1.1. Summary of general formulae

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In an ideal crystal structure, the arrangement of atoms is three-dimensionally periodic. This periodicity is usually described in terms of point lattices, vector lattices, and translation groups [*cf. IT* A (1983, Section 8.1.3)].

1.1.1. General relations between direct and reciprocal lattices

1.1.1.1. *Primitive crystallographic bases*

The vectors **a**, **b**, **c** form a primitive crystallographic basis of the vector lattice **L**, if each translation vector $\mathbf{t} \in \mathbf{L}$ may be expressed as

$$\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

with u, v, w being integers.

A primitive basis defines a primitive unit cell for a corresponding point lattice. Its volume V may be calculated as the mixed product (triple scalar product) of the three basis vectors:

$$\begin{aligned} V &= (\mathbf{abc}) = \mathbf{a} \times \mathbf{b} \cdot \mathbf{c} \\ &= \left[\begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{vmatrix} \right]^{1/2} \\ &= abc[1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma \\ &\quad + 2\cos\alpha\cos\beta\cos\gamma]^{1/2} \\ &= 2abc\left[\sin\frac{\alpha+\beta+\gamma}{2} \sin\frac{-\alpha+\beta+\gamma}{2} \right. \\ &\quad \left. \times \sin\frac{\alpha-\beta+\gamma}{2} \sin\frac{\alpha+\beta-\gamma}{2} \right]^{1/2}. \end{aligned} \tag{1.1.1.1}$$

Here a, b and c designate the lengths of the three basis vectors and $\alpha = \mathbf{b} \wedge \mathbf{c}$, $\beta = \mathbf{c} \wedge \mathbf{a}$ and $\gamma = \mathbf{a} \wedge \mathbf{b}$ the angles between them.

Each vector lattice **L** and each primitive crystallographic basis **a**, **b**, **c** is uniquely related to a reciprocal vector lattice $\mathbf{L}^*$ and a primitive reciprocal basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$:

$$\left.\begin{aligned} \mathbf{a}^* &= \frac{\mathbf{b}\times\mathbf{c}}{V} \quad \text{or} \quad \mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = 0, \quad \mathbf{a}^*\cdot\mathbf{a} = 1; \\ \mathbf{b}^* &= \frac{\mathbf{c}\times\mathbf{a}}{V} \quad \text{or} \quad \mathbf{b}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{c} = 0, \quad \mathbf{b}^*\cdot\mathbf{b} = 1; \\ \mathbf{c}^* &= \frac{\mathbf{a}\times\mathbf{b}}{V} \quad \text{or} \quad \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0, \quad \mathbf{c}^*\cdot\mathbf{c} = 1. \end{aligned}\right\} \tag{1.1.1.2}$$

$$\mathbf{L}^* = \{\mathbf{r}^* | \mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \text{ and } h, k, l \text{ integers}\}.$$

The lengths a^*, b^* and c^* of the reciprocal basis vectors and the angles $\alpha^* = \mathbf{b}^* \wedge \mathbf{c}^*$, $\beta^* = \mathbf{c}^* \wedge \mathbf{a}^*$ and $\gamma^* = \mathbf{a}^* \wedge \mathbf{b}^*$ are given by:

$$\left.\begin{aligned} a^* &= \frac{bc\sin\alpha}{V}, \quad b^* = \frac{ac\sin\beta}{V}, \quad c^* = \frac{ab\sin\gamma}{V}, \\ \cos\alpha^* &= \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}, \\ \cos\beta^* &= \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}, \\ \cos\gamma^* &= \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}. \end{aligned}\right\} \tag{1.1.1.3}$$

