Introduction to Solid State Physics

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TU Graz

MAS.020UF Introduction to Solid State Physics

Course outline

- **Crystal structure**
  - Crystal structure W
  - Unit cell W
  - Bravais lattices W
  - Miller indices W
  - Wigner Seitz cell W
    - Drawing Wigner-Seitz cells in two dimensions
    - Drawing Wigner-Seitz cells in three dimensions
  - Asymmetric unit
  - Examples of crystal structures
    - simple cubic, fcc, bcc, hcp, diamond, silicon, zincblende, ZnO wurzite, NaCl, CsCl, sugar
    - More crystal structures, CIF files, and programs to visualize crystal structures
    - The AFLOW standard encyclopedia of crystallographic prototypes
  - Symmetries
    - Point groups W
      - Table of crystal classes and their associated point groups
      - Flowchart to determine the point group of a crystal
    - Space groups W
    - Space Group → Bravais Lattice, Point Group

Exercises to 'Introduction to Solid State Physics'

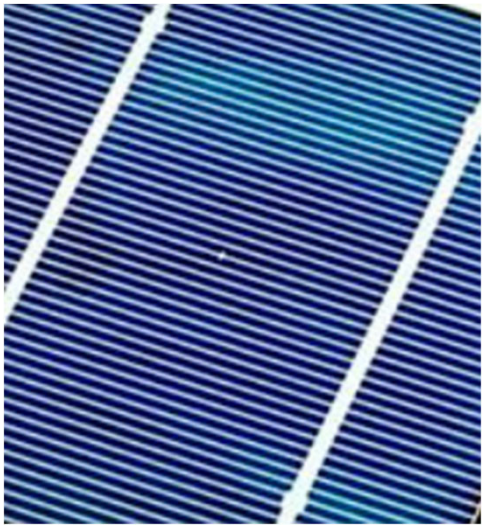
- **Repetition**
- **Examples and Training**
- **Identifying open questions**
- **Preparation for the Exam**
- **(Potential exam question will be given)**

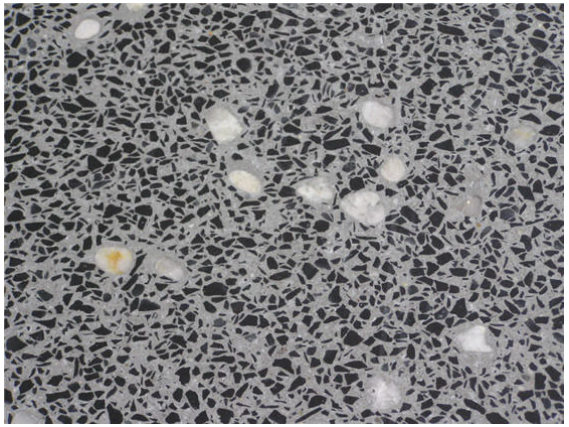
Exam

Written exam on November 20.
Similar to other written exams.

Solid materials

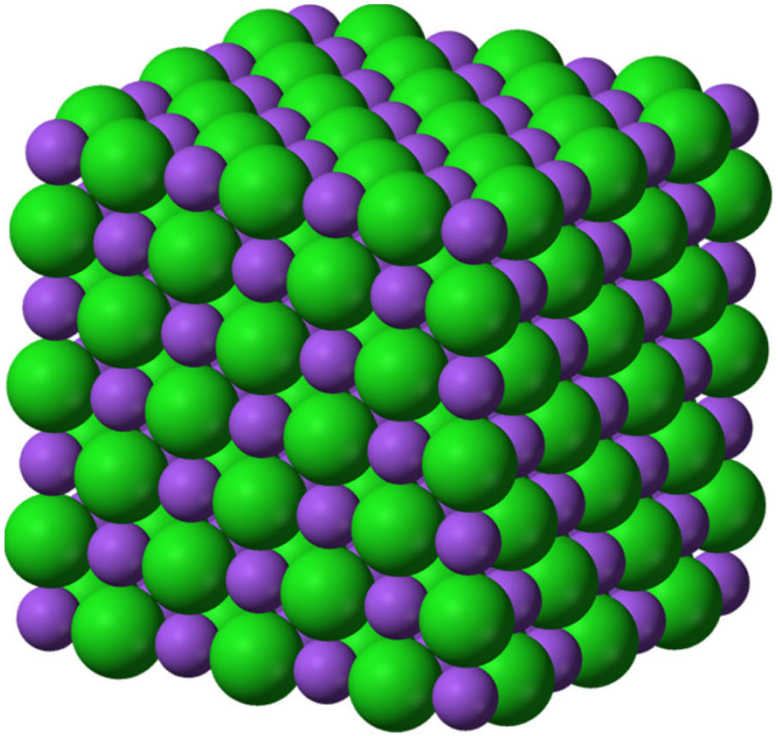
Metals and alloys
Plastics
Ceramics
Biological materials
Composite materials



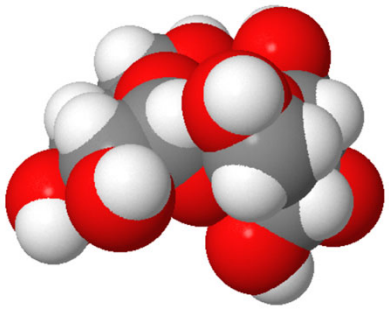


Crystal structure

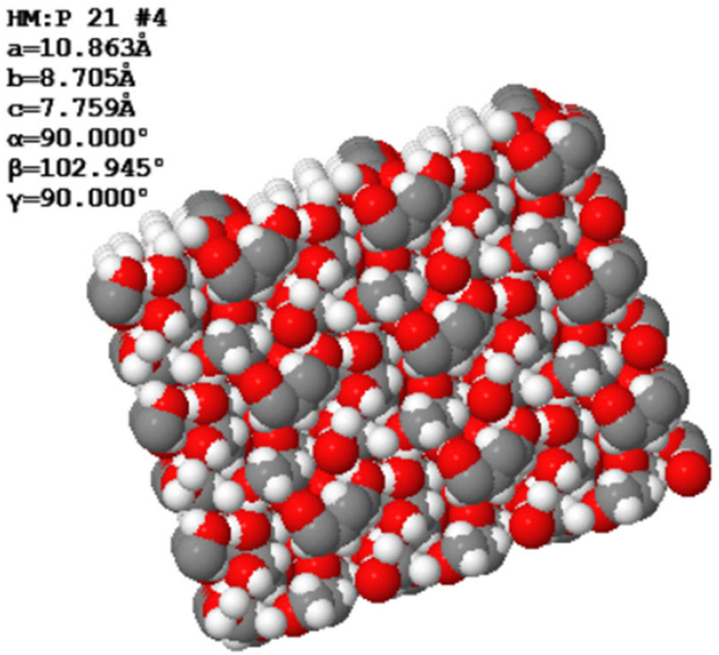
A crystal is a three dimensional periodic arrangement of atoms.



