SYMMETRY OF CRYSTALS

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The ability of a body to coincide with itself in its different positions regarding a coordinate system is called its symmetry. This property reveals itself in iteration of the parts of the body in space. The iteration may be done by reflection in mirror planes, rotation about certain axes, inversions and translations. These actions are called the symmetry operations. The planes, axes, points, etc., are known as symmetry elements. Essentially, mirror reflection is the only truly primitive symmetry operation. All other operations may be done by a sequence of reflections in certain mirror planes. Hence, the mirror plane is the only true basic symmetry element. But for clarity, it is convenient to use the other symmetry operations, and accordingly, the other aforementioned symmetry elements. The symmetry elements and operations are presented in Table 1.

The entire set of symmetry elements of a body is called its symmetry class. There are thirty-two symmetry classes that describe all crystals which have ever been noted in mineralogy or been synthesized (more than 150,000). The denominations and symbols of the symmetry classes are presented in Table 2.

There are several known approaches to classification of individual crystals in accordance with their symmetry and crystallochemistry. The particles which form a crystal are distributed in certain points in space. These points are separated by certain distances (translations) equal to each other in any chosen direction in the crystal. Crystal lattice is a diagram that describes the location of particles (individual or groups) in a crystal. The lattice parameters are three non-coplanar translations that form the crystal lattice. Three basic translations form the unit cell of a crystal. August Bravais (1848) has shown that all possible crystal lattice structures belong to one or another of fourteen lattice types (Bravais lattices). The Bravais lattices, both primitive and non-primitive, are the contents of Table 3.

Among the three-dimensional figures, there is a group of polyhedrons that are called regular, which have all faces of the same shape and all edges of the same size (regular polygons). It has been shown that there are only five regular polyhedrons. Because of their importance in crystallography and solid state physics, a brief description of these polyhedrons is included in Table 4.

The systematic description of crystal structures is presented primarily in the well known *Structurbericht*. The classification of crystals by the Structurbericht does not reflect their crystal class, the Bravais lattice, but is based on the crystallochemical type. This makes it inconvenient to use the Structurbericht categories for comparison of some individual crystals. Thus, there have been several attempts to provide a more convenient classification of crystals. Table 5 presents a compilation of different classifications which allows the reader to correlate the Structurbericht type with the international and Schoenflies point and space groups and with Pearson's symbols, based on the Bravais lattice and chemical composition of the class prototype. The information included in Table 5 has been chosen as an introduction to a more detailed crystallophysical and crystallochemical description of solids.

TABLE 1. Symmetry Operations and Elements

	Symmetry element			
		Symbol		
Symmetry operation	**Name**	**International (Hermann-Mauguin)**	**Schoenflies**	**Presentation on the stereographic projection** Parallel / Perpendicular
Reflection in a plane	Plane	m	C_s	
Rotation by angle $\alpha = 360°/n$ about an axis	Axis	n = 1, 2, 3, 4 or 6	C_n	
		n = 2	C_2	
		n = 3	C_3	
		n = 4	C_4	
		n = 6	C_6	
Rotation about an axis and inversion in a symmetry center lying on the axis	Inversion (improper) axis	$\bar{n} = \bar{3}, \bar{4}, \bar{6}$	C_{ni}	
		$\bar{n} = \bar{3}$	C_{3i}	
		$\bar{n} = \bar{4}$	C_{4i}	

TABLE 1. Symmetry Operations and Elements

Symmetry operation	Symmetry element: Name	Symbol: International (Hermann-Mauguin)	Symbol: Schoenflies	Presentation on the stereographic projection: Parallel	Perpendicular
		$\tilde{n} = \bar{6}$	C_{6i}		
Inversion in a point	Center	$\bar{1}$	C_i		
Parallel translation	Translation vector $\vec{a}, \vec{b}, \vec{c}$				
Reflection in a plane and translation parallel to the plane	Glide–plane	a, b, c, n, d			
Rotation about an axis and translation parallel to the axis	Screw axis	n_m ($m = 1, 2, .., n - 1$)			
Rotation about an axis and reflection in a plane perpendicular to the axis	Rotatory-reflection axis	$\tilde{n}$ $\tilde{n} = \tilde{1}, \tilde{2}, \tilde{3}, \tilde{4}, \tilde{6}$	S_n		