$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ define a primitive unit cell in a corresponding reciprocal point lattice. Its volume V^* may be expressed by analogy with V [equation (1.1.1.1)]:

$$\begin{aligned} V^* &= (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \mathbf{a}^* \times \mathbf{b}^* \cdot \mathbf{c}^* \\ &= \left[\begin{vmatrix} a^{*2} & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ a^*b^*\cos\gamma^* & b^{*2} & b^*c^*\cos\alpha^* \\ a^*c^*\cos\beta^* & b^*c^*\cos\alpha^* & c^{*2} \end{vmatrix} \right]^{1/2} \\ &= a^*b^*c^*[1 - \cos^2\alpha^* - \cos^2\beta^* - \cos^2\gamma^* \\ &\quad + 2\cos\alpha^*\cos\beta^*\cos\gamma^*]^{1/2} \\ &= 2a^*b^*c^*\left[\sin\frac{\alpha^*+\beta^*+\gamma^*}{2} \sin\frac{-\alpha^*+\beta^*+\gamma^*}{2} \right. \\ &\quad \left. \times \sin\frac{\alpha^*-\beta^*+\gamma^*}{2} \sin\frac{\alpha^*+\beta^*-\gamma^*}{2} \right]^{1/2}. \end{aligned} \tag{1.1.1.4}$$

In addition, the following equation holds:

$$VV^* = 1. \tag{1.1.1.5}$$

As all relations between direct and reciprocal lattices are symmetrical, one can calculate **a**, **b**, **c** from $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$:

$$\mathbf{a} = \frac{\mathbf{b}^*\times\mathbf{c}^*}{V^*}, \quad \mathbf{b} = \frac{\mathbf{c}^*\times\mathbf{a}^*}{V^*}, \quad \mathbf{c} = \frac{\mathbf{a}^*\times\mathbf{b}^*}{V^*}, \tag{1.1.1.6}$$

$$\left.\begin{aligned} a &= \frac{b^*c^*\sin\alpha^*}{V^*}, \\ b &= \frac{a^*c^*\sin\beta^*}{V^*}, \\ c &= \frac{a^*b^*\sin\gamma^*}{V^*}, \\ \cos\alpha &= \frac{\cos\beta^*\cos\gamma^* - \cos\alpha^*}{\sin\beta^*\sin\gamma^*}, \\ \cos\beta &= \frac{\cos\alpha^*\cos\gamma^* - \cos\beta^*}{\sin\alpha^*\sin\gamma^*}, \\ \cos\gamma &= \frac{\cos\alpha^*\cos\beta^* - \cos\gamma^*}{\sin\alpha^*\sin\beta^*}. \end{aligned}\right\} \tag{1.1.1.7}$$

The unit-cell volumes V and V^* may also be obtained from:

$$\begin{aligned} V &= abc\sin\alpha^*\sin\beta\sin\gamma \\ &= abc\sin\alpha\sin\beta^*\sin\gamma \\ &= abc\sin\alpha\sin\beta\sin\gamma^*, \end{aligned} \tag{1.1.1.8}$$

Table 1.1.1.1. *Direct and reciprocal lattices described with respect to conventional basis systems*

Direct lattice $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$			Reciprocal lattice		
			$\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$		
Bravais letter	Centring vectors	Unit-cell volume V_c	Conditions for reciprocal-lattice vectors $h\mathbf{a}_c^* + k\mathbf{b}_c^* + l\mathbf{c}_c^*$	Unit-cell volume V_c^*	Bravais letter
A	$\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$k + l = 2n$	$\frac{1}{2}V^*$	A
B	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + l = 2n$	$\frac{1}{2}V^*$	B
C	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c$	$2V$	$h + k = 2n$	$\frac{1}{2}V^*$	C
I	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + k + l = 2n$	$\frac{1}{2}V^*$	F
F	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c$, $\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c$, $\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$4V$	$h + k = 2n$, $h + l = 2n$, $k + l = 2n$	$\frac{1}{4}V^*$	I
R	$\frac{1}{3}\mathbf{a}_c + \frac{2}{3}\mathbf{b}_c + \frac{2}{3}\mathbf{c}_c$, $\frac{2}{3}\mathbf{a}_c + \frac{1}{3}\mathbf{b}_c + \frac{1}{3}\mathbf{c}_c$	$3V$	$-h + k + l = 3n$	$\frac{1}{3}V^*$	R