Sugar (Sucrose)

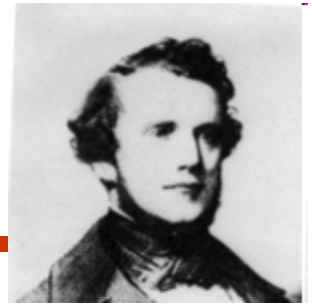


basis

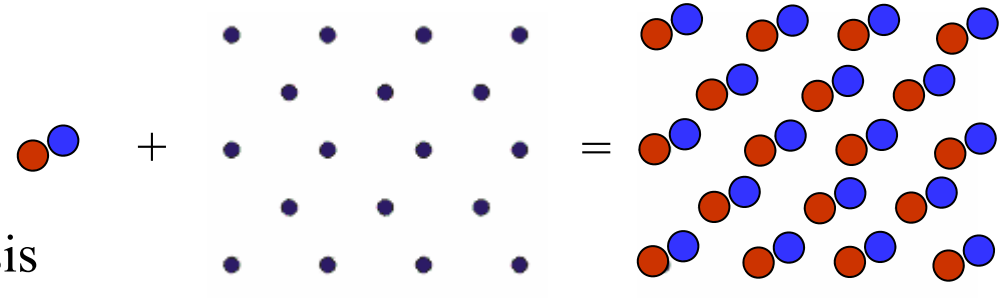


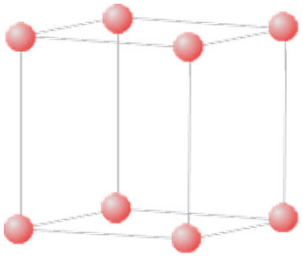
crystal

Bravais lattice

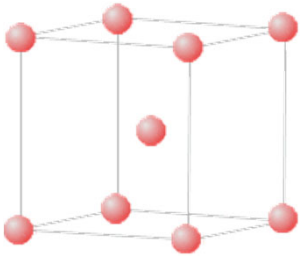


Auguste Bravais

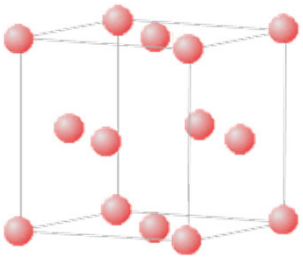




simple cubic



body centered cubic, bcc

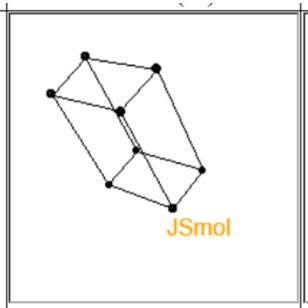
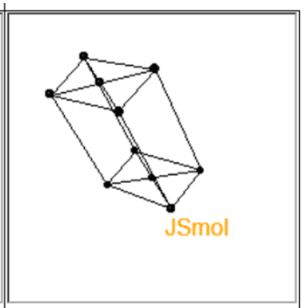
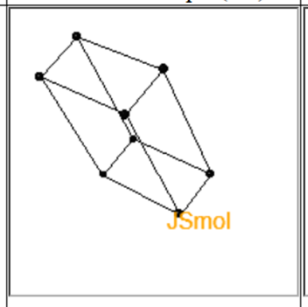
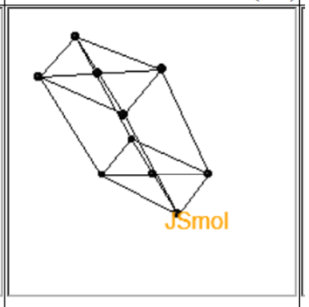
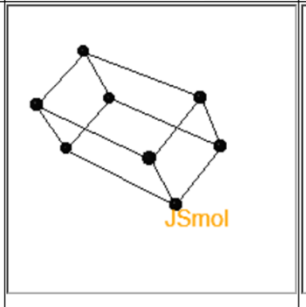
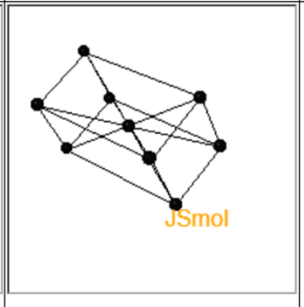
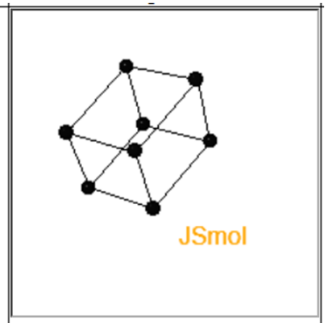