TABLE 2. The Thirty-Two Symmetry Classes

Crystal symbol	Class name[a] and its symbol – International (Int) and Schoenflies (Sch): Primitive Int	Primitive Sch	Central Int	Central Sch	Planal Int	Planal Sch	Axial Int	Axial Sch	Plane-axial Int	Plane-axial Sch	Inversion primitive Int	Inversion primitive Sch	Inversion-planal Int	Inversion-planal Sch
Triclinic	1	C_1	$\bar{1}$	C_i										
Monoclinic					m	C_s	2	C_2	2/m	C_{2h}				
Ortho-rhombic					mm2	C_{2v}	222	D_2	mmm	D_{2h}				
Trigonal	3	C_3	$\bar{3}$	C_{3i}	3m	C_{3v}	32	D_3	$\bar{3}$m	C_{3d}				
Tetragonal	4	C_4	4/m	C_{4h}	4mm	C_{4v}	422	D_4	4/mmm	D_{4h}	$\bar{4}$	S_4	$\bar{4}$2m	D_{2d}
Hexagonal	6	C_6	6/m	C_{6h}	6mm	C_{6v}	622	D_6	6/mmm	D_{6h}	$\bar{6}$	C_{3h}	$\bar{6}$m2	D_{3h}
Cubic	23	T	m3	T_h	$\bar{4}$3m	T_d	432	O	m3m	O_h				

[a] Per Fedorov Institute of Crystallography, USSR Academy of Sciences, nomenclature.

TABLE 3. The Fourteen Possible Space Lattices (Bravais Lattices)

Crystal system	Metric category of the system	No. of different lattices in the system	Lattice type[a] (marked by +): P	C	I	F	R	No. of identi-points per unit cell	Characteristic parameters (marked by +): a	b	c	α	β	γ	Description of characteristic parameters a⊂X, b⊂Y, c⊂Z α≡(b,c), β≡(a,c), γ≡(a,b)	Symmetry of the lattice: Int	Sch
Triclinic	Trimetric	1	+					1	+	+	+	+	+	+	$a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$	1	C
Monoclinic	Trimetric	2	+	+				1 or 2	+	+	+		+		$a \neq b \neq c$, $\alpha = \gamma = 90° \neq \beta$	2/m	C_{2h}
Orthorhombic	Trimetric	4	+	+	+	+		1, 2 or 4	+	+	+				$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$	mmm	D_{2h}
Trigonal (rhombohedral)	Dimetric	1					+	1	+			+			$a = b = c$, $120° > \alpha = \beta = \gamma \neq 90°$	3m	D_{3d}
Tetragonal	Dimetric	2	+		+			1 or 2	+		+				$a = b \neq c$, $\alpha = \beta = \gamma = 90°$	4/mmm	D_{4h}
Hexagonal	Dimetric	1	+					1	+		+				$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$	6/mmm	D_{6h}
Isometric (cubic)	Monometric	3	+		+	+		1, 2 or 4	+						$a = b = c$, $\alpha = \beta = \gamma = 90°$	m3m	O_h

[a] Designations of the space-lattice types: P – primitive, C – side-centered (base-centered), I – body-centered, F – face-centered, R – rhombohedral.