$$\begin{aligned} V^* &= a^*b^*c^* \sin\alpha \sin\beta^* \sin\gamma^* \\ &= a^*b^*c^* \sin\alpha^* \sin\beta \sin\gamma^* \\ &= a^*b^*c^* \sin\alpha^* \sin\beta^* \sin\gamma. \end{aligned} \tag{1.1.1.9}$$

1.1.1.2. *Non-primitive crystallographic bases*

For certain lattice types, it is usual in crystallography to refer to a 'conventional' crystallographic basis $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ instead of a primitive basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. In that case, $\mathbf{a}_c$, $\mathbf{b}_c$, and $\mathbf{c}_c$ with all their integral linear combinations are lattice vectors again, but there exist other lattice vectors $\mathbf{t} \in \mathbf{L}$,

$$\mathbf{t} = t_1\mathbf{a}_c + t_2\mathbf{b}_c + t_3\mathbf{c}_c,$$

with at least two of the coefficients t_1, t_2, t_3 being fractional.

Such a conventional basis defines a conventional or centred unit cell for a corresponding point lattice, the volume V_c of which may be calculated by analogy with V by substituting $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ for $\mathbf{a}, \mathbf{b}$, and $\mathbf{c}$ in (1.1.1.1).

If m designates the number of centring lattice vectors $\mathbf{t}$ with $0 \le t_1, t_2, t_3 < 1$, V_c may be expressed as a multiple of the primitive unit-cell volume V:

$$V_c = mV. \tag{1.1.1.10}$$

With the aid of equations (1.1.1.2) and (1.1.1.3), the reciprocal basis $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$ may be derived from $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$. Again, each reciprocal-lattice vector

$$\mathbf{r}^* = h\mathbf{a}_c^* + k\mathbf{b}_c^* + l\mathbf{c}_c^* \in \mathbf{L}^*$$

is an integral linear combination of the reciprocal basis vectors, but in contrast to the use of a primitive basis only certain triplets h, k, l refer to reciprocal-lattice vectors.

Equation (1.1.1.5) also relates V_c to V_c^*, the reciprocal cell volume referred to $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$. From this it follows that

$$V_c^* = \frac{1}{m}V^*. \tag{1.1.1.11}$$

Table 1.1.1.1 contains detailed information on 'centred lattices' described with respect to conventional basis systems.

As a direct lattice and its corresponding reciprocal lattice do not necessarily belong to the same type of Bravais lattices [*IT* A (1987, Section 8.2.4)], the Bravais letter of $\mathbf{L}^*$ is given in the last column of Table 1.1.1.1. Except for *P* lattices, a conventionally chosen basis for $\mathbf{L}^*$ coincides neither with $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ nor with $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$. This third basis, however, is not used in crystallography. The designation of scattering vectors and the indexing of Bragg reflections usually refers to $\mathbf{a}_c^*, \mathbf{b}_c^*, \mathbf{c}_c^*$.

If the differences with respect to the coefficients of direct- and reciprocal-lattice vectors are disregarded, all other relations discussed in Part 1 are equally true for primitive bases and for conventional bases.

1.1.2. Lattice vectors, point rows, and net planes

The length t of a vector $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ is given by

$$\begin{aligned} t^2 = {} & u^2\mathbf{a}^2 + v^2\mathbf{b}^2 + w^2\mathbf{c}^2 + 2uvab\cos\gamma \\ & + 2uwac\cos\beta + 2vwbc\cos\alpha. \end{aligned} \tag{1.1.2.1}$$

Accordingly, the length r^* of a reciprocal-lattice vector $\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ may be calculated from

$$\begin{aligned} r^{*2} = {} & h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^* \\ & + 2hla^*c^*\cos\beta^* + 2klb^*c^*\cos\alpha^*. \end{aligned} \tag{1.1.2.2}$$

If the coefficients u, v, w of a vector $\mathbf{t} \in \mathbf{L}$ are coprime, $[uvw]$ symbolizes the direction parallel to $\mathbf{t}$. In particular, $[uvw]$ is used to designate a crystal edge, a zone axis, or a point row with that direction.