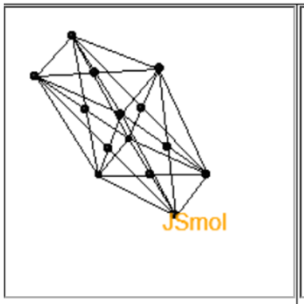
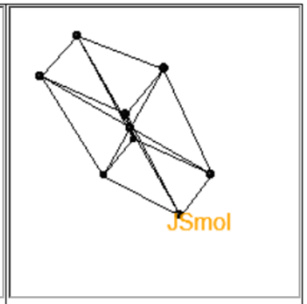
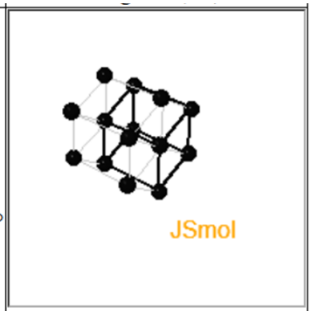
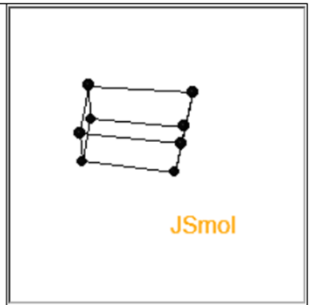
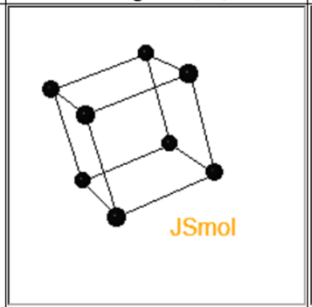
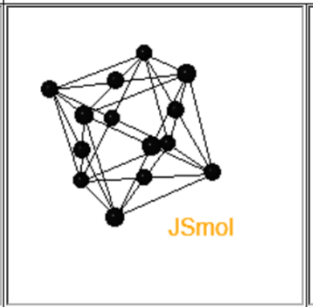
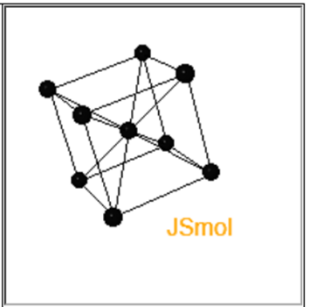
face centered cubic, fcc

14 Bravais lattices

Points of a Bravais lattice do not necessarily represent atoms.

P … primitive
I … body centered
F … face centered
S … centered
R … Rhombohedral

Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$ $\beta = \gamma = 90°$	 Monoclinic simple (mP)	 Monoclinic Base centered (mS)
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	 Orthorhombic simple (oP)	 Base centered (oS)
Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90°$	 Simple (tP)	 Body centered (tI)
Trigonal $a = b = c$ $\alpha = \beta = \gamma \neq 90°$	 Trigonal (hR)	

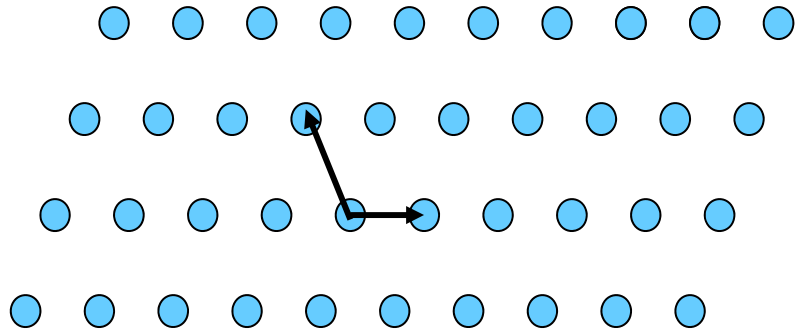
	 Face centered (oF)	 Body centered (oI)
Hexagonal $a = b \neq c$ $\alpha = 120°, \beta = \gamma = 90°$	 Hexagonal (hP)	
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	 Triclinic (aP)	
Cubic $a = b = c$ $\alpha = \beta = \gamma = 90°$	 Simple (cP)	 Face centered (cF)
		 Body centered (cI)

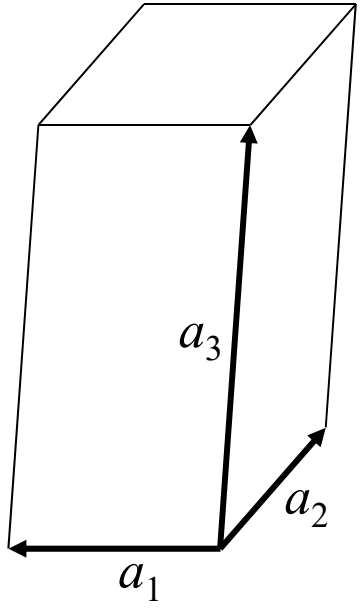
Primitive lattice vectors

Every point of a Bravais lattice can be reached from another point on the lattice by a translation vector

Translation vector

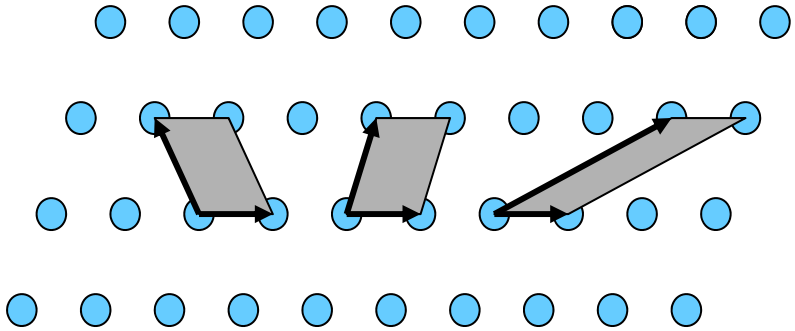
$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$



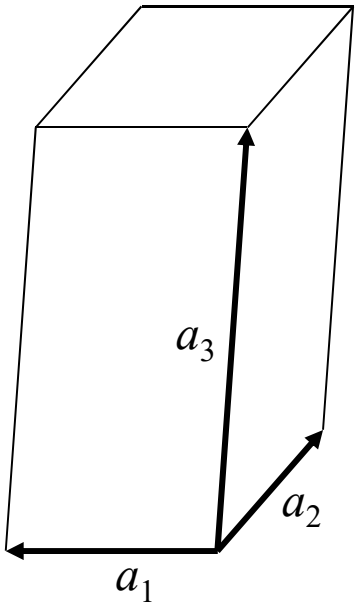


Primitive lattice vectors

Primitive Unit Cell



There is more than one choice for a primitive unit cell



volume of a unit cell =

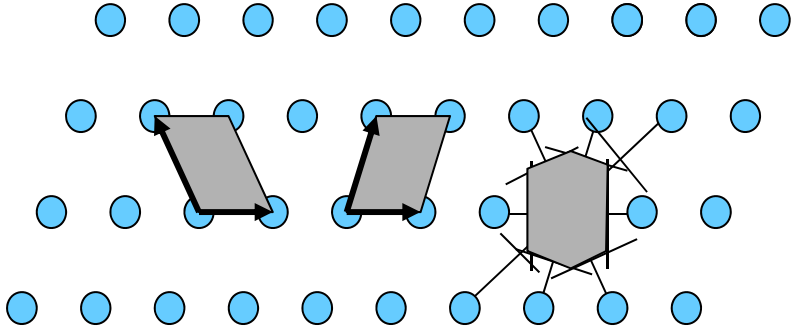
$$|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad n_1, n_2, n_3 = \cdots -2, -1, 0, 1, 2, \cdots$$

There is one primitive unit cell per Bravais lattice point.

