

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Table 3.1.2.3
Delaunay types of lattices (‘Symmetrische Sorten’)

Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
<i>K1 V1</i> <i>cI</i> $\frac{4}{3} \frac{2}{m} \frac{2}{m}$ $v s s^2$	—						$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
<i>K2 V3</i> <i>cF</i> $\frac{4}{3} \frac{2}{m} \frac{2}{m}$ $v^4 v^3 v$	—						$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}$
<i>K3 V5</i> <i>cP</i> $\frac{4}{3} \frac{2}{m} \frac{2}{m}$ $v v^3 v^2$	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$
							$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
<i>H V4</i> <i>hP</i> $\frac{6}{m} \frac{2}{m} \frac{2}{m}$ $s v v^2$	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
<i>R1 V1</i> <i>hR</i> $\frac{2}{3} \frac{2}{m}$ $s s^2$	$2c^2 < 3a^2$				—		$\begin{pmatrix} 1 & 0 & 1 \\ -1 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix}$
<i>R2 V3</i> <i>hR</i> $\frac{2}{3} \frac{2}{m}$ $v^3 v$	$2c^2 > 3a^2$				—		$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 3 \\ 0 & 1 & 2 \end{pmatrix}$
<i>Q1 V1</i> <i>iI</i> $\frac{4}{m} \frac{2}{m} \frac{2}{m}$ $v v s^2$	$c^2 < 2a^2$						$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$

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Table 3.1.2.3 (continued)

Delaunay-Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
$Q2 V2$ iI $\frac{4\ 2\ 2}{mmm}$ $v^4\ s\ s^2$	$c^2 > 2a^2$						$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}$
$Q3 V5$ iP $\frac{4\ 2\ 2}{mmm}$ $v\ v\ v^2$	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
							$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$
							$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$O1 V1$ oF $\frac{2\ 2\ 2}{mmm}$ $s^2\ v\ s^2$	—						$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}$
$O2 V1$ oI $\frac{2\ 2\ 2}{mmm}$ $v\ v\ v$	$a^2 + b^2 > c^2$						$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
$O3 V2$ oI $\frac{2\ 2\ 2}{mmm}$ $s\ s\ v^4$	$a^2 + b^2 < c^2$						$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}$
$O4 V3$ oI $\frac{2\ 2\ 2}{mmm}$ $v\ v\ v^4$	$a^2 + b^2 = c^2$						$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$
							$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}$

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Table 3.1.2.3 (continued)

Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
$O5 V4$ $o(AB)C$ $\frac{2\ 2\ 2}{m\ m\ m}$ $s\ v^2\ v$	—						$\begin{pmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
							$\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$O6 V5$ oP $\frac{2\ 2\ 2}{m\ m\ m}$ $v\ v\ v$	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
							$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$

Table 3.1.2.3 (continued)

Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell			Transformation to the conventional cell
$M1 V1$ $m(AC)I$ $\frac{2}{m}$ s^2	$b^2 > p^2$						$\begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$
				$A: b^2 > c^2$	$C: b^2 > a^2$	$I: b^2 > f^2$	
$M2 V1$ $m(AC)I$ $\frac{2}{m}$ v	$p^2 > b^2,$ $b^2 > r^2 - q^2$						$\begin{pmatrix} 0 & 1 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \end{pmatrix}$
				$A: c^2 > b^2 > f^2 - a^2$	$C: a^2 > b^2 > f^2 - c^2$	$I: f^2 > b^2 > c^2 - a^2$	
$M3 V2$ $m(AC)I$ $\frac{2}{m}$ s	$r^2 - q^2 > b^2$						$\begin{pmatrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -2 & 0 & 0 \end{pmatrix}$
				$A: f^2 - a^2 > b^2$	$C: f^2 - c^2 > b^2$	$I: c^2 - a^2 > b^2$	
$M4 V4$ $m(AC)I$ $\frac{2}{m}$ s^2	$b^2 = p^2$						$\begin{pmatrix} 0 & 1 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \end{pmatrix}$ $\begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$
				$A: b^2 = c^2$	$C: b^2 = a^2$	$I: b^2 = f^2$	

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Table 3.1.2.3 (continued)

Delauany-Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell			Transformation to the conventional cell
M5 V3 m(AC)I $\frac{2}{m}$ v	$b^2 = r^2 - q^2$						$\begin{pmatrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -2 & 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$
				A: $b^2 = f^2 - a^2$	C: $b^2 = f^2 - c^2$	I: $b^2 = c^2 - a^2$	
M6 V4 mP $\frac{2}{m}$ s	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
T1 V1 aP 1	—						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
T2 V2 aP 1	$\mathbf{a} \cdot \mathbf{b} = 0$						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
T3 V3 aP 1	$\mathbf{a} \cdot \mathbf{b} = 0$ $(\mathbf{a} + \mathbf{b} + \mathbf{c}) \cdot \mathbf{c} = 0$						$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

In some cases, different Selling patterns are given for one ‘Symmetrische Sorte’. This procedure avoids a final reduction step (cf. Patterson & Love, 1957) and simplifies the computational treatment significantly. The number of ‘Symmetrische Sorten’, and thus the number of transformations which have to be applied, is smaller than the number of lattice characters according to Niggli. Note that the introduction of reduced bases using shortest lattice vectors causes complications in more than three dimensions (cf. Schwarzenberger, 1980).

3.1.2.4. Example of Delaunay reduction and standardization of the basis

Let the basis $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ given by the scalar products

$$\begin{pmatrix} g_{11} & g_{22} & g_{33} \\ g_{23} & g_{31} & g_{12} \end{pmatrix} = \begin{pmatrix} 6 & 8 & 8 \\ 4 & 2 & 3 \end{pmatrix}$$

or by $b_1 = 2.449 (\sqrt{6})$, $b_2 = b_3 = 2.828 (\sqrt{8})$ (in arbitrary units), β_{23}

$= 60^\circ$ ($\cos \beta_{23} = \frac{1}{2}$), $\beta_{13} = 73.22^\circ$ ($\cos \beta_{13} = \sqrt{3}/6$), $\beta_{12} = 64.34^\circ$ ($\cos \beta_{12} = \sqrt{3}/4$).

The aim is to find a standardized basis of shortest lattice vectors using Delaunay reduction. This example, given by B. Gruber (cf. Burzlaff & Zimmermann, 1985), shows the standardization problems remaining after the reduction.

The general reduction step can be described using Selling four flats. The corners are designated by the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} = -\mathbf{a} - \mathbf{b} - \mathbf{c}$. The edges are marked by the scalar products among these vectors. If positive scalar products can be found, choose the largest: $\mathbf{a} \cdot \mathbf{b}$ (indicated as \mathbf{ab} in Fig. 3.1.2.2a). The reduction transformation is: $\mathbf{a}_D = \mathbf{a}, \mathbf{b}_D = -\mathbf{b}, \mathbf{c}_D = \mathbf{c} + \mathbf{b}, \mathbf{d}_D = \mathbf{d} + \mathbf{b}$ (see Fig. 3.1.2.2a). In this example, this results in the Selling four flat shown in Fig. 3.1.2.2(b). The next step, shown in Fig. 3.1.2.2(c), uses the (maximal) positive scalar product for further reduction. Finally, using $\mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4 = -\mathbf{b}_1$ we get the result shown in Fig. 3.1.2.2(d).

The complete procedure can be expressed in a table, as shown in Table 3.1.2.4. Each pair of lines contains the starting basis and