AC III

Moderne Anorganische Molekül- und Festkörperchemie (MAMF)

Dr. Günther Thiele

Terminübersicht

- Vorlesung: Dienstags 9.15 Uhr – 10 Uhr
  Mittwochs 10.15 Uhr – 12 Uhr
- Übungen: Dienstags 8.15 Uhr – 9 Uhr
  Erster Termin: 16.04

  Gruppe 1: HS AC (Leitung: Moritz Ernst)
  Gruppe 2: SR AC (Leitung: Jonas Schmid)
  28.05 - SR 34.16/17
- Klausur: Mittwoch, 10.07, 10.00 Uhr – 12:00 Uhr
  Q&A Session: Dienstag, 09.07, 8:15 Uhr
  Notenveröffentlichung (online): Montag, 15.07, 18:00 Uhr
  Noteneinsicht (C009): Dienstag, 16.07, 9-10 Uhr
- Anwendung: AC-Kolloquium 18. Juni, 17:15 Uhr: A. Möller

Übungen, Folien: Online

https://www.bcp.fu-berlin.de/chemie/chemie/forschung/InorgChem/agthiele/lehre/AC-III-SoSe-2019/index.html

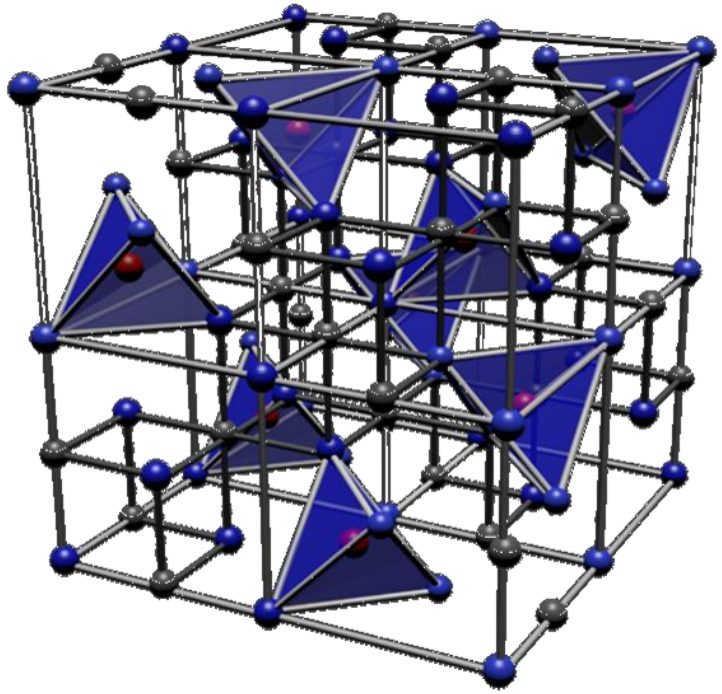
Festkörperfahrplan: B.Sc./M.Sc.

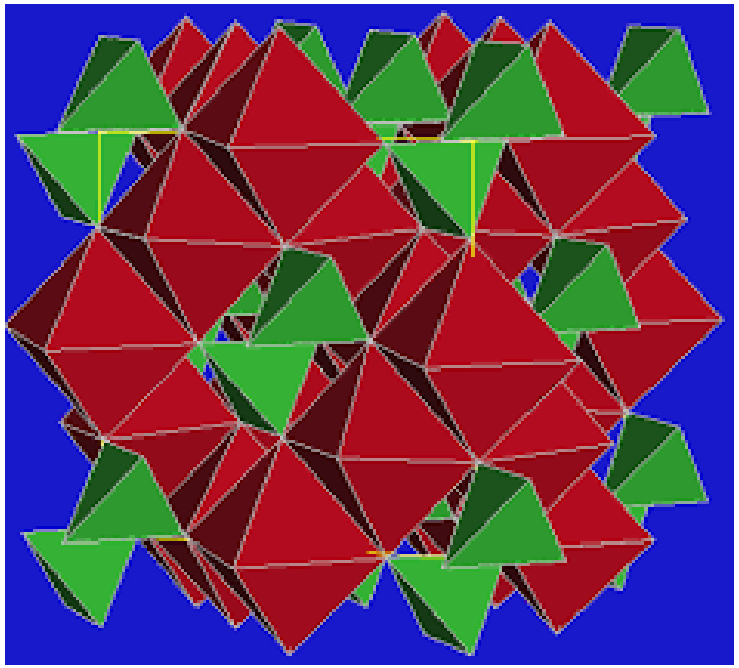
- B.Sc.
  - **AC III**: Einführung, Allgemeine Konzepte, wichtigste Strukturtypen
- M.Sc.
  - **Solids and Interfaces**: Beschreibung der elektronischen Struktur und Grenzflächenphänomene
  - **Structure Determination**: Röntgenbeugungsmethoden, Festkörper-NMR
  - **Elektronenstrukturmethoden**: Quantentheorie periodischer Systeme
  - **Solid State and Materials**: Spezielle Konzepte, Synthesen, Struktur-Eigenschaftsbeziehungen, Symmetrietheorie