Unit Cells

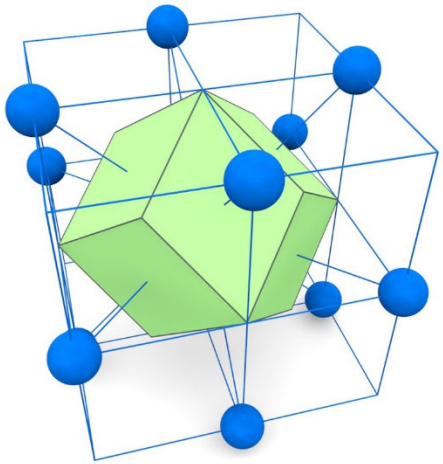
There is more than one choice for a primitive unit cell



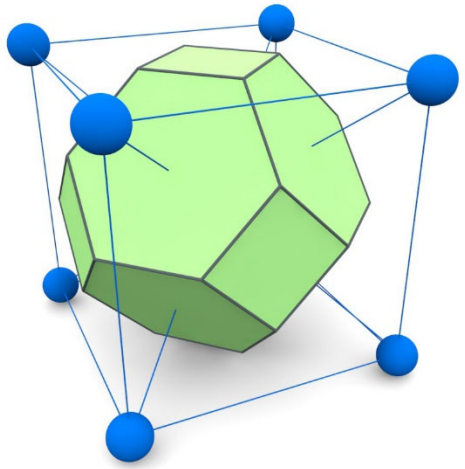
Eugene Wigner

Frederick Seitz

Wigner-Seitz primitive unit cell

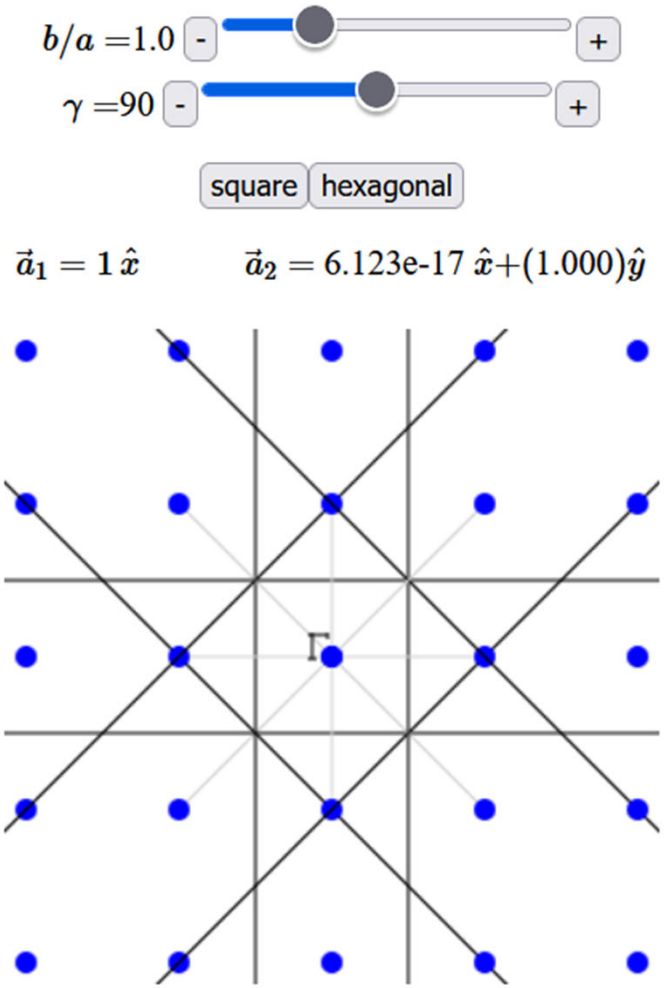


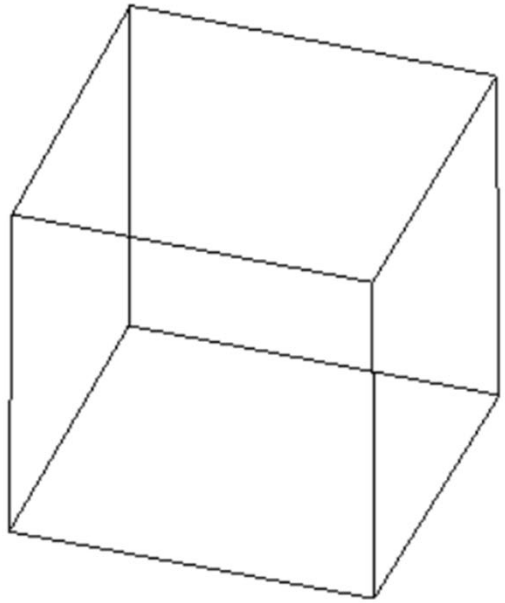
fcc



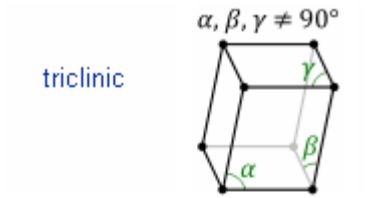
bcc

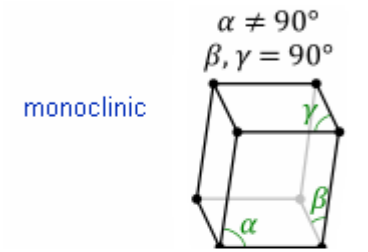
Wigner-Seitz cells

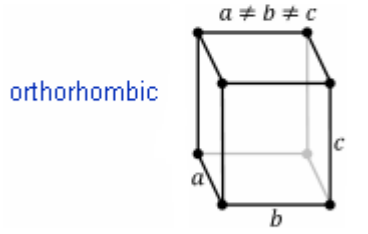


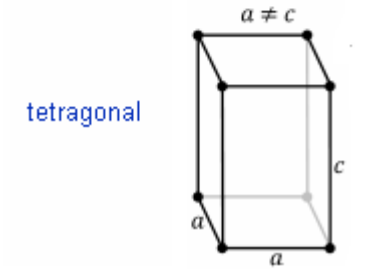


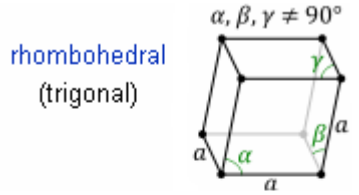
Conventional (crystallographic) unit cell