TABLE 4. The Five Possible Regular Polyhedrons

Polyhedron	Symmetry (Schoenflies)		Form of faces	Number of[a]		
	Class	Elements		Faces (F)	Edges (E)	Vertices (V)
Tetrahedron	T	$4C_3 3C_2$	Equilateral triangle	4	6	4
Cube (hexahedron)	O	$3C_4 4C_3 6C_2$	Square	6	12	8
Octahedron	O	$3C_4 4C_3 6C_2$	Equilateral triangle	8	12	6
Pentagonal dodecahedron	J	$6C_5 10C_3 15C_2$	Regular pentagon	12	30	20
Icosahedron	J	$6C_5 10C_3 15C_2$	Equilateral triangle	20	30	12

[a] Per formula by Leonhard Euler: F + V − E = 2

TABLE 5. Classification of Crystals

Strukturbericht symbol	Structure name	Symmetry group		Pearson symbol[a]	Standard ASTM E157-82a symbol[b]
		International	Schoenflies		
1	2	3	4	5	6
A1	Cu	Fm3m	O^4_h	cF4	F
A2	W	Im3m	O^9_h	cI2	B
A3	Mg	$P6_3/mmc$	D^4_{6h}	hP2	H
A4	C	Fd3m	O^7_h	cF8	F
A5	Sn	If_1/amd	D^{19}_{4h}	tI4	U
A6	In	I4/mmm	D^{17}_{4h}	tI2	U
A7	As	$R\bar{3}m$	D^5_{3d}	hR2	R
A8	Se	$P3_121$ or $P3_221$	D^4_3 (D^6_3)	hP3	H
A10	Hg	$R\bar{3}m$	D^5_{3d}	hR1	R
A11	Ga	Cmca	D^{18}_{2h}	oC8	Q
A12	α-Mn	$I4\bar{3}m$	T^3_d	cI58	B
A13	β-Mn	$P4_132$	O^7	cP20	C
A15	OW_3	Pm3n	O^3_h	cP8	C
A20	α-U	Cmcm	D^{17}_{2h}	oC4	Q
B1	ClNa	Fm3m	O^5_h	cF8	F
B2	ClCs	Pm3m	O^1_h	cP2	C
B3	SZn	$F\bar{4}3m$	T^2_d	cF8	F
B4	SZn	$P6_3mc$	C^4_{6v}	hP4	H
$B8_1$	AsNi	$P6_3/mmc$	D^4_{6h}	hP4	H
$B8_2$	$InNi_2$	$P6_3/mmc$	D^4_{6h}	hP6	H
B9	HgS	$P3_121$ or $P3_221$	D^4_3 or D^6_3	hP6	H
B10	OPb	P4/nmm	D^7_{4h}	tP4	T
B11	γ-CuTi	P4/nmm	D^7_{4h}	tP4	T
B13	NiS	$R\bar{3}m$	D^5_{3d}	hR6	R
B16	GeS	Pnma	D^{16}_{2h}	oP8	O
B17	PtS	$P4_2/mmc$	D^9_{4h}	tP4	T
B18	CuS	$P6_3/mmc$	D^4_{6h}	hP12	H
B19	AuCd	Pmma	D^5_{2h}	oP4	O
B20	FeSi	$P2_13$	T^4	cP8	C
B27	BFe	Pnma	D^{16}_{2h}	oP8	O
B31	MnP	Pnma	D^{16}_{2h}	oP8	O
B32	NaTl	Fd3m	O^7_h	cF16	F
B34	Pds	$P4_2/m$	C^2_{4h}	tP16	T
B35	CoSn	P6/mmm	D^1_{6h}	hP6	H
B37	SeTl	I4/mcm	D^{18}_{4h}	tI16	U
B_e	CdSb	Pbca	D^{15}_{2h}	oP16	O
B_f (B33)	ξ-BCr	Cmcm	D^{17}_{2h}	oC8	Q
B_g	BMo	$I4_1/amd$	D^{19}_{4h}	tI4	U
B_h	CW	P6m2	D^1_{3h}	hP2	H
B_i	γ′CMo (AsTi)	$P6_3/mmc$	D^4_{6h}	hP8	H
C1	CaF_2	$Fm\bar{3}m$	O^5_h	cF12	F
$C1_b$	AgAsMg	$F\bar{4}3m$	T^2_d	cF12	F
C2	FeS_2	Pa3	T^6_h	cP12	C