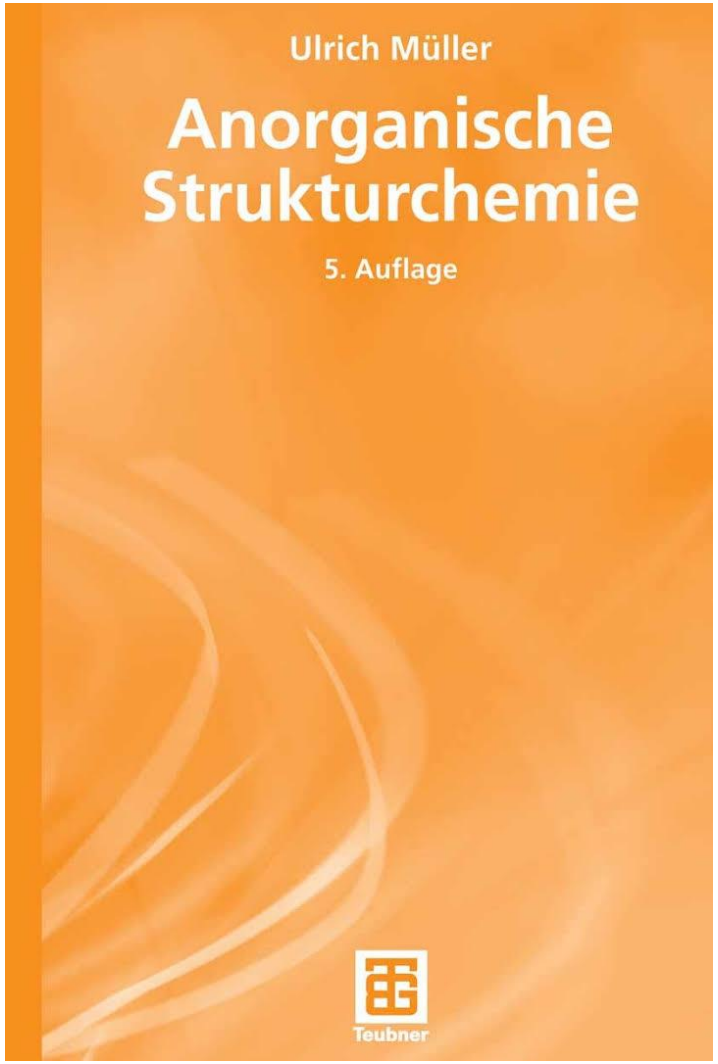
0. **Wiederholung Symmetrie und Translation**
1. **Strukturchemie**
    1. Kugelpackungen, Metallstrukturen, Elementstrukturen
    2. Spezielle Strukturtypen: AB, AB_2, AB_3, A_2B_3, …
    3. Legierungen und intermetallische Phasen
    4. Verknüpfte Polyeder: Heusler-Phasen, Polyoxometallate und Silikate
    5. Defektstrukturen, Gläser
    6. Nanostrukturen, Quantenpunkte, innere und äußere Grenzflächen
2. **Energetische Beschreibung und Bindungstheorien**
    1. Ionenverbindungen, Gitterenergie, Pauling-Regeln
    2. Hauptgruppenverbindungen, VSEPR-Konzept
    3. Nebengruppenverbindungen, Ligandenfeldtheorie
    4. Bändertheorie, Peierls-Verzerrungen, Kristall-Orbital-Überlappungspopulation Relativistische Effekte
    5. Phasenumwandlungen
3. **Physikalische Eigenschaften von Festkörpern**
    1. Mechanische Eigenschaften
    2. Elektrizität, Ferroelektrika, Piezoelektrika, Seebeck-Effekt
    3. Magnetische Eigenschaften
    4. Leitfähigkeiten: thermisch, elektrisch, ionisch, Supraleitung
    5. Optische Eigenschaften
    6. Spintronics

Strukturpräsentationen

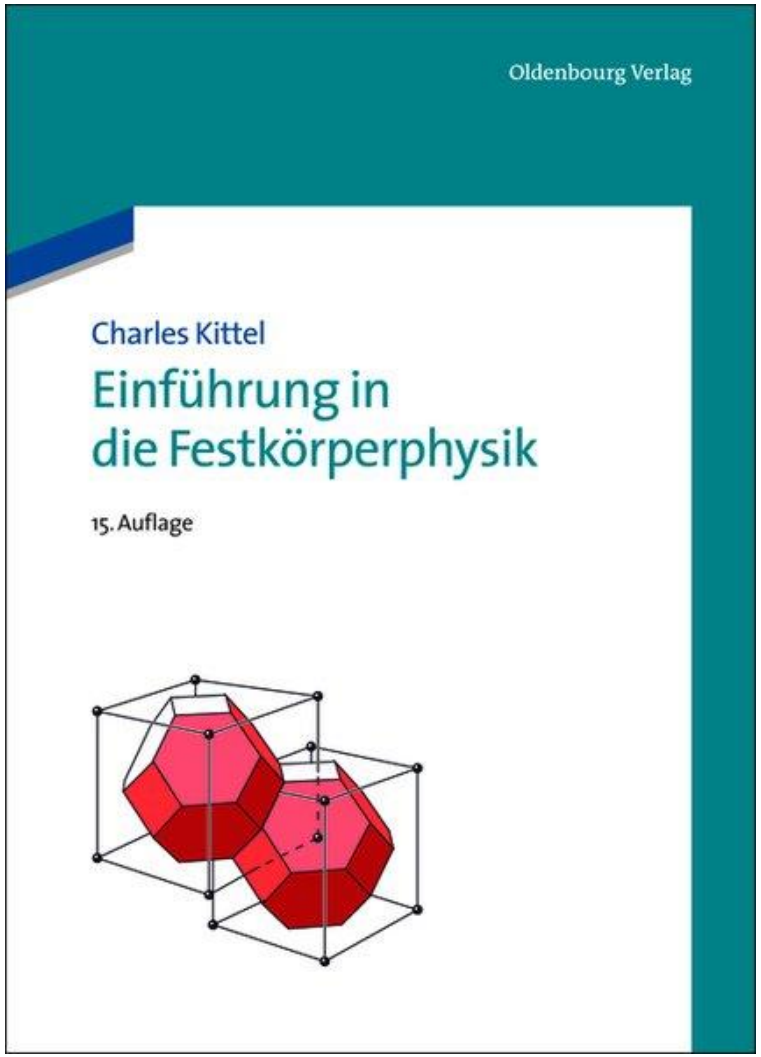
- Je 2 Personen einen Vortrag (max 5 Min.) und ein HandOut (max ein A4 PDF)
- Eine Woche vor Präsentation: Rücksprache!
- Termine: Online Anmeldung via doodle first come – first serve, einfach…komplex
- Wie erstellen? Guidelines online.