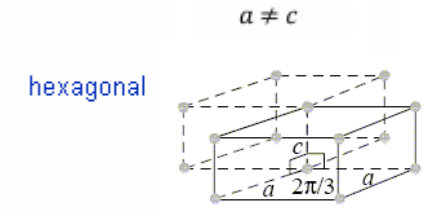


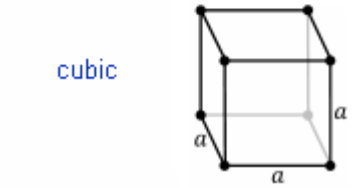












α is the angle between *b* and *c*
β is the angle between *a* and *c*
γ is the angle between *a* and *b*

6 faces, 8 corners

http://en.wikipedia.org/wiki/Bravais_lattice

Symmetries

$$\mathbf{E} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{i} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Identity Inversion

$$\mathbf{C_4} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{C_{4i}} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad \sigma_{\mathbf{h}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Rotation Rotoinversion Reflection

Symmetries form Groups

$$\mathbf{E} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{i} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\mathbf{E} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{C_4} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{C_2} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{C_4^3} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Point group symmetries can be represented by matrices.
All such matrices that bring the crystal into itself form the group of the crystal.

$AB \in G$ for $A, B \in \mathbf{G}$

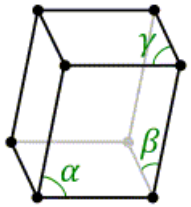
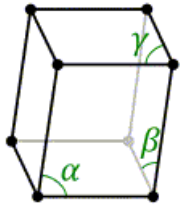
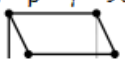
32 point groups (one point remains fixed during transformation)
230 space groups

Space Group → Bravais lattice

ıely determines the Bravais lattice.

Space Group	Bravais lattice
1	Triclinic
2	Triclinic
3	Simple Monoclinic
4	Simple Monoclinic
5	Base-Centered Monoclinic
6	Simple Monoclinic
7	Simple Monoclinic
8	Base-Centered Monoclinic
9	Base-Centered Monoclinic
10	Simple Monoclinic
11	Simple Monoclinic
12	Base-Centered Monoclinic
13	Simple Monoclinic
14	Simple Monoclinic
15	Base-Centered Monoclinic
16	Simple Orthorhombic
17	Simple Orthorhombic
18	Simple Orthorhombic
19	Simple Orthorhombic
20	Base-Centered Orthorhombic
21	Base-Centered Orthorhombic
22	Face-Centered Orthorhombic
23	Body-Centered Orthorhombic
24	Body-Centered Orthorhombic
25	Simple Orthorhombic
26	Simple Orthorhombic
27	Simple Orthorhombic
28	Simple Orthorhombic

The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: P$\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2_1, 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$2/m$	C_{2h}	10: P2/m, 11: P2_1/m, 12: C2/m, 13: P2/c, 14: P2_1/c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222_1, 18: P2_12_12, 19: P$2_12_12_1$, 20: C222_1, 21: C222, 22: F222, 23: I222, 24: I$2_12_12_1$	3	-	-	-	-	n		4

Physical properties exhibit crystal symmetries

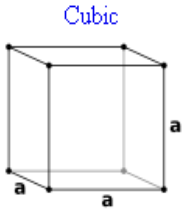
Electrical conductivity
Thermal conductivity
Dielectic constant
Magnetic susceptibility
Thermal expansion
Piezoelectricity
Piezoconductivity

Cubic crystals

All second rank tensors of cubic crystals reduce to constants

Electrical conductivity, thermal conductivity, electric susceptibility, magnetic susceptibility, Peltier effect (heat current due to electrical current), Seebeck effect (Electric field due to thermal gradient)

216: ZnS, GaAs, GaP, InAs, SiC
221: CsCl, cubic perovskite
225: Al, Cu, Ni, Ag, Pt, Au, Pb, NaCl
227: C, Si, Ge, spinel
229: Na, K, Cr, Fe, Nb, Mo, Ta



23	T	195-199		12
$m3$	T_h	200-206		24
432	O	207-214		24
$\bar{4}3m$	T_d	215-220	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
$m3m$	O_h	221-230	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ-Fe, NaCl 227: diamond, C, Si,	48

