

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 \mathbf{a} , \mathbf{b} , \mathbf{c} form a primitive crystallographic basis of the vector lattice \mathbf{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:

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

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

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

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

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:

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

\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)]:

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

In addition, the following equation holds:

$$VV^* = 1. \quad (1.1.1.5)$$

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

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

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

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

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

1.1. SUMMARY OF GENERAL FORMULAE

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
<i>A</i>	$\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$k + l = 2n$	$\frac{1}{2}V^*$	<i>A</i>
<i>B</i>	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + l = 2n$	$\frac{1}{2}V^*$	<i>B</i>
<i>C</i>	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c$	$2V$	$h + k = 2n$	$\frac{1}{2}V^*$	<i>C</i>
<i>I</i>	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$2V$	$h + k + l = 2n$	$\frac{1}{2}V^*$	<i>F</i>
<i>F</i>	$\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{b}_c,$ $\frac{1}{2}\mathbf{a}_c + \frac{1}{2}\mathbf{c}_c,$ $\frac{1}{2}\mathbf{b}_c + \frac{1}{2}\mathbf{c}_c$	$4V$	$h + k = 2n,$ $h + l = 2n,$ $k + l = 2n$	$\frac{1}{4}V^*$	<i>I</i>
<i>R</i>	$\frac{1}{3}\mathbf{a}_c + \frac{2}{3}\mathbf{b}_c + \frac{2}{3}\mathbf{c}_c,$ $\frac{2}{3}\mathbf{a}_c + \frac{1}{3}\mathbf{b}_c + \frac{1}{3}\mathbf{c}_c$	$3V$	$-h + k + l = 3n$	$\frac{1}{3}V^*$	<i>R</i>

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

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 $0 \leq t_1, t_2, t_3 < 1$, V_c may be expressed as a multiple of the primitive unit-cell volume V :

$$V_c = mV. \quad (1.1.1.10)$$

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

$$V_c^* = \frac{1}{m}V^*. \quad (1.1.1.11)$$

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

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

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

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

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