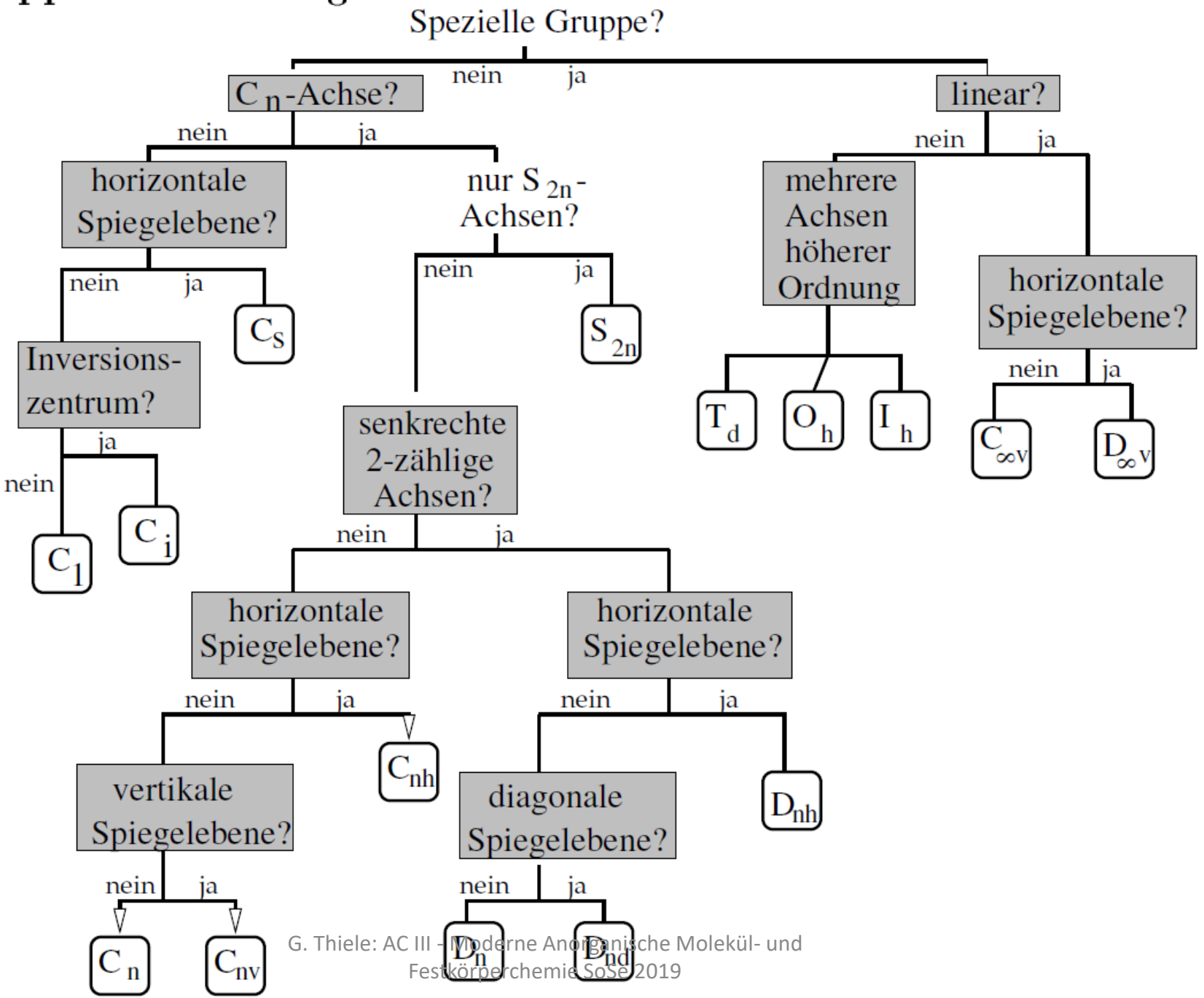
Müller: Anorganische Strukturchemie.
€ 29,99 (e-pdf)



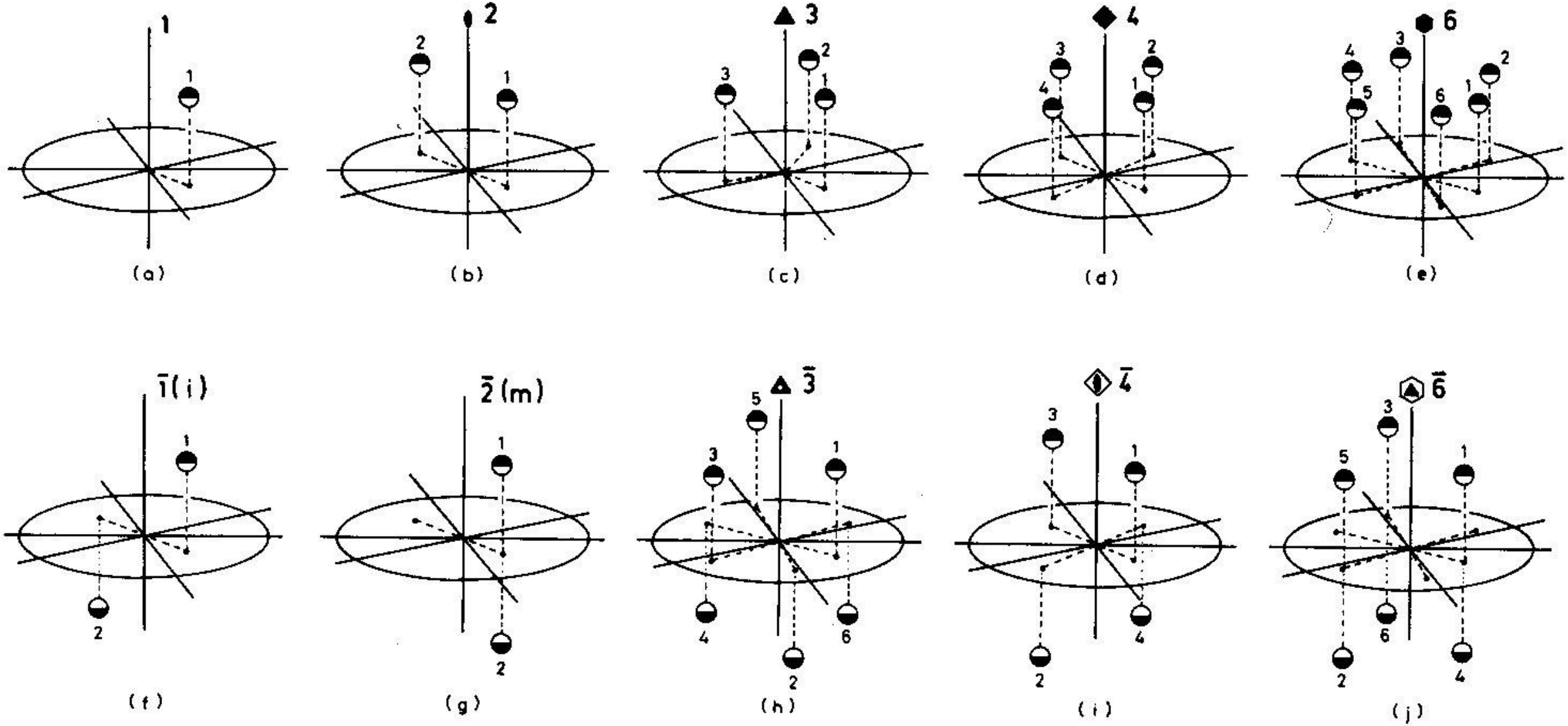
Kittel: Einführung in die Festkörperphysik. € 69,80
Verfügbar @ UB

