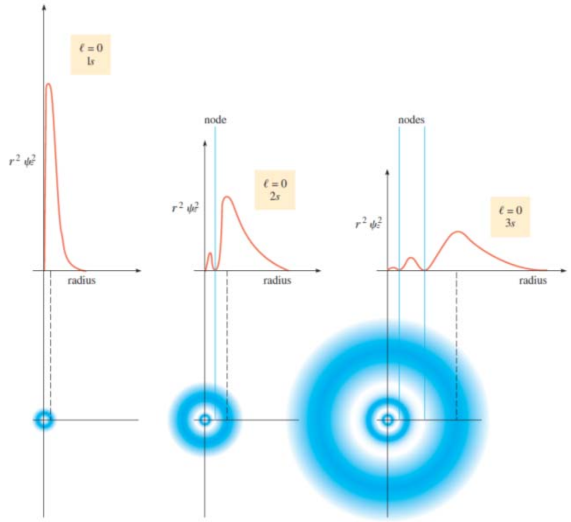
Standing waves



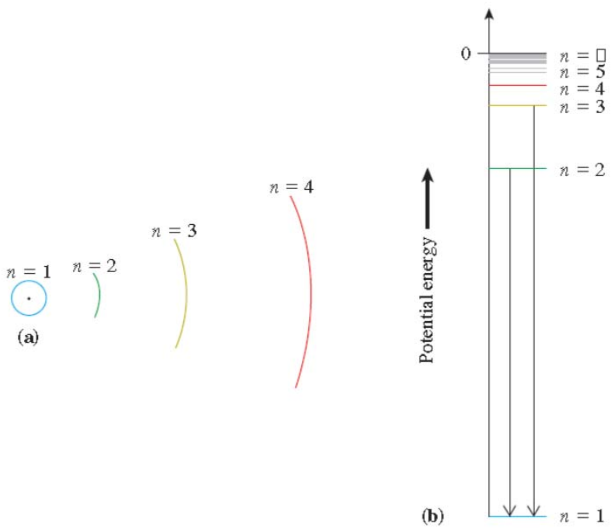
Two dimensional standing waves



Three dimensional standing waves



Bohr‘s atomic model



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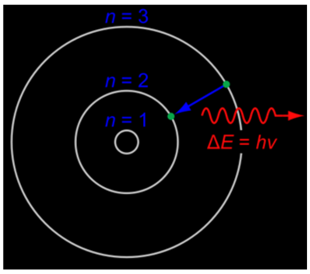
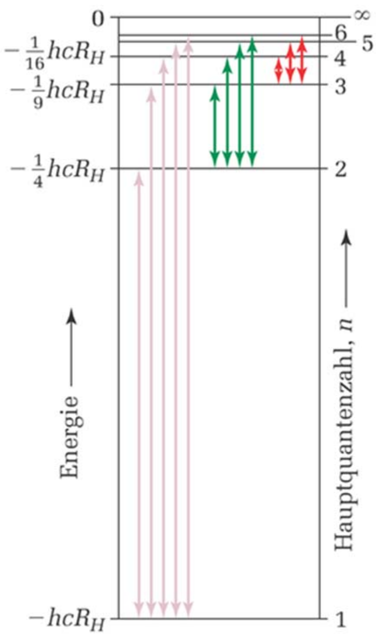
Bohr‘s atomic model

