

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Table 3.1.2.2

Three-dimensional Bravais types of lattices

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
<i>aP</i>	<i>a, b, c</i> α, β, γ	<i>a, b, c</i> α, β, γ	$g_{11} \ g_{12} \ g_{13}$ $g_{22} \ g_{23}$ g_{33}	$g_{11} \ g_{12} \ g_{13}$ $g_{22} \ g_{23}$ g_{33}		
<i>mP</i>	<i>a, b, c</i> $\beta, \alpha = \gamma = 90^\circ$	<i>a, b, c</i> $\beta, \alpha = \gamma = 90^\circ$	$g_{11} \ 0 \ g_{13}$ $g_{22} \ 0$ g_{33}	$g_{11} \ 0 \ g_{13}$ $g_{22} \ 0$ g_{33}		
<i>mC</i> (<i>mS</i>)		$a_1 = a_2, c$ $\gamma, \alpha = \beta$		$P(C)$ $\tilde{g}'_{11} \ \tilde{g}'_{12} \ \tilde{g}'_{13}$ $\tilde{g}'_{11} \ \tilde{g}'_{13}$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2}g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
<i>oP</i>	<i>a, b, c</i> $\alpha = \beta = \gamma = 90^\circ$	<i>a, b, c</i> $\alpha = \beta = \gamma = 90^\circ$	$g_{11} \ 0 \ 0$ $g_{22} \ 0$ g_{33}	$g_{11} \ 0 \ 0$ $g_{22} \ 0$ g_{33}		
<i>oC</i> (<i>oS</i>)		$a_1 = a_2, c$ $\gamma, \alpha = \beta = 90^\circ$		$P(C)$ $\tilde{g}'_{11} \ \tilde{g}'_{12} \ 0$ $\tilde{g}'_{11} \ 0$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
<i>oI</i>		$a_1 = a_2 = a_3$ α, β, γ $\cos \alpha + \cos \beta + \cos \gamma = -1$		$P(I)$ $-\tilde{g} \ \tilde{g}'_{12} \ \tilde{g}'_{13}$ $-\tilde{g} \ \tilde{g}'_{23}$ $-\tilde{g}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
<i>oF</i>		<i>a, b, c</i> α, β, γ $\cos \alpha = \frac{-a^2 + b^2 + c^2}{2bc}$ $\cos \beta = \frac{a^2 + b^2 - c^2}{2ac}$ $\cos \gamma = \frac{a^2 + b^2 - c^2}{2ab}$		$P(F)$ $\tilde{g}_1 \ \tilde{g}'_{12} \ \tilde{g}'_{13}$ $\tilde{g}_2 \ \tilde{g}'_{23}$ \tilde{g}_3	$g'_{12} = \frac{1}{4}g_{33}$ $g'_{13} = \frac{1}{4}g_{22}$ $g'_{23} = \frac{1}{4}g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Column 1 contains the Delaunay description followed by the Voronoi type. Beneath these, the Bravais lattice and the symbol of its holohedry are given. Next the topological features that are compatible with the symmetry axes referred to the 'blickrichtungen' of the holohedry are listed. Column 2 gives the metric

conditions for the occurrence of certain Voronoi types. For the monoclinic cases with centred cells (*M1–M5*) it is useful to introduce in addition to the vectors **a, c, f = a + c** special parameters (*p*², *q*², *r*²). **p** designates the vector below the centring point in the projection in the net perpendicular to **b**. **q** is the

3.1. CRYSTAL LATTICES

Table 3.1.2.2 (continued)