http://ruby.chemie.uni-freiburg.de/Vorlesung/

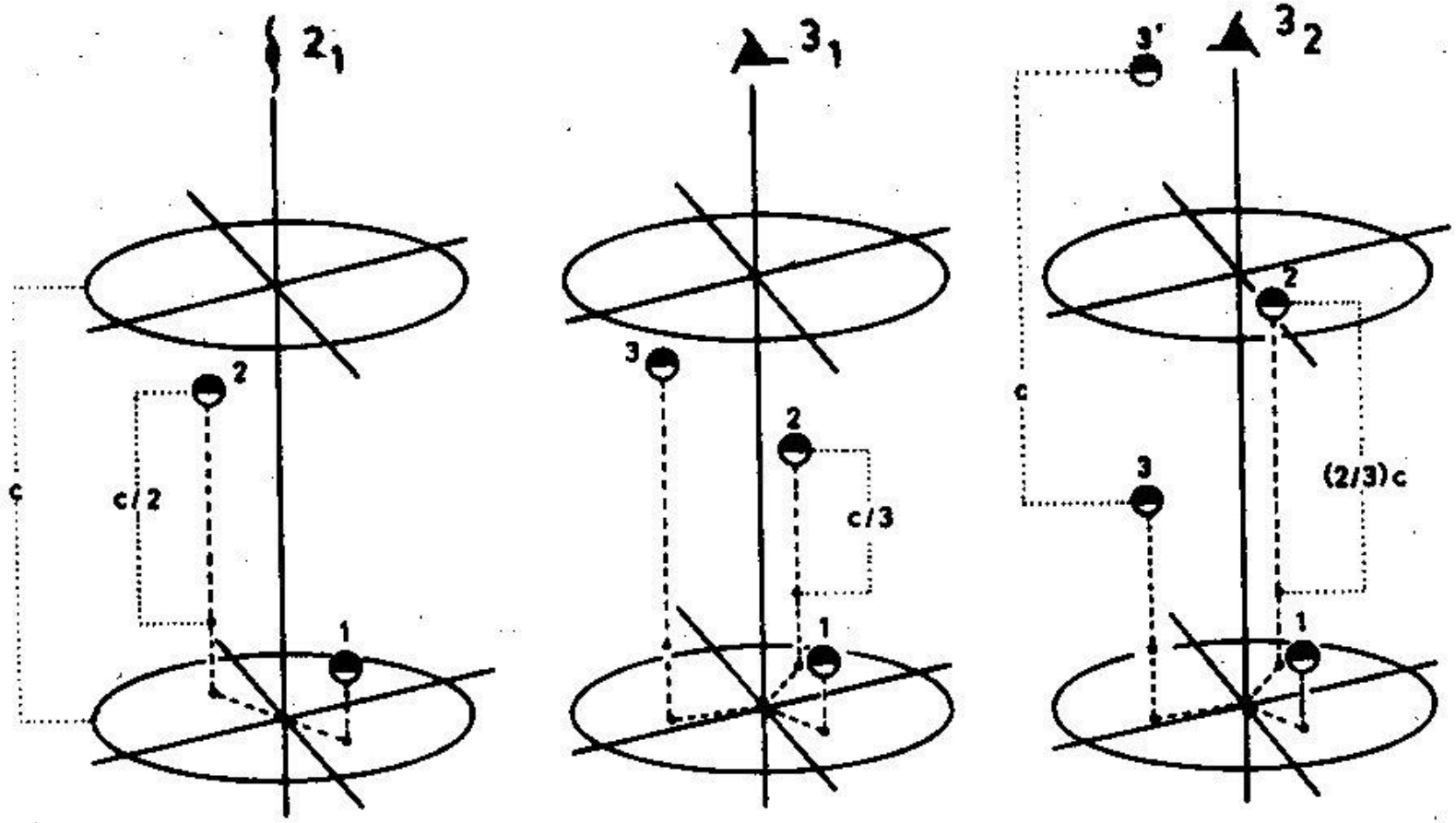
Punktgruppenbestimmung



Hermann-Mauguin

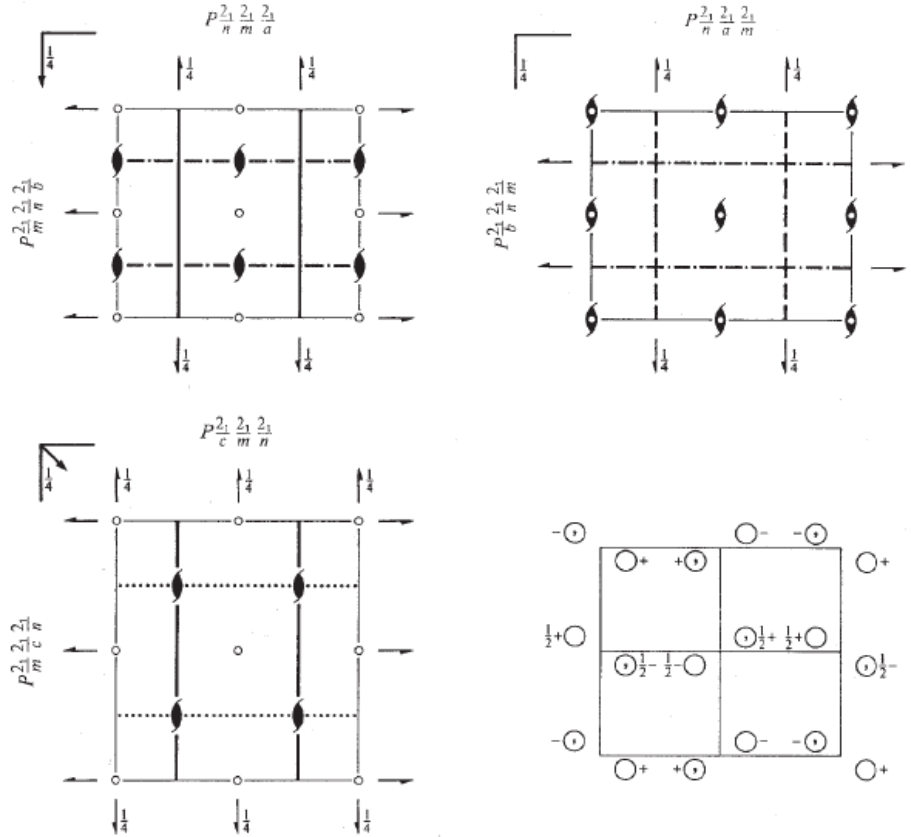


Schraubenachsen



$Pnma$ D_{2h}^{16} mmm Orthorhombic

No. 62 $P\,2_1/n\,2_1/m\,2_1/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0\le x\le\frac{1}{4}$; $0\le y\le\frac{1}{4}$; $0\le z\le 1$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{4},0)$ $0,y,0$	(4) $2(\frac{1}{4},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8 d 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$		$0kl$: $k+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,z+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$		Special: as above, plus
4 c $.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$		no extra conditions
4 b $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		hkl : $h+l,k=2n$
4 a $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		hkl : $h+l,k=2n$