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Strukturbericht symbol	Structure name	Symmetry group		Pearson symbol[a]	Standard ASTM E157-82a symbol[b]
		International	Schoenflies		
1	2	3	4	5	6
C3	Cu_2O	Pn3m	O^4_h	cP6	C
C4	O_2Ti	$P4_2/mnm$	D^{14}_{4h}	tP6	T
C6	CdI_2	P3m1	D^3_{3d}	hP3	H
C7	MoS_2	$P6_3/mmc$	D^4_{6h}	hP6	H
$C11_a$	C_2Ca	I4/mmm	D^{17}_{4h}	tI6	U
$C11_b$	$MoSi_2$	I4/mmm	D^{17}_{4h}	tI6	U
C12	$CaSi_2$	$R\bar{3}m$	D^5_{3d}	hR6	R
C14	$MgZn_2$	$P6_3/mmc$	D^4_{6h}	hP12	H
C15	Cu_2Mg	Fd3m	O^7_h	cF24	F
$C15_b$	$AuBe_5$	$F\bar{4}3m$ or F23	T^2_d or T^2	cF24	F
C16	Al_2Cu	I4/mcm	D^{18}_{4h}	tI12	U
C18	FeS_2	Pnnm	D^{12}_{2h}	oP6	O
C19	$CdCl_2$	$R\bar{3}m$	D^5_{3d}	hR3	R
C22	Fe_2P	$P2\bar{6}m$	D^1_{3h}	hP9	H
C23	Cl_2Pb	Pnma	D^{16}_{2h}	oP12	O
C32	AlB_2	P6/mmm	D^1_{6h}	hP3	H
C33	Bi_2STe_2	$R\bar{3}m$	D^5_{3d}	hR5	R
C34	$AuTe_2$	C2/m (P2/m)	C^3_{2h} (C^1_{2h})	mC6	N
C36	$MgNi_2$	$P6_3/mmc$	D^4_{6h}	hP24	H
C38	Cu_2Sb	P4/nmm	D^7_{4h}	tP6	T
C40	$CrSi_2$	$P6_222$	D^4_6	hP9	H
C42	SiS_2	Ibam	D^{26}_{2h}	oI12	P
C44	GeS_2	Fdd2	C^{19}_{2v}	oF72	S
C46	$AuTe_2$	Pma2	C^4_{2v}	oP24	O
C49	Si_2Zr	Cmcm	D^{17}_{2h}	oC12	Q
C54	Si_2Ti	Fddd	D^{24}_{2h}	oF24	S
C_c	Si_2Th	$I4_1/amd$	D^{19}_{4h}	tI12	U
C_e	$CoGe_2$	Aba2	C^{17}_{2v}	oC23	Q
DO_2	As_3Co	Im3	T^5_h	cI32	B
DO_3	BiF_3	Fm3m	O^5_h	cF16	F
DO_9	O_3Re	Pm3m	O^1_h	cP4	C
DO_{11}	CFe_3	Pnma	D^{16}_{2h}	oP16	O
DO_{18}	$AsNa_3$	$P6_3/mmc$	D^4_{6h}	hP8	H
DO_{19}	Ni_3Sn	$P6_3/mmc$	D^4_{6h}	hP8	H
DO_{20}	Al_3Ni	Pnma	D^{16}_{2h}	oP16	O
DO_{21}	Cu_3P	$P\bar{3}c1$	D^4_{3d}	hP24	H
DO_{22}	Cu_3P	I4/mmm	D^{17}_{4h}	tI8	U
DO_{23}	Al_3Zr	I4/mmm	D^{17}_{4h}	tI16	U
DO_{24}	Ni_3Ti	$P6_3/mmc$	D^4_{6h}	hP16	H
DO_c	SiU_3	I4/mcm	D^{18}_{4h}	tI16	U
DO_e	Ni_3P	$I\bar{4}$	S^2_4	tI32	U
$D1_3$	Al_4Ba	I4/mmm	D^{17}_{4h}	tI10	U
$D1_a$	$MoNi_4$	I4/m	C^5_{4h}	tI10	U
$D1_b$	Al_4U	Imma	D^{28}_{2h}	oI20	P
$D1_c$	$PtSn_4$	Aba2	C^{17}_{2v}	oC20	Q
$D1_e$	B_4Th	P4/mbm	D^5_{4h}	tP20	T
$D1_f$	BMn_4	Fddd	D^{24}_{2h}	oF40	S
$D2_1$	B_6Ca	Pm3m	O^1_h	cP7	C
$D2_3$	$NaZn_{13}$	Fm3m	O^5_h	cF112	F
$D2_b$	$Mn_{12}Th$	I4/mmm	D^{17}_{4h}	tI26	U
$D2_c$	MnU_6	I4/mcm	D^{18}_{4h}	tI28	U
$D2_d$	$CaCu_5$	P6/mmm	D^1_{6h}	hP6	H
$D2_f$	$B_{12}U$	Fm3m	O^5_h	cF52	F
$D2_h$	Al_6Mn	Cmcm	D^{17}_{2h}	oC28	Q
$D5_1$	α-Al_2O_3	R3c	D^6_{3d}	hR10	R
$D5_2$	La_2O_3	$P\bar{3}m1$	D^3_{3d}	hP5	H
$D5_3$	Mn_2O_3	Ia3	T^7_h	cI80	B