$$\begin{bmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{bmatrix}$$

Material	ρ (Ω•m) at 20 °C	σ (S/m) at 20 °C	Temperature coefficient[note 1] (K^{-1})	Reference
Silver	1.59×10^{-8}	6.30×10^{7}	0.0038	[7][8]
Copper	1.68×10^{-8}	5.96×10^{7}	0.0039	[8]
Annealed copper[note 2]	1.72×10^{-8}	5.80×10^{7}		[*citation needed*]
Gold[note 3]	2.44×10^{-8}	4.10×10^{7}	0.0034	[7]
Aluminium[note 4]	2.82×10^{-8}	3.5×10^{7}	0.0039	[7]
Calcium	3.36×10^{-8}	2.98×10^{7}	0.0041	
Tungsten	5.60×10^{-8}	1.79×10^{7}	0.0045	[7]
Zinc	5.90×10^{-8}	1.69×10^{7}	0.0037	[9]
Nickel	6.99×10^{-8}	1.43×10^{7}	0.006	
Lithium	9.28×10^{-8}	1.08×10^{7}	0.006	
Iron	1.0×10^{-7}	1.00×10^{7}	0.005	[7]
Platinum	1.06×10^{-7}	9.43×10^{6}	0.00392	[7]
Tin	1.09×10^{-7}	9.17×10^{6}	0.0045	
Carbon steel (1010)	1.43×10^{-7}	6.99×10^{6}		[10]
Lead	2.2×10^{-7}	4.55×10^{6}	0.0039	[7]
Titanium	4.20×10^{-7}	2.38×10^{6}	X	
Grain oriented electrical steel	4.60×10^{-7}	2.17×10^{6}		[11]
Manganin	4.82×10^{-7}	2.07×10^{6}	0.000002	[12]
Constantan	4.9×10^{-7}	2.04×10^{6}	0.000008	[13]
Stainless steel[note 5]	6.9×10^{-7}	1.45×10^{6}		[14]
Mercury	9.8×10^{-7}	1.02×10^{6}	0.0009	[12]
Nichrome[note 6]	1.10×10^{-6}	9.09×10^{5}	0.0004	[7]
GaAs	5×10^{-7} to 10×10^{-3}	5×10^{-8} to 10^{3}		[15]
Carbon (amorphous)	5×10^{-4} to 8×10^{-4}	1.25 to 2×10^{3}	−0.0005	[7][16]
Carbon (graphite)[note 7]	$2.5e\times10^{-6}$ to 5.0×10^{-6} //basal plane 3.0×10^{-3} ⊥basal plane	2 to 3×10^{5} //basal plane 3.3×10^{2} ⊥basal plane		[17]
Carbon (diamond)[note 8]	1×10^{12}	$\sim10^{-13}$		[18]
Germanium[note 8]	4.6×10^{-1}	2.17	−0.048	[7][8]
Sea water[note 9]	2×10^{-1}	4.8		[19]
[note 10]				[*citation needed*]

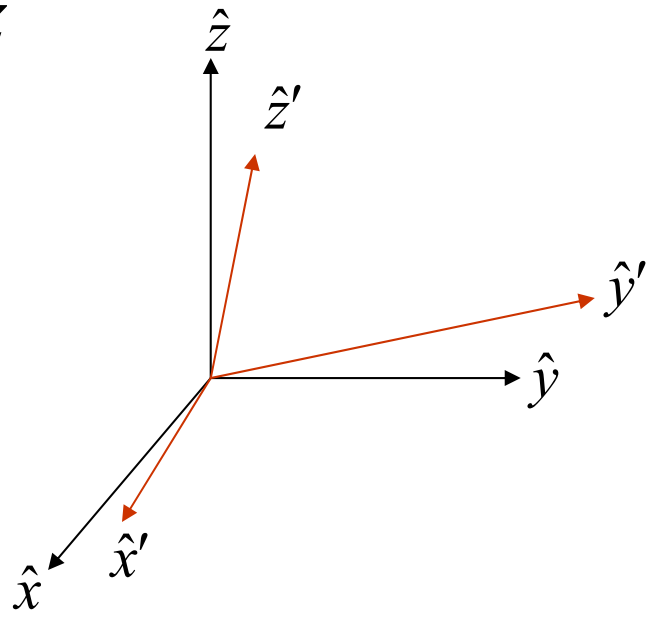
Strain

A distortion of a material is described by the strain matrix

$$x' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$

$$y' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$

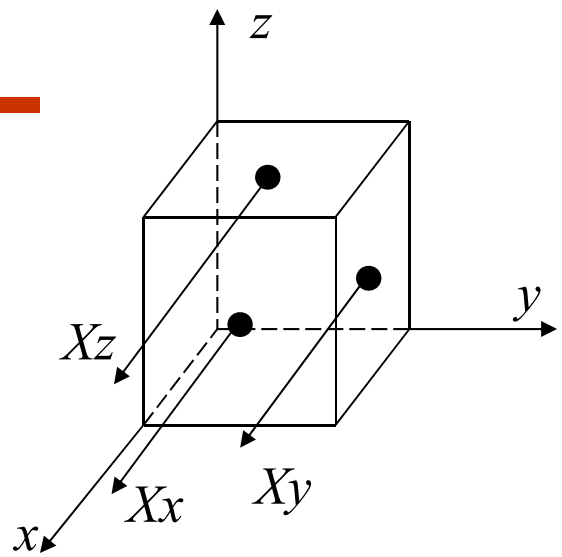
$$z' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$



Stress

9 forces describe the stress

Xx, Xy, Xz, Yx, Yy, Yz, Zx, Zy, Zz



Xx is a force applied in the *x*-direction to the plane normal to *x*

Xy is a sheer force applied in the *x*-direction to the plane normal to *y*

stress tensor:

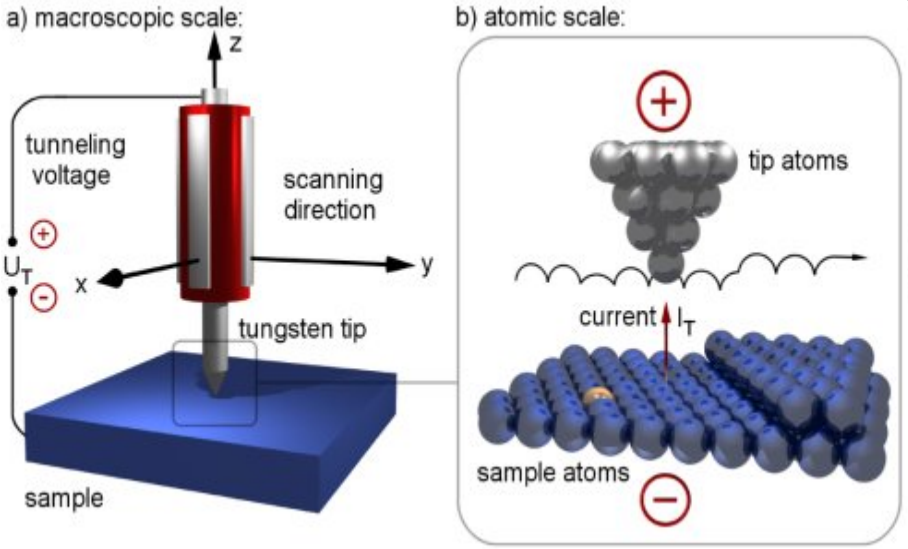
$$\sigma = \begin{bmatrix} \frac{X_x}{A_x} & \frac{X_y}{A_y} & \frac{X_z}{A_z} \\ \frac{Y_x}{A_x} & \frac{Y_y}{A_y} & \frac{Y_z}{A_z} \\ \frac{Z_x}{A_x} & \frac{Z_y}{A_y} & \frac{Z_z}{A_z} \end{bmatrix}$$