Symmetry of special projections

Along [001] $p\,2g\,m$
$\boldsymbol{a'}=\frac{1}{2}\boldsymbol{a}$ $\boldsymbol{b'}=\boldsymbol{b}$
Origin at $0,0,z$

Along [100] $c\,2m\,m$
$\boldsymbol{a'}=\boldsymbol{b}$ $\boldsymbol{b'}=\boldsymbol{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p\,2g\,g$
$\boldsymbol{a'}=\boldsymbol{c}$ $\boldsymbol{b'}=\boldsymbol{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	$[2]P\,2_1\,2_1\,2_1$	1; 2; 3; 4
	$[2]P\,1\,1\,2_1/a$ $(P\,2_1/c)$	1; 2; 5; 6
	$[2]P\,1\,2_1/m\,1$ $(P\,2_1/m)$	1; 3; 5; 7
	$[2]P\,2_1/n\,1\,1$ $(P\,2_1/c)$	1; 4; 5; 8
	$[2]Pnm\,2_1$ $(Pmn\,2_1)$	1; 2; 7; 8
	$[2]Pn\,2_1a$ $(Pna\,2_1)$	1; 3; 6; 8
	$[2]P\,2_1ma$ $(Pmc\,2_1)$	1; 4; 6; 7
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc $[3]Pnma(\boldsymbol{a'}=3\boldsymbol{a})$; $[3]Pnma(\boldsymbol{b'}=3\boldsymbol{b})$; $[3]Pnma(\boldsymbol{c'}=3\boldsymbol{c})$

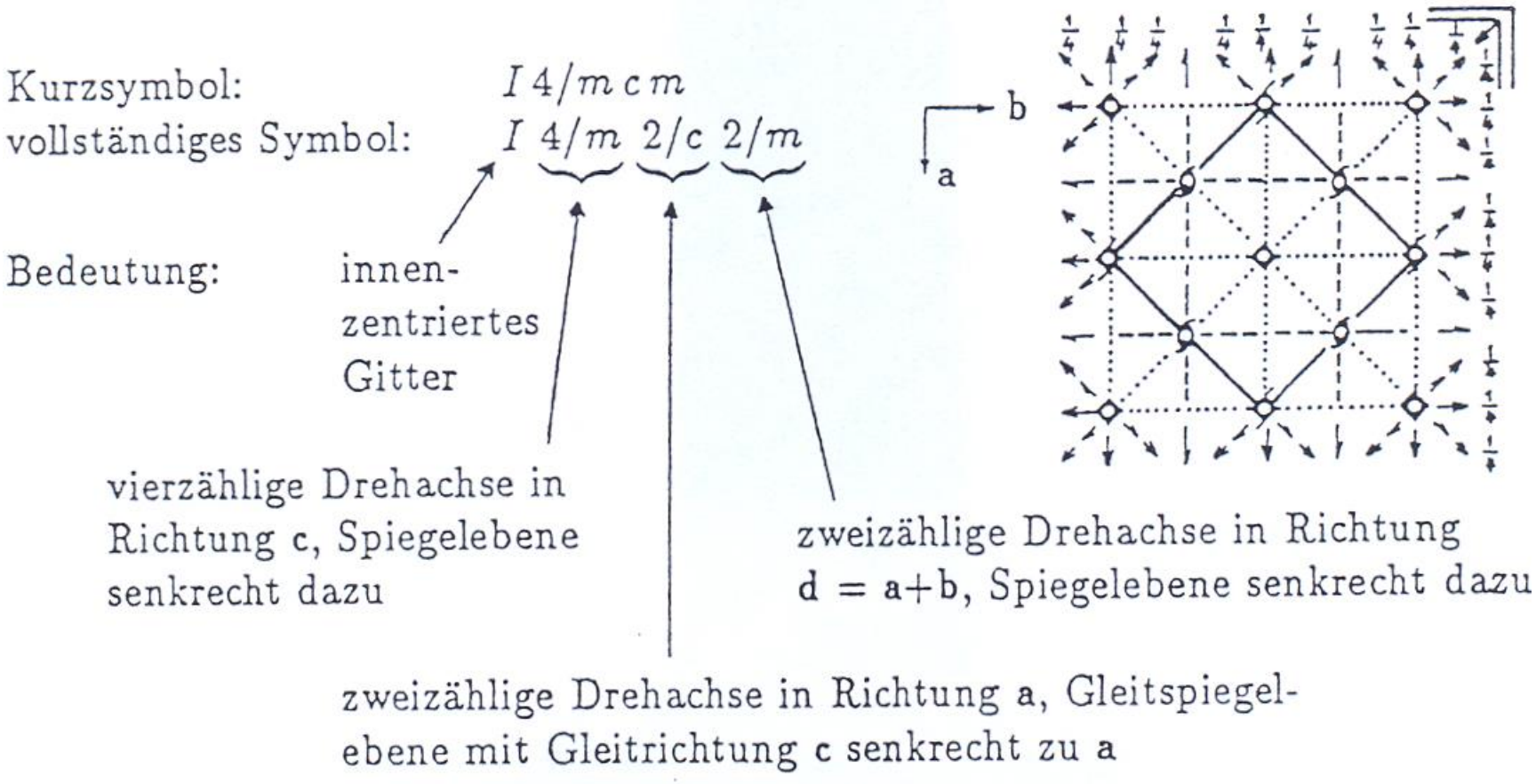
Minimal non-isomorphic supergroups

I none

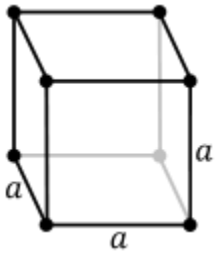
II $[2]Amma(Cmcm)$; $[2]Bbmm(Cmcm)$; $[2]Ccmb(Cmca)$; $[2]Immm$; $[2]Pnmm(2\boldsymbol{a'}=\boldsymbol{a})(Pmmn)$; $[2]Pcma(2\boldsymbol{b'}=\boldsymbol{b})(Pbam)$; $[2]Pbma(2\boldsymbol{c'}=\boldsymbol{c})(Pbcm)$