The integer coefficients h, k, l of a vector $\mathbf{r}^* \in \mathbf{L}^*$ are also the coordinates of a point of the corresponding reciprocal lattice and designate the Bragg reflection with scattering vector $\mathbf{r}^*$. If h, k, l are coprime, the direction parallel to $\mathbf{r}^*$ is symbolized by $[hkl]^*$.

Each vector $\mathbf{r}^*$ is perpendicular to a family of equidistant parallel nets within a corresponding direct point lattice. If the coefficients h, k, l of $\mathbf{r}^*$ are coprime, the symbol (hkl) describes that family of nets. The distance $d(hkl)$ between two neighbouring nets is given by

$$d(hkl) = r^{*-1}. \tag{1.1.2.3}$$

Parallel to such a family of nets, there may be a face or a cleavage plane of a crystal.

The net planes (hkl) obey the equation

$$hx + ky + lz = n \quad (n = \text{integer}). \tag{1.1.2.4}$$

Different values of n distinguish between the individual nets of the family; x, y, z are the coordinates of points on the net planes (not necessarily of lattice points). They are expressed in units a, b, and c, respectively.

Similarly, each vector $\mathbf{t} \in \mathbf{L}$ with coprime coefficients u, v, w is perpendicular to a family of equidistant parallel nets within a corresponding reciprocal point lattice. This family of nets may be symbolized $(uvw)^*$. The distance $d^*(uvw)$ between two neighbouring nets can be calculated from

$$d^*(uvw) = t^{-1}. \tag{1.1.2.5}$$

A layer line on a rotation pattern or a Weissenberg photograph with rotation axis $[uvw]$ corresponds to one such net of the family $(uvw)^*$ of the reciprocal lattice.

The nets $(uvw)^*$ obey the equation

$$uh + vk + wl = n \quad (n = \text{integer}). \tag{1.1.2.6}$$

Equations (1.1.2.6) and (1.1.2.4) are essentially the same, but may be interpreted differently. Again, n distinguishes between the individual nets out of the family $(uvw)^*$. h, k, l are the coordinates of the reciprocal-lattice points, expressed in units a^*, b^*, c^*, respectively.

A family of nets (hkl) and a point row with direction $[uvw]$ out of the same point lattice are parallel if and only if the following equation is satisfied:

$$hu + kv + lw = 0. \tag{1.1.2.7}$$

This equation is called the 'zone equation' because it must also hold if a face (hkl) of a crystal belongs to a zone $[uvw]$.

Two (non-parallel) nets $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect in a point row with direction $[uvw]$ if the indices satisfy the condition

$$u : v : w = \begin{vmatrix} k_1 l_1 \\ k_2 l_2 \end{vmatrix} : \begin{vmatrix} l_1 h_1 \\ l_2 h_2 \end{vmatrix} : \begin{vmatrix} h_1 k_1 \\ h_2 k_2 \end{vmatrix}. \tag{1.1.2.8}$$

The same condition must be satisfied for a zone axis $[uvw]$ defined by the crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$.