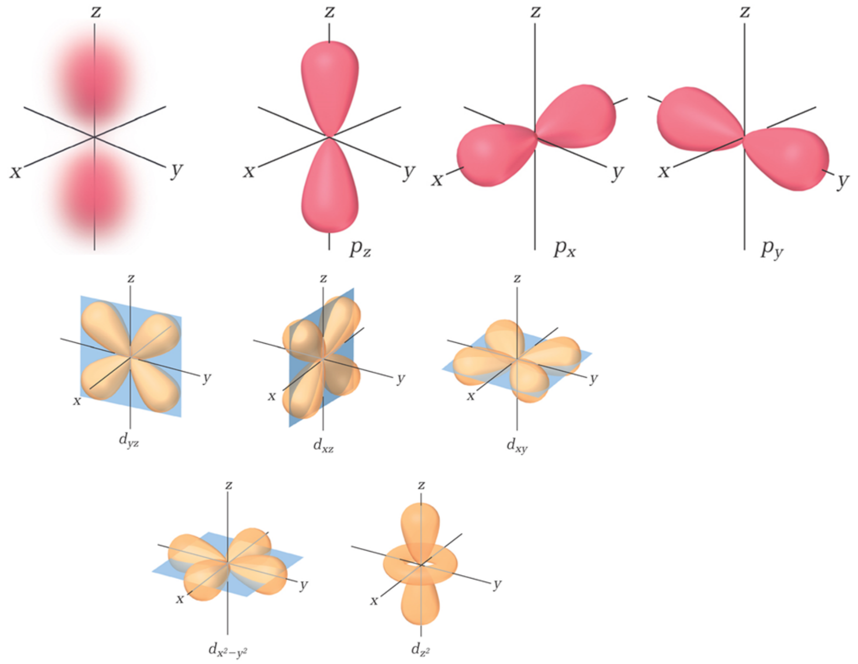


$$\frac{1}{\lambda} = R\left(\frac{1}{n_2{}^2} - \frac{1}{n_1{}^2}\right)$$

$R = 1{,}1 \cdot 10^7\,\mathrm{m}^{-1}$

Rydberg-Konstant





Abbildungen aus: Brown-LeMay, Chemie
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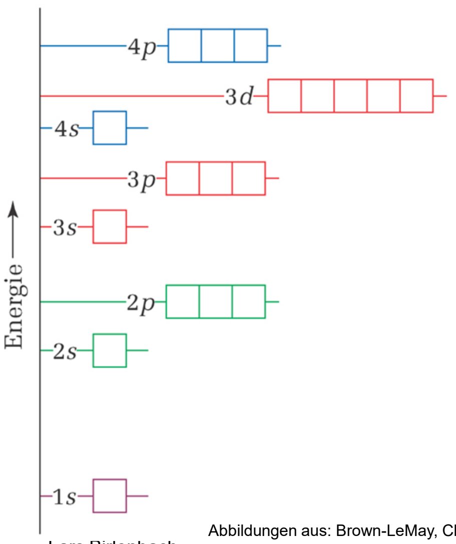
Energy levels of the orbitals



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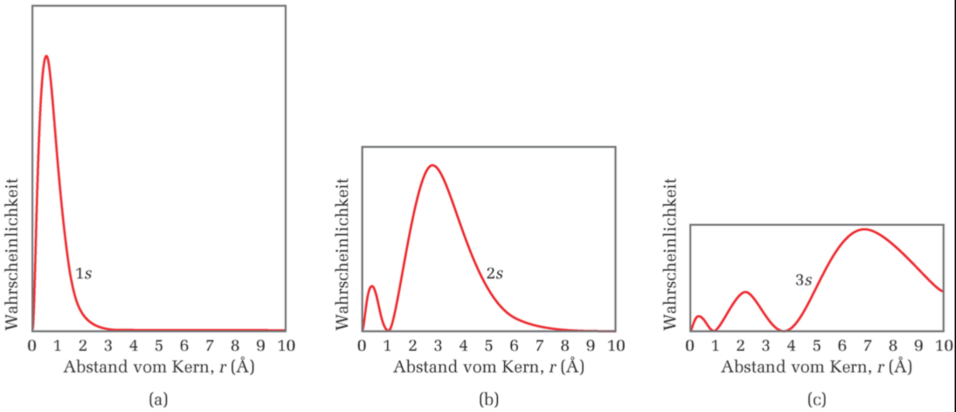
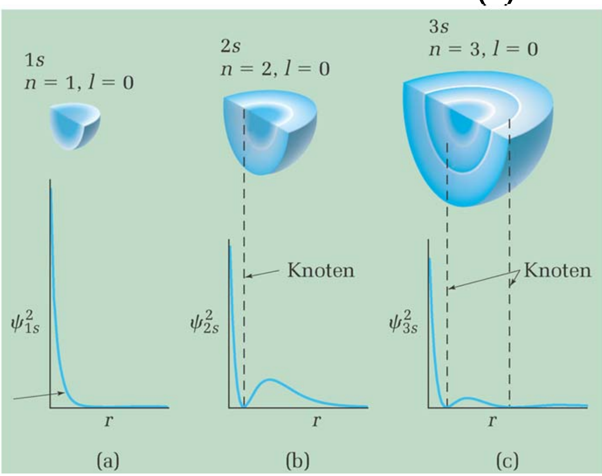
Ions in s-Orbitals