Space group Symbolism according to Herrmann-Mauguin

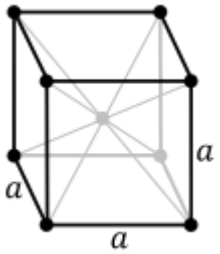
(Int.Tables for X-Ray Crystallography)



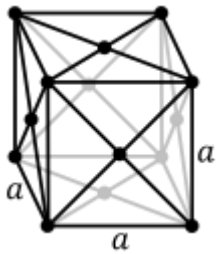
14 Bravais Gitter



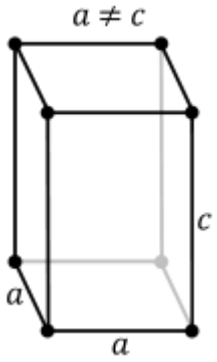
cP



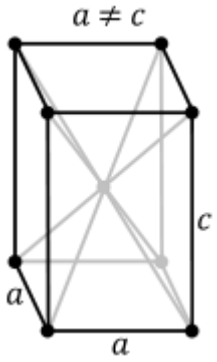
cI



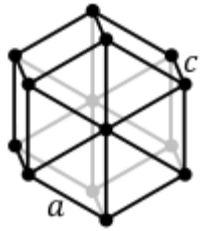
cF



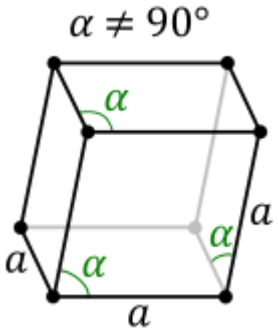
tP



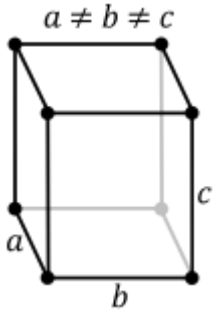
tI



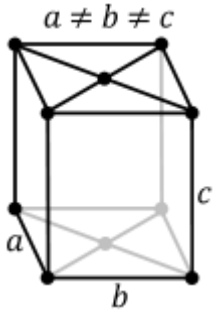
hP



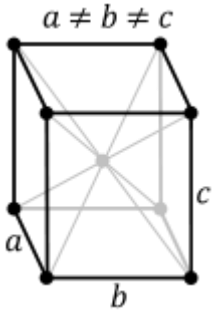
hR



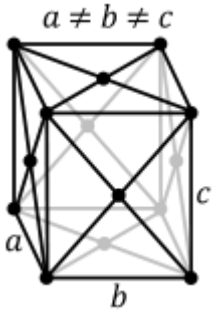
oP



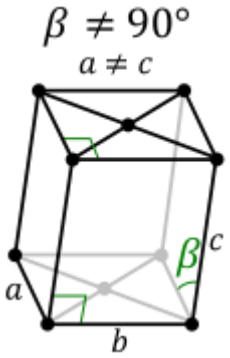
oC



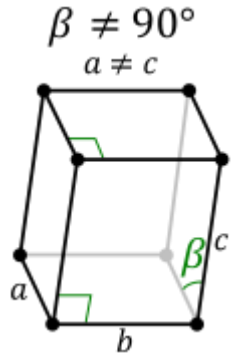
oI



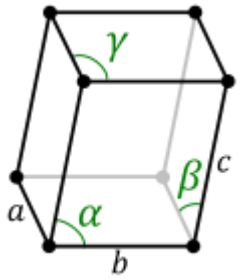
oF



mC



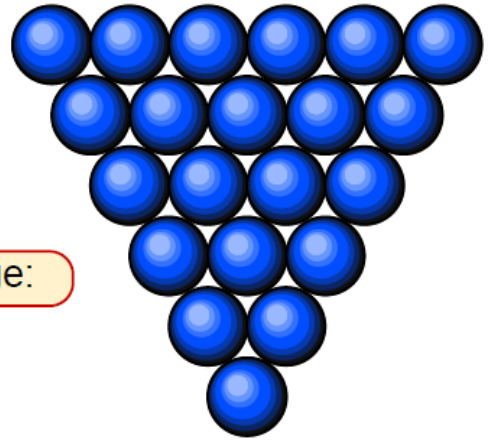
mP



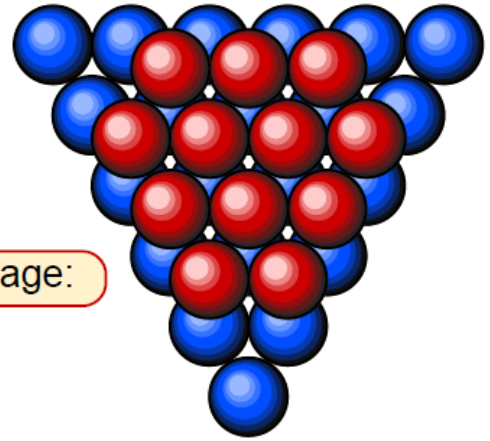
aP

Dichteste Kugelpackung

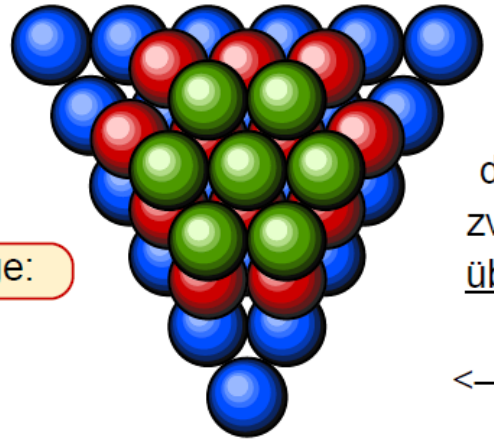
erste Lage:



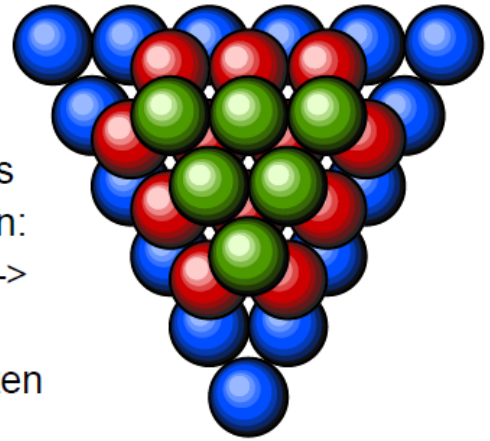
zweite Lage:



dritte Lage:



für die
dritte Lage gibt es
zwei Möglichkeiten:
über der ersten —>
oder
<— neben der ersten