Three nets $(h_1k_1l_1)$, $(h_2k_2l_2)$, and $(h_3k_3l_3)$ intersect in parallel rows, or three faces with these indices belong to one zone if

$$\begin{vmatrix} h_1 k_1 l_1 \\ h_2 k_2 l_2 \\ h_3 k_3 l_3 \end{vmatrix} = 0. \tag{1.1.2.9}$$

Two (non-parallel) point rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ in the direct lattice are parallel to a family of nets (hkl) if

$$h : k : l = \begin{vmatrix} v_1 w_1 \\ v_2 w_2 \end{vmatrix} : \begin{vmatrix} w_1 u_1 \\ w_2 u_2 \end{vmatrix} : \begin{vmatrix} u_1 v_1 \\ u_2 v_2 \end{vmatrix}. \tag{1.1.2.10}$$

The same condition holds for a face (hkl) belonging to two zones $[u_1v_1w_1]$ and $[u_2v_2w_2]$.

Three point rows $[u_1v_1w_1]$, $[u_2v_2w_2]$, and $[u_3v_3w_3]$ are parallel to a net (hkl), or three zones of a crystal with these indices have a common face (hkl) if

$$\begin{vmatrix} u_1 v_1 w_1 \\ u_2 v_2 w_2 \\ u_3 v_3 w_3 \end{vmatrix} = 0. \tag{1.1.2.11}$$

A net (hkl) is perpendicular to a point row $[uvw]$ if

$$\begin{aligned} &\frac{a}{h}(au + bv\cos\gamma + cw\cos\beta) \\ &\quad = \frac{b}{k}(au\cos\gamma + bv + cw\cos\alpha) \\ &\quad = \frac{c}{l}(au\cos\beta + bv\cos\alpha + cw). \end{aligned} \tag{1.1.2.12}$$

1.1.3. Angles in direct and reciprocal space

The angles between the normal of a crystal face and the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called the direction angles of that face. They may be calculated as angles between the corresponding reciprocal-lattice vector $\mathbf{r}^*$ and the basis vectors $\lambda = \mathbf{r}^* \wedge \mathbf{a}$, $\mu = \mathbf{r}^* \wedge \mathbf{b}$ and $\nu = \mathbf{r}^* \wedge \mathbf{c}$:

$$\left.\begin{aligned} \cos\lambda = \frac{h}{a}d(hkl), \quad \cos\mu = \frac{k}{b}d(hkl), \\ \cos\nu = \frac{l}{c}d(hkl). \end{aligned}\right\} \tag{1.1.3.1}$$

The three equations can be combined to give

$$\left.\begin{aligned} a : b : c = \frac{h}{\cos\lambda} : \frac{k}{\cos\mu} : \frac{l}{\cos\nu} \\ \text{or} \\ h : k : l = a\cos\lambda : b\cos\mu : c\cos\nu. \end{aligned}\right\} \tag{1.1.3.2}$$

The first formula gives the ratios between a, b, and c, if for any face of the crystal the indices (hkl) and the direction angles λ, μ, and ν are known. Once the axial ratios are known, the indices of any other face can be obtained from its direction angles by using the second formula.

Similarly, the angles between a direct-lattice vector $\mathbf{t}$ and the reciprocal basis vectors $\lambda^* = \mathbf{t} \wedge \mathbf{a}^*$, $\mu^* = \mathbf{t} \wedge \mathbf{b}^*$ and $\nu^* = \mathbf{t} \wedge \mathbf{c}^*$ are given by

$$\left.\begin{aligned} \cos\lambda^* = \frac{u}{a^*}d^*(uvw), \quad \cos\mu^* = \frac{v}{b^*}d^*(uvw), \\ \cos\nu^* = \frac{w}{c^*}d^*(uvw). \end{aligned}\right\} \tag{1.1.3.3}$$