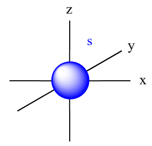


$$\text{probability} \propto 4\pi r^2 \Psi^2$$

Wave function $\Psi = f(r)$

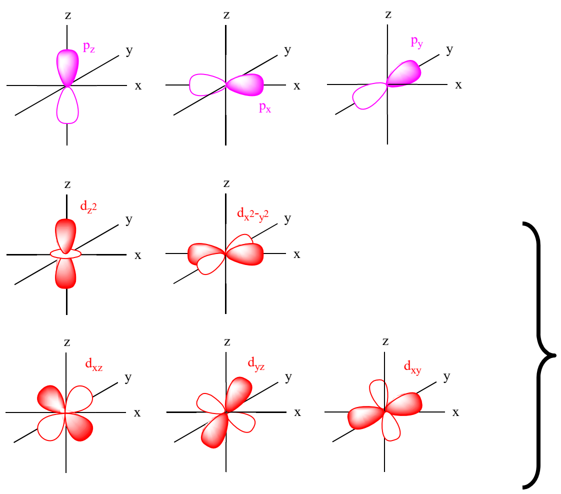


Elektrons in atoms



Standing three-dimensional waves

0 nodal planes
s-Orbitals



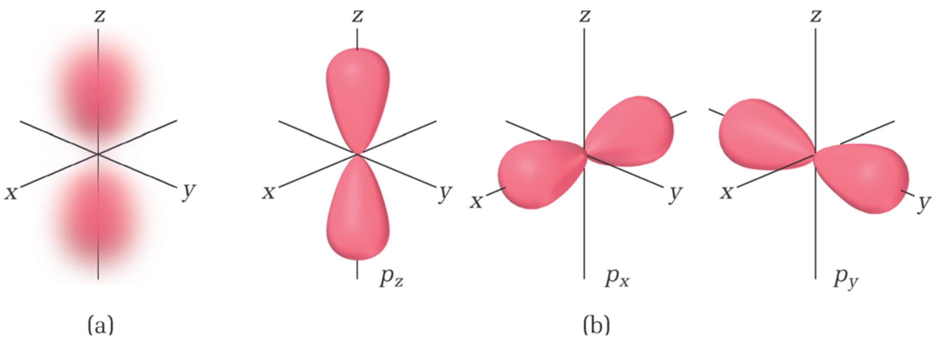
1 nodal plane

p-Orbitals

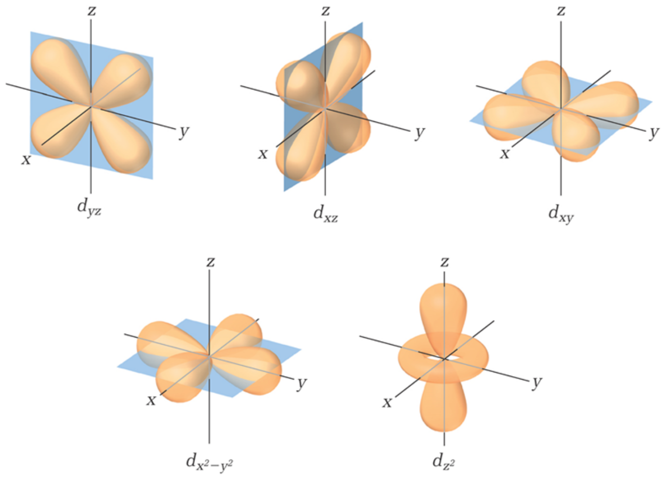
2 nodal planes

d-Orbitals

p-Orbitals



d-Orbitals



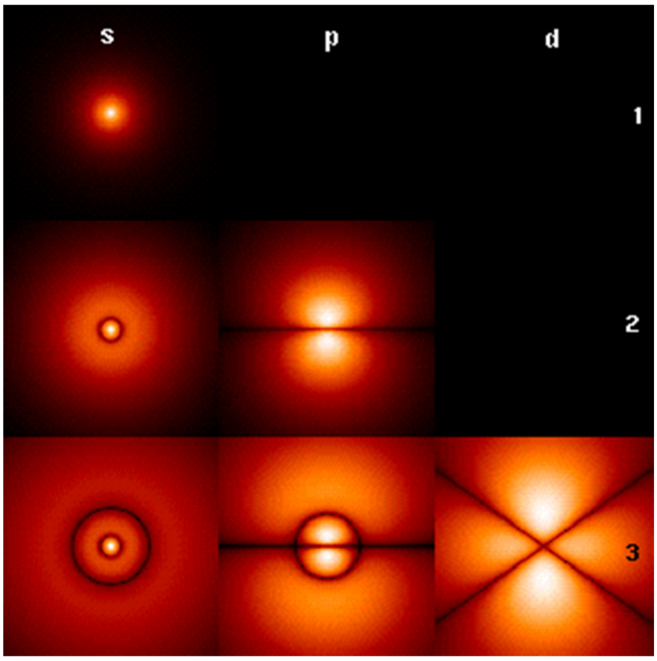


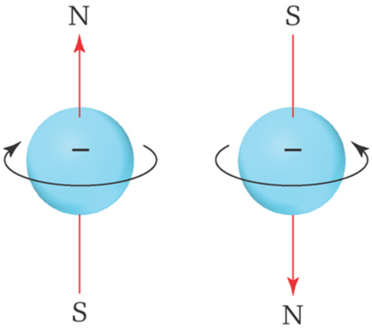
TABLE 6.5

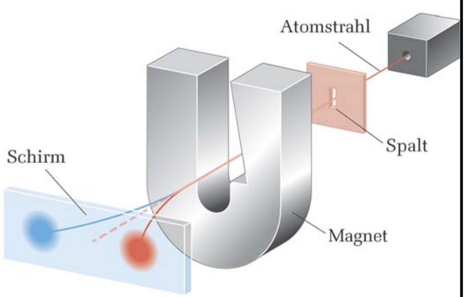
The complete hydrogenlike atomic wave functions for $n = 1, 2,$ and 3. The quantity Z is the atomic number of the nucleus, and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{200} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{210} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{21\pm1} = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta e^{\pm i\phi}$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27 - 18\sigma + 2\sigma^2)e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{310} = \frac{1}{81}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2)e^{-\sigma/3}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2)e^{-\sigma/3}\sin\theta e^{\pm i\phi}$
	$l = 2,$	$m = 0$	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}(3\cos^2\theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin\theta\cos\theta e^{\pm i\phi}$
	$l = 2,$	$m = \pm 2$	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin^2\theta e^{\pm 2i\phi}$

aus: McQuarrie, Simon: Physical Chemistry. University Science Books

Electron spin





Abbildungen aus: Brown-LeMay, Chemie
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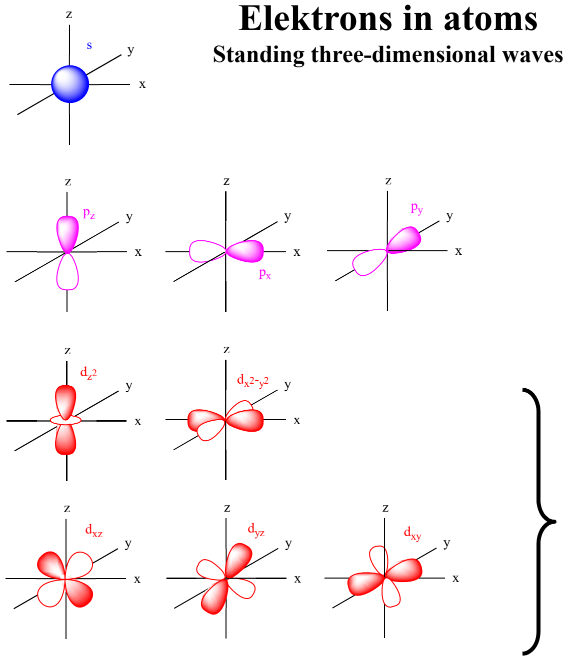