TABLE 5. Classification of Crystals

Strukturbericht symbol	Structure name	Symmetry group		Pearson symbol[a]	Standard ASTM E157-82a symbol[b]
		International	Schoenflies		
1	2	3	4	5	6
$D5_8$	S_3Sb_2	Pnma	D^{16}_{2h}	oP20	O
$D5_9$	P_2Zn_3	$P4_2/mmc$	D^{9}_{4h}	tP40	T
$D5_{10}$	C_2C_3	Pnma	D^{16}_{2h}	oP20	O
$D5_{13}$	Al_3Ni_2	$P\bar{3}m1$	D^{3}_{3d}	hP5	H
$D5_a$	Si_2U_3	P4/mbm	D^{5}_{4h}	tP10	T
$D5_c$	C_3Pu_2	$I\bar{4}3d$	T^{6}_{d}	cI40	B
$D7_1$	Al_4C_3	$R\bar{3}m$	D^{5}_{3d}	hR7	R
$D7_3$	P_4Th_3	$I\bar{4}3d$	T^{6}_{d}	cI28	B
$D7_b$	B_4Ta_3	Immm	D^{25}_{2h}	oI14	P
$D8_1$	Fe_3Zn_{10}	Im3m	O^{9}_{h}	cI52	B
$D8_2$	Cu_5Zn_8	$I\bar{4}3m$	T^{3}_{d}	cI52	B
$D8_3$	Al_4Cu_9	P43m	T^{1}_{d}	cP52	C
$D8_4$	C_6Cr23	Fm3m	O^{5}_{h}	cF116	F
$D8_5$	Fe_7W_6	$R\bar{3}m$	D^{5}_{3d}	hR13	R
$D8_6$	$Cu_{15}Si_4$	$I\bar{4}3m$	T^{3}_{d}	cI76	B
$D8_8$	Mn_5Si_3	$P6_3/mcm$	D^{3}_{6h}	hP16	H
$D8_9$	Co_9S_8	Fm3m	O^{5}_{h}	cF68	F
$D8_{10}$	Al_8Cr_5	R3m	C^{5}_{3v}	hR26	R
$D8_{11}$	Al_5Co_2	$P6_3/mcm$	D^{3}_{6h}	hP28	H
$D8_a$	$Mn_{23}Th_6$	Fm3m	O^{5}_{h}	cF116	F
$D8_b$	σ-phase of Cr-Fe	$p\bar{4}_2/mnm$	D^{14}_{4h}	tP30	T
$D8_e$	$(Al,Zn)_{49}Mg_{32}$	Im3	T^{5}_{h}	cI162	B
$D8_f$	Ge_7Ir_3	Im3m	O^{9}_{h}	cI40	B
$D8_h$	B_5W_2	$P6_3/mmc$	D^{4}_{6h}	hP14	H
$D8_i$	B_5Mo_2	$R\bar{3}m$	D^{5}_{3d}	hR7	R
$D8_l$	B_3Cr_5	I4/mcm	D^{18}_{4h}	tI32	U
$D8_m$	Si_3W_5	I4/mcm	D^{18}_{4h}	tI32	U
$D10_1$	C_3Cr_7	P31c	C^{4}_{3v}	hP80	H
$D10_2$	Fe_3Th_7	$P6_3mc$	C^{4}_{6v}	hP20	H
$E0_1$	ClFPb	P4/nmm	D^{7}_{4h}	tP6	T
$E1_1$	$CuFeS_2$	$I\bar{4}2d$	D^{12}_{2d}	tI16	U
$E2_1$	CaO_3Ti	Pm3m	O^{1}_{h}	cP5	C
$E2_4$	S_3Sn_2	Pnma	D^{16}_{2h}	oP20	O