Stress is force/m^2

Piezoelectricity (rank 3 tensor)

AFM's, STM's
Quartz crystal oscillators
Surface acoustic wave generators
Pressure sensors - Epcos
Fuel injectors - Bosch
Inkjet printers

No inversion symmetry



lead zirconate titanate ($Pb[Zr_xTi_{1-x}]O_3$ $0<x<1$)
—more commonly known as PZT
barium titanate ($BaTiO_3$)
lead titanate ($PbTiO_3$)
potassium niobate ($KNbO_3$)
lithium niobate ($LiNbO_3$)
lithium tantalate ($LiTaO_3$)
sodium tungstate (Na_2WO_3)
$Ba_2NaNb_5O_5$
$Pb_2KNb_5O_{15}$

Piezoelectric crystal classes: 1, 2, m, 222, mm2, 4, -4, 422, 4mm, -42m, 3, 32, 3m, 6, -6, 622, 6mm, -62m, 23, -43m

International Tables for Crystallography
Volume A: Space-group symmetry

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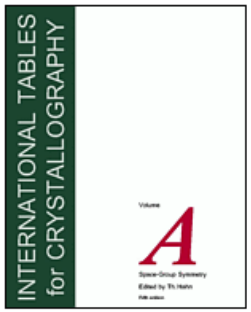
Edited by Th. Hahn



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10 (P 2/m)
11 (P 21/m)
12 (C 2/m)
13 (P 2/c)
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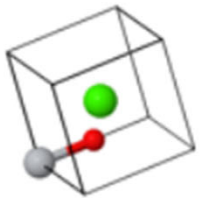
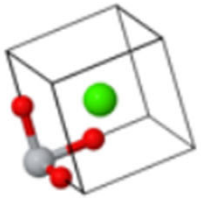
- extensive subgroup and supergroup data.

Parts 8 to 15 deal with the following aspects of symmetry theory: the mathematical approach to space groups; crystal lattices; point groups and crystal classes; symbols for symmetry operations; symbols for space groups; isomorphic subgroups of space groups; lattice complexes; and normalizers of space groups.

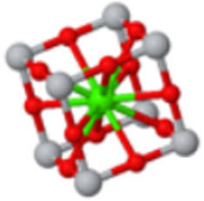
Asymmetric unit



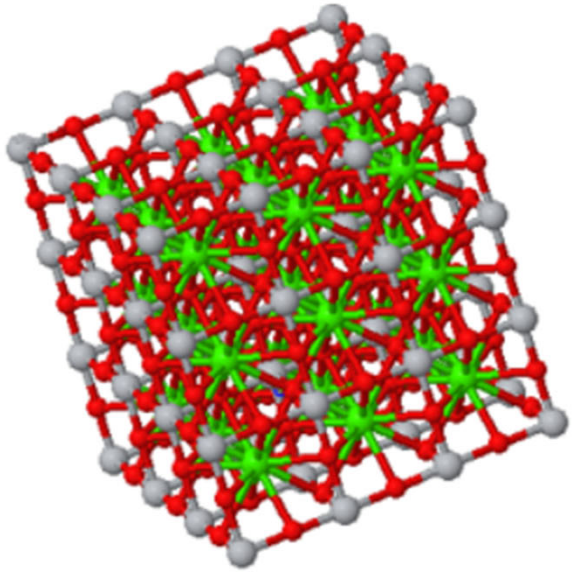
Asymmetric unit



Primitive unit cell



Conventional unit cell

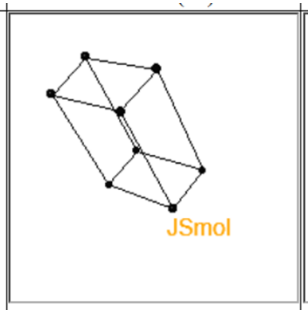
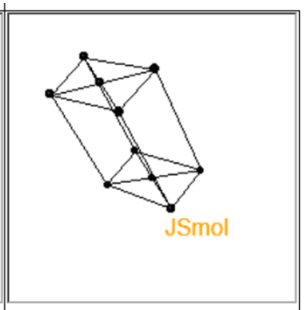
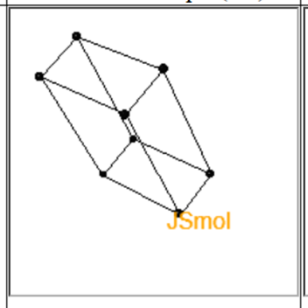
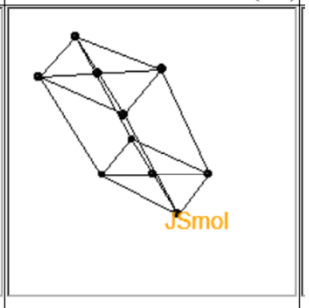
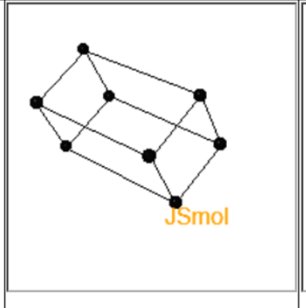
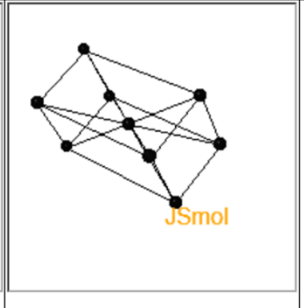
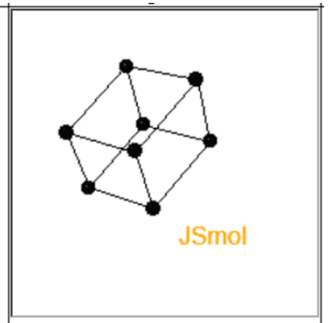