Quantum numbers

- Main quantum number *n*: Size of wave function
  - $n = 1, 2, \ldots$
- Azimutal quantum number *l*: number of nodal planes
  - $l = 0$ no nodal plane
  - $l = 1$ one nodal plane
  - $l = 2$, two nodal planes
  - $l = 0, 1, 2, \ldots n-1$
- Magnetic quantum number *m*: distribution in space
  - $m = -l, \ldots, 0, \ldots, +l$
- Spin quantum number *s*: angular momentum
  - +½ , -½

Elektrons in atoms

Standing three-dimensional waves



0 nodal planes
s-Orbitals

1 nodal plane

p-Orbitals

2 nodal planes

d-Orbitals

Electronic configuration for Chlorine

Electron	n	ℓ	m_ℓ	m_s	e^- Configuration
1, 2	1	0	0	$\pm\frac{1}{2}$	$1s^2$
3, 4	2	0	0	$\pm\frac{1}{2}$	$2s^2$
5–10	2	1	−1	$\pm\frac{1}{2}$	$2p^6$
	2	1	0	$\pm\frac{1}{2}$	
	2	1	+1	$\pm\frac{1}{2}$	
11, 12	3	0	0	$\pm\frac{1}{2}$	$3s^2$
13–17	3	1	−1	$\pm\frac{1}{2}$	$3p^5$
	3	1	0	$\pm\frac{1}{2}$	
	3	1	+1	$+\frac{1}{2}$ or $-\frac{1}{2}$*	

Electronic configurations

n	ℓ	m_ℓ	m_s	Electron Capacity of Subshell = $4\ell + 2$	Electron Capacity of Shell = $2n^2$
1	0(1*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	2
2	0(2*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	8
	1(2*p*)	−1, 0, +1	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
3	0(3*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	18
	1(3*p*)	−1, 0, +1	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
	2(3*d*)	−2, −1, 0, +1, +2	$\pm\frac{1}{2}$ for each value of m_ℓ	10	
4	0(4*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	32
	1(4*p*)	−1, 0, +1	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
	2(4*d*)	−2, −1, 0, +1, +2	$\pm\frac{1}{2}$ for each value of m_ℓ	10	
	3(4*f*)	−3, −2, −1, 0, +1, +2, +3	$\pm\frac{1}{2}$ for each value of m_ℓ	14	