Stapelfolge ABCABCABC…
"kubisch flächenzentriert" =
face centered cubic = fcc

Stapelfolge ABABABAB…
"hexagonal dicht gepackt" =
hexagonal close packed = hcp

Dichteste Kugelpackung

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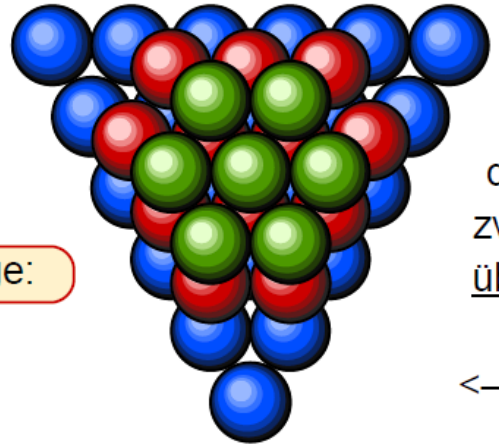

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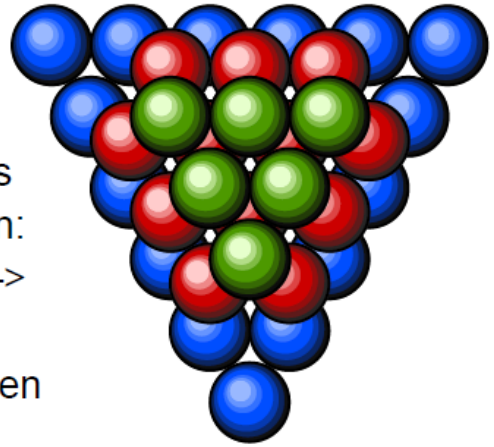

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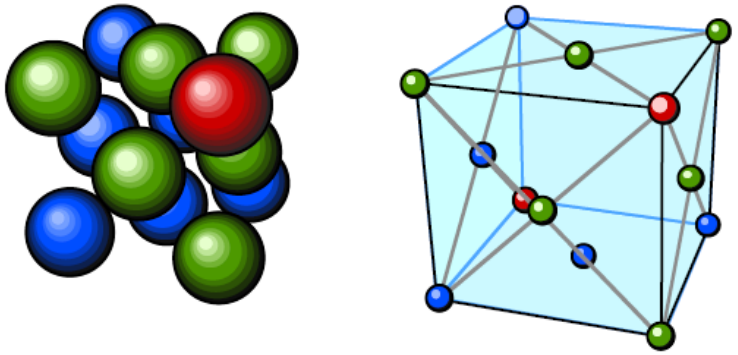
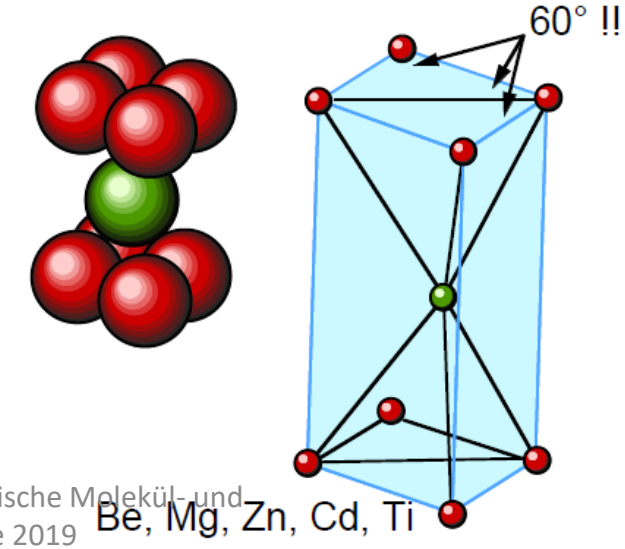
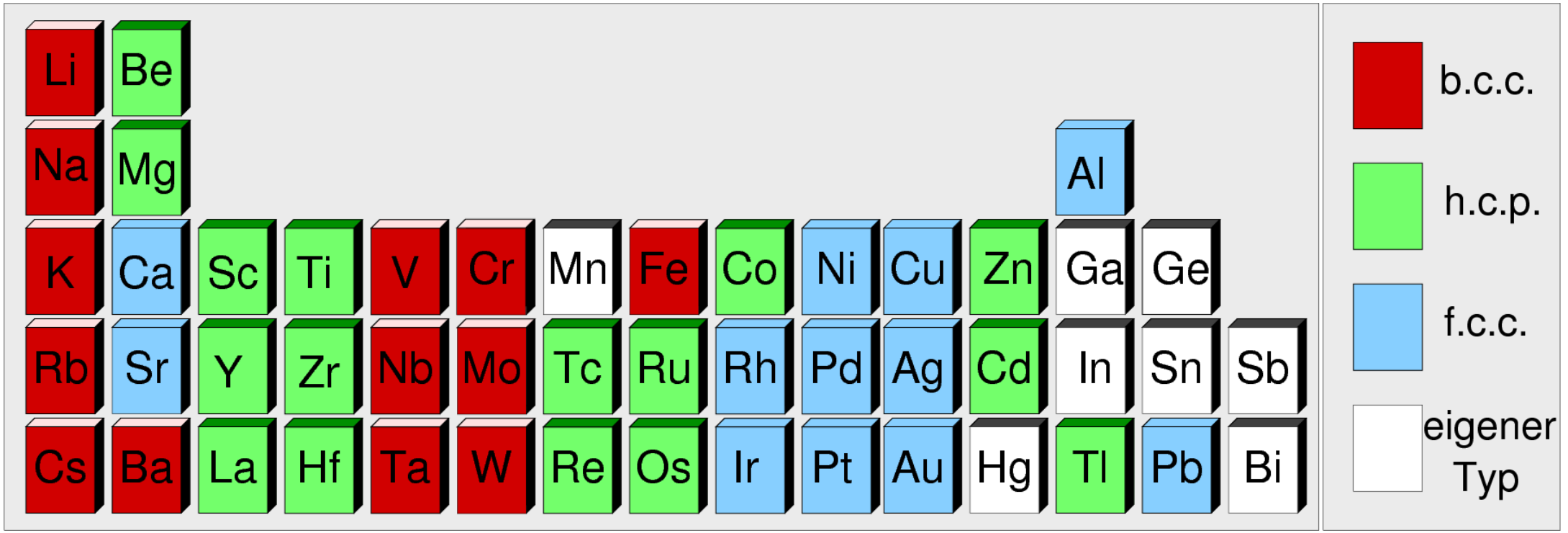