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
<i>tP</i>	$a_1 = a_2, c$ $\alpha = \beta = \gamma = 90^\circ$	$a_1 = a_2, c$ $\alpha = \beta = \gamma = 90^\circ$	$g_{11} \ 0 \ 0$ $g_{11} \ 0$ g_{33}	$g_{11} \ 0 \ 0$ $g_{11} \ 0$ g_{33}		
<i>tI</i>		$a_1 = a_2 = a_3$ $\gamma, \alpha = \beta$ $2 \cos \alpha + \cos \gamma = -1$		$\begin{matrix} \bar{g} & g'_{12} & g'_{13} \\ & \bar{g} & g'_{13} \\ & & \bar{g} \end{matrix}$ $\bar{g} = -(g'_{12} + 2g'_{13})$	$\begin{matrix} g'_{12} = \frac{1}{4}(-2g_{11} + g_{33}) \\ g'_{13} = -\frac{1}{4}g_{33} \end{matrix}$ $g_{11} = 2(g'_{12} + g'_{13})$ $g_{33} = -4g'_{13}$	
<i>hR</i>	$a_1 = a_2, c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma$	$g_{11} \ -\frac{1}{2}g_{11} \ 0$ $g_{11} \ 0$ g_{33}	$\begin{matrix} g'_{11} & g'_{12} & g'_{12} \\ & g'_{11} & g'_{12} \\ & & g'_{11} \end{matrix}$	$\begin{matrix} g'_{11} = \frac{1}{9}(3g_{11} + g_{33}) \\ g'_{12} = \frac{1}{3}(-\frac{3}{2}g_{11} + g_{33}) \\ g_{11} = 2(g'_{11} - g'_{12}) \\ g_{33} = 3(g'_{11} + 2g'_{12}) \end{matrix}$	
<i>hP</i>		$a_1 = a_2, c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$		$g_{11} \ -\frac{1}{2}g_{11} \ 0$ $g_{11} \ 0$ g_{33}		
<i>cP</i>	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$	$g_{11} \ 0 \ 0$ $g_{11} \ 0$ g_{11}	$g_{11} \ 0 \ 0$ $g_{11} \ 0$ g_{11}		
<i>cI</i>		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 109.5^\circ$ $\cos \alpha = -\frac{1}{3}$		$\begin{matrix} g'_{11} & -\frac{1}{3}g'_{11} & -\frac{1}{3}g'_{11} \\ & g'_{11} & -\frac{1}{3}g'_{11} \\ & & g'_{11} \end{matrix}$	$\begin{matrix} g'_{11} = \frac{3}{4}g_{11} \\ g_{11} = \frac{4}{3}g'_{11} \end{matrix}$	
<i>cF</i>		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60^\circ$		$\begin{matrix} g'_{11} & \frac{1}{2}g'_{11} & \frac{1}{2}g'_{11} \\ & g'_{11} & \frac{1}{2}g'_{11} \\ & & g'_{11} \end{matrix}$	$\begin{matrix} g'_{11} = \frac{1}{2}g_{11} \\ g_{11} = 2g'_{11} \end{matrix}$	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; cf. de Wolff *et al.* (1985). Symbols in parentheses are standard symbols, see Table 2.1.1.1. ‡ $\mathbf{P}(C) = \frac{1}{2}(110/\bar{1}10/002)$, $\mathbf{P}(I) = \frac{1}{2}(\bar{1}11/111/111)$, $\mathbf{P}(F) = \frac{1}{2}(011/101/110)$, $\mathbf{P}(R) = \frac{1}{3}(\bar{1}21/\bar{2}11/111)$.

shorter one of the other two vectors and **r** labels the remaining one (cf. Burzlaff & Zimmermann, 1985).

For practical applications, it is useful to classify the patterns of the resulting six scalar products regarding their equivalence or zero values in the form of a symbolic (Selling) tetrahedron (column 3). These classes of patterns correspond to the reduced bases. They result in 24 ‘Symmetrische Sorten’ (Delaunay, 1933) that fix the Voronoi types and the holohedries, and simultaneously lead directly to the conventional crystallographic cells by

fixed transformations (cf. Patterson & Love, 1957; Burzlaff & Zimmermann, 1993).

Column 4 contains projections of the Dirichlet domain along the symmetry directions indicated by the topological/symmetry symbol in column 1. Column 5 shows the relation between the Dirichlet domain and the conventional cell. Column 6 contains the transformation matrix from the reduced basis to the conventional basis. (Note: In the monoclinic centred case it leads to the *I* centring.)