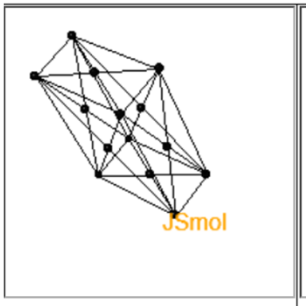
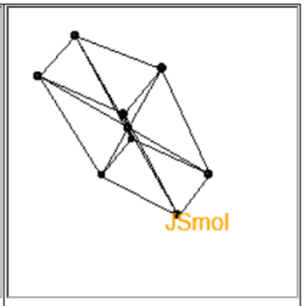
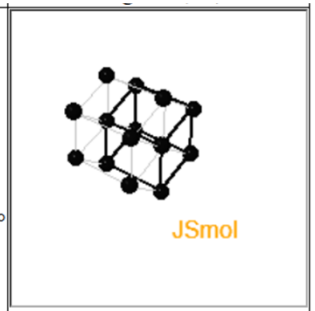
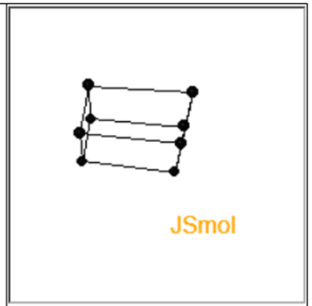
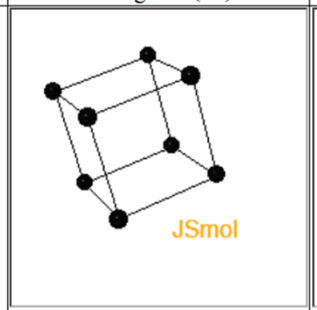
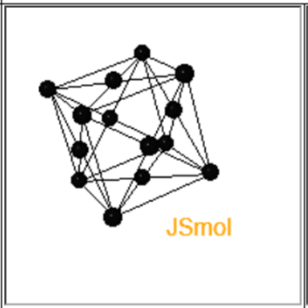
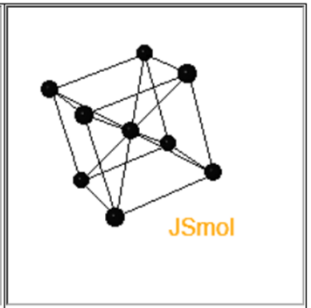
Crystal

14 Bravais lattices

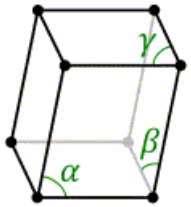
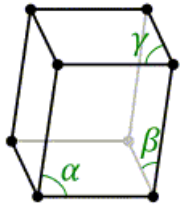
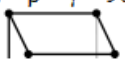
Points of a Bravais lattice do not necessarily represent atoms.

P … primitive
I … body centered
F … face centered
A,C … centered
R … Rhombohedral

Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$ $\beta = \gamma = 90°$	 Monoclinic simple (mP)	 Monoclinic Base centered (mS)
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	 Orthorhombic simple (oP)	 Base centered (oS)
Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90°$	 Simple (tP)	 Body centered (tI)
Trigonal $a = b = c$ $\alpha = \beta = \gamma \neq 90°$	 Trigonal (hR)	

	 Face centered (oF)	 Body centered (oI)
Hexagonal $a = b \neq c$ $\alpha = 120°, \beta = \gamma = 90°$	 Hexagonal (hP)	
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	 Triclinic (aP)	
Cubic $a = b = c$ $\alpha = \beta = \gamma = 90°$	 Simple (cP)	 Face centered (cF)
		 Body centered (cI)

The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	triclinic-pedial	1	C_1	1: P1	-	-	-	-	-	n		1
	triclinic-pinacoidal	$\bar{1}$	$S_2 = C_i$	2: P$\bar{1}$	-	-	-	-	-	y		2
Monoclinic $a \neq b \neq c$ $\alpha \neq 90°$, $\beta = \gamma = 90°$ 	monoclinic-sphenoidal	2	C_2	3: P2, 4: P2_1, 5: C2	1	-	-	-	-	n		2
	monoclinic-domatic	m	$C_{1h} = C_s$	6: Pm, 7: Pc, 8: Cm, 9: Cc	-	-	-	-	1	n		2
	monoclinic-prismatic	$2/m$	C_{2h}	10: P2/m, 11: P2_1/m, 12: C2/m, 13: P2/c, 14: P2_1/c, 15: C2/c	1	-	-	-	1	y		4
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ 	orthorhombic-disphenoidal	222	$V = D_2$	16: P222, 17: P222_1, 18: P2_12_12, 19: P$2_12_12_1$, 20: C222_1, 21: C222, 22: F222, 23: I222, 24: I$2_12_12_1$	3	-	-	-	-	n		4

Space Group → Bravais lattice

ıely determines the Bravais lattice.

Space Group	Bravais lattice
1	Triclinic
2	Triclinic
3	Simple Monoclinic
4	Simple Monoclinic
5	Base-Centered Monoclinic
6	Simple Monoclinic
7	Simple Monoclinic
8	Base-Centered Monoclinic
9	Base-Centered Monoclinic
10	Simple Monoclinic
11	Simple Monoclinic
12	Base-Centered Monoclinic
13	Simple Monoclinic
14	Simple Monoclinic
15	Base-Centered Monoclinic
16	Simple Orthorhombic
17	Simple Orthorhombic
18	Simple Orthorhombic
19	Simple Orthorhombic
20	Base-Centered Orthorhombic
21	Base-Centered Orthorhombic
22	Face-Centered Orthorhombic
23	Body-Centered Orthorhombic
24	Body-Centered Orthorhombic
25	Simple Orthorhombic
26	Simple Orthorhombic
27	Simple Orthorhombic
28	Simple Orthorhombic

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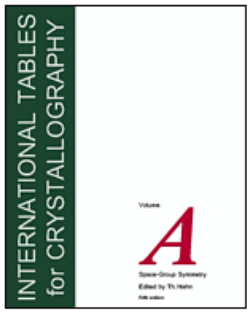

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4 (P 21)
5 (C 2)
6 (P m)
7 (P c)
8 (C m)
9 (C c)
10 (P 2/m)
11 (P 21/m)
12 (C 2/m)
13 (P 2/c)
14 (P 21/c)
15 (C 2/c)
16 (P 2 2 2)
17 (P 2 2 21)
18 (P 21 21 2)
19 (P 21 21 21)
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- general and special positions with multiplicities, site symmetries, coordinates and re
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- extensive subgroup and supergroup data.

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