E3	Al_2CdS_4	$I\bar{4}$	S^{2}_{4}	tI14	U
$E9_3$	$SiFe_3W_3$	Fd3m	O^{7}_{h}	cF112	F
$E9_a$	Al_7Cu_2Fe	P4/mnc	D^{6}_{4h}	tP40	T
$E9_b$	$AlLi_3N_2$	Ia3	T^{7}_{h}	cI96	B
$F0_1$	NiSSb	$P2_13$	T^{4}	cP12	C
$F5_1$	$CrNaS_2$	R3m or R32	D^{5}_{3d} or D^{7}_{3}	hR4	R
$F5_6$	CuS_2Sb	Pnma	D^{16}_{2h}	oP16	O
$H1_1$	Al_2MgO_4	Fd3m	O^{7}_{h}	cF56	F
$H2_4$	Cu_3S_4V	P43m	T^{1}_{d}	cP8	C
$H2_5$	$AsCu_3S_4$	$Pmn2_1$	C^{7}_{2v}	oP16	O
$L1_0$	AuCu	P4/mmm	D^{1}_{4h}	tP4	T
$L1_2$	$AlCu_3$	Pm3m	O^{1}_{h}	cP4	C
$L2_1$	$AlCu_2Mn$	Fm3m	O^{5}_{h}	cF16	F
$L2_2$	Sb_2Tl_7	Im3m	O^{9}_{h}	cI54	B
$L'2_b$	H_2Th	I4/mmm	D^{17}_{4h}	tI6	U
L′3	Fe_2N	$P6_3/mmc$	D^{4}_{6h}	hP3	H
$L6_0$	$CuTi_3$	P4/mmm	D^{1}_{4h}	tP4	T

[a] The first letter denotes the crystal system: triclinic (a), monoclinic (m), orthorhombic (o), tetragonal (t), hexagonal (h) and cubic (c). Trigonal (rhombohedral) system is denoted by combination hR. The second letter of Pearson's symbol denotes lattice type: primitive (P), edge-(base-) centered (C), body-centered (I) or face-centered (F). The following number denotes number of atoms in the crystal unit cell.

[b] Standard ASTM E157-82a has the Bravais lattices designations as following: C – primitive cubic; B – body-centered cubic; F – face-centered cubic; T – primitive tetragonal; U – body-centered tetragonal; R – rhombohedral; H – hexagonal; O – primitive orthorhombic; P – body-centered orthorhombic; Q – base-centered orthorhombic; S – face-centered orthorhombic; M – primitive monoclinic; N – centered monoclinic; A – triclinic.

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