The angle ψ between two direct-lattice vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ or between two corresponding point rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ may be derived from the scalar product

$$\begin{aligned} \mathbf{t}_1 \cdot \mathbf{t}_2 = {} & u_1u_2a^2 + v_1v_2b^2 + w_1w_2c^2 + (u_1v_2 + u_2v_1)ab\cos\gamma \\ & + (u_1w_2 + u_2w_1)ac\cos\beta + (v_1w_2 + v_2w_1)bc\cos\alpha \end{aligned} \tag{1.1.3.4}$$

as

$$\cos\psi = \frac{\mathbf{t}_1 \cdot \mathbf{t}_2}{t_1 t_2}. \tag{1.1.3.5}$$

Analogously, the angle φ between two reciprocal-lattice vectors $\mathbf{r}_1^*$ and $\mathbf{r}_2^*$ or between two corresponding point rows $[h_1k_1l_1]^*$ and $[h_2k_2l_2]^*$ or between the normals of two corresponding crystal faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$ may be calculated as

$$\cos\varphi = \frac{\mathbf{r}_1^* \cdot \mathbf{r}_2^*}{r_1 r_2} \tag{1.1.3.6}$$

with

$$\begin{aligned} \mathbf{r}_1^* \cdot \mathbf{r}_2^* = {} & h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2} \\ & + (h_1k_2 + h_2k_1)a^*b^*\cos\gamma^* \\ & + (h_1l_2 + h_2l_1)a^*c^*\cos\beta^* \\ & + (k_1l_2 + k_2l_1)b^*c^*\cos\alpha^*. \end{aligned} \tag{1.1.3.7}$$

Finally, the angle ω between a first direction $[uvw]$ of the direct lattice and a second direction $[hkl]$ of the reciprocal lattice may also be derived from the scalar product of the corresponding vectors $\mathbf{t}$ and $\mathbf{r}^*$.

$$\cos\omega = \frac{\mathbf{t}\cdot\mathbf{r}^*}{tr^*} = \frac{uh+vk+wl}{tr^*}. \qquad (1.1.3.8)$$

1.1.4. The Miller formulae

Consider four faces of a crystal that belong to the same zone in consecutive order: $(h_1k_1l_1)$, $(h_2k_2l_2)$, $(h_3k_3l_3)$, and $(h_4k_4l_4)$. The angles between the ith and the jth face normals are designated φ_{ij}. Then the Miller formulae relate the indices of these faces to the angles φ_{ij}:

$$\frac{\sin\varphi_{12}\sin\varphi_{43}}{\sin\varphi_{13}\sin\varphi_{42}} = \frac{u_{12}u_{43}}{u_{13}u_{42}} = \frac{v_{12}v_{43}}{v_{13}v_{42}} = \frac{w_{12}w_{43}}{w_{13}w_{42}} \qquad (1.1.4.1)$$

with

$$u_{ij} = \begin{vmatrix} k_i & l_i \\ k_j & l_j \end{vmatrix}, \quad v_{ij} = \begin{vmatrix} l_i & h_i \\ l_j & h_j \end{vmatrix}, \quad w_{ij} = \begin{vmatrix} h_i & k_i \\ h_j & k_j \end{vmatrix}.$$

If all angles between the face normals and also the indices for three of the faces are known, the indices of the fourth face may be calculated. Equation (1.1.4.1) cannot be used if two of the faces are parallel.

From the definition of u_{ij}, v_{ij}, and w_{ij}, it follows that all fractions in (1.1.4.1) are rational:

$$\frac{\sin\varphi_{12}\sin\varphi_{43}}{\sin\varphi_{13}\sin\varphi_{42}} = \frac{p}{q} \quad \text{with } p, q \text{ integers.}$$

Therefore, (1.1.4.1) may be rearranged to

$$p\cot\varphi_{12} - q\cot\varphi_{13} = (p-q)\cot\varphi_{14}. \qquad (1.1.4.2)$$

This equation allows the determination of one angle if two of the angles and the indices of all four faces are known.

1.4.2.1. *Symmorphic space groups*

The 73 space groups known as 'symmorphic' are in one-to-one correspondence with the arithmetic crystal classes, and their standard 'short' symbols (Bertaut, 1995) are obtained by interchanging the order of the geometric crystal class and the Bravais cell in the symbol for the arithmetic space group. In fact, conventional crystallographic symbolism did not distinguish between arithmetic crystal classes and symmorphic space groups until recently (de Wolff *et al.*, 1985); the symbol of the symmorphic group was used also for the arithmetic class.