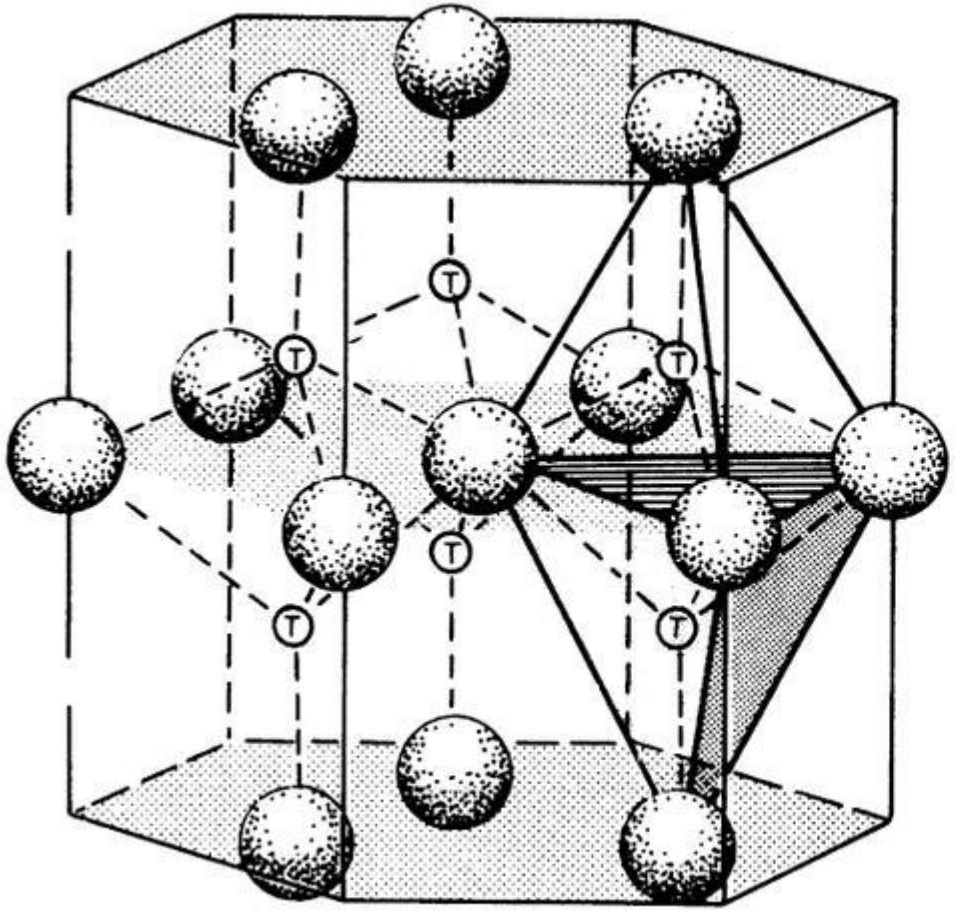
Beispiele:
Cu, Ag, Au, Al, Pb, Co, Ir, Pt

Be, Mg, Zn, Cd, Ti

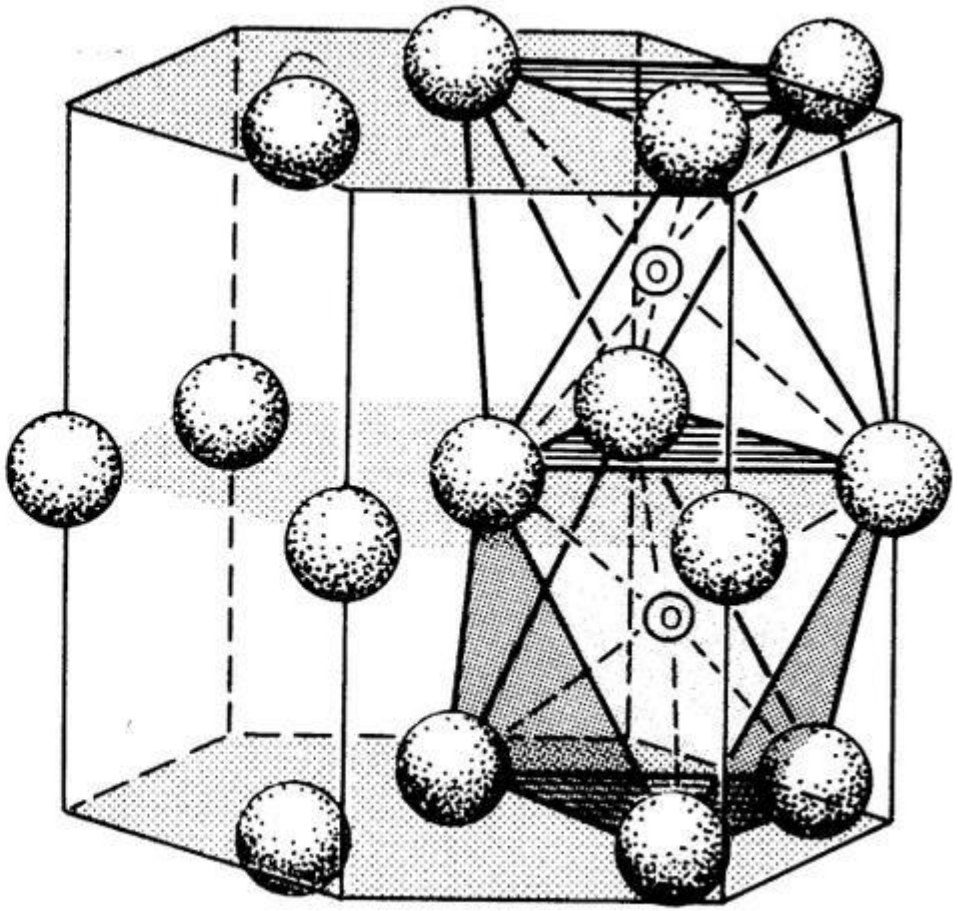
Metallstrukturen



Lücken in hexagonal dichtesten Packungen



A



B