This relationship between the symbols, and the equivalent rule-of-thumb *symmorphic space groups are those whose standard (short) symbols do not contain glide planes or screw axes*, reveal nothing fundamental about the nature of symmorphism; they are simply a consequence of the conventions governing the construction of symbols in *International Tables for Crystallography*.*

Although the *standard* symbols of the symmorphic space groups do not contain screw axes or glide planes, this is a result of the manner in which the space-group symbols have been devised. Most symmorphic space groups do in fact contain screw axes and/or glide planes. This is immediately obvious for the symmorphic space groups based on centred cells; *C*2 contains equal numbers of diad rotation axes and diad screw axes, and *Cm* contains equal numbers of reflection planes and glide planes. This is recognized in the 'extended' space-group symbols (Bertaut, 1995), but these are clumsy and not commonly used; those for *C*2 and *Cm* are $C1^{2}_{2_1}1$ and $C1^{m}_{a}1$, respectively. In the more symmetric crystal systems, even symmorphic space groups with primitive cells contain screw axes and/or glide planes; *P*422 ($P42^{2}_{2_1}$) contains many diad screw axes and *P*4/*mmm* ($P4/m2/m^{2/m}_{2_1/g}$) contains both screw axes and glide planes.

The balance of symmetry elements within the symmorphic space groups is discussed in more detail in Subsection 9.7.1.2.

1.4.3. Effect of dispersion on diffraction symmetry

In the absence of dispersion ('anomalous scattering'), the intensities of the reflections *hkl* and $\bar{h}\bar{k}\bar{l}$ are equal (Friedel's law), and statements about the symmetry of the weighted reciprocal lattice and quantities derived from it often rest on the tacit or explicit assumption of this law – the condition underlying it being forgotten. In particular, if dispersion is appreciable, the symmetry of the Patterson synthesis and the 'Laue' symmetry are altered.

1.4.3.1. *Symmetry of the Patterson function*

In Volume A of *International Tables*, the symmetry of the Patterson synthesis is derived in two stages. First, any glide planes and screw axes are replaced by mirror planes and the corresponding rotation axes, giving a symmorphic space group (Subsection 1.4.2.1). Second, a centre of symmetry is added. This second step involves the tacit assumption of Friedel's law, and should not be taken if any atomic scattering factors have appreciable imaginary components. In such cases, the symmetry of the Patterson synthesis will not be that of one of the 24 centrosymmetric symmorphic space groups, as given in Volume A, but will be that of the symmorphic space group belonging to the arithmetic crystal class to which the space group of the structure belongs. There are thus 73 possible Patterson symmetries.

An equivalent description of such symmetries, in terms of 73 of the 1651 dichromatic colour groups, has been given by Fischer & Knop (1987); see also Wilson (1993).

1.4.3.2. *'Laue' symmetry*

Similarly, the eleven conventional 'Laue' symmetries [*International Tables for Crystallography* (1995), Volume A, p. 40 and elsewhere] involve the explicit assumption of Friedel's law. If dispersion is appreciable, the 'Laue' symmetry may be that of any of the 32 point groups. The point group, in correct orientation, is obtained by dropping the Bravais-lattice symbol from the symbol of the arithmetic crystal class or of the Patterson symmetry.

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* Three examples of informative definitions are:

1. The space group corresponding to the zero solution of the Frobenius congruences is called a symmorphic space group (Engel, 1986, p. 155).

2. A space group *F* is called *symmorphic* if one of its finite subgroups (and therefore an infinity of them) is of an order equal to the order of the point group R_r (Opechowski, 1986, p. 255).

3. A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed (Wondratschek, 1995, p. 717).

Even in context, these are pretty opaque.

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1.1–1.3

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