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Zones and sublattices of integral lattices

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Methods are presented for an analysis of zones and sublattices of integral lattices, whose relevance is revealed by sharp peaks in the frequency distribution of hexagonal and tetragonal lattices, as a function of the axial ratio c/a. Starting from a few examples, zone symmetries, lattice–sublattice relations and integral scaling transformations are derived for hexagonal lattices with axial ratios $\sqrt{\frac{3}{2}}$, $\sqrt{3}$, $\sqrt{2}$ and 1 (the isometric case) and for the related $\sqrt{3}$ and $\sqrt{2}$ tetragonal lattices. Sublattices and zones connected by linear rational transformations lead to rational equivalence classes of integral lattices. For properties like the axial ratio and the point-group symmetry (lattice holohedry), rational equivalence can be extended so that also metric tensors differing by an integral factor become equivalent. These two types of equivalence classes are determined for the lattices mentioned above.

1. Introduction

The distribution of hexagonal and tetragonal crystals as a function of the axial ratio $\gamma = c/a$ of the lattice parameters shows sharp peaks at (or near to) rational values of γ^2. This implies that the corresponding lattices are integral (Janner, 2004; de Gelder & Janner, 2004*a*).

In order to get a better understanding of the structural basis of this empirical observation, properties of crystal structures with integral lattices are investigated. Several different approaches are possible, as already considered for crystal structures, like hexagonal close packing, or B8 compounds with a Frank's cubic hexagonal lattice:

(*a*) diffraction symmetry of zone patterns (Singh *et al.*, 1998; Ranganathan *et al.*, 2002);

(*b*) building block units (Singh *et al.*, 1998; Lidin, 1998; Ranganathan *et al.*, 2002);

(*c*) multimetrical symmetry (Janner, 1997);

(*d*) projection and section of higher-dimensional lattices (Frank, 1965);

(*e*) integral quadratic forms, positive definite and indefinite (Conway & Sloane, 1988).

In this note, attention is focused on the identification of square and hexagonal zones. This problem is equivalent to that of determining hexagonal and tetragonal sublattices. Ways of constructing new solutions from a given one are discussed.

2. Basic definitions and notation

Consider a γ hexagonal lattice Λ with rational axial ratio squared $\gamma^2 \in \mathbb{Q}$. The cubic hexagonal Frank lattice (Frank, 1965) represents the special case $\gamma = \sqrt{\frac{3}{2}}$ and the lattice of a hexagonal close packing (h.c.p.) that of $\gamma = \sqrt{\frac{8}{3}}$. The normalized hexagonal basis $a = (a_1, a_2, a_3)$ with components expressed with respect to an orthonormal reference system is given by

$$a_1 = (1, 0, 0), \quad a_2 = \left(-\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}, 0\right), \quad a_3 = (0, 0, \gamma). \tag{1}$$

The reciprocal basis $a^* = (a_1^*, a_2^*, a_3^*)$ is then

$$a_1^* = \left(1, \tfrac{1}{\sqrt{3}}, 0\right), \quad a_2^* = \left(0, \tfrac{2}{\sqrt{3}}, 0\right), \quad a_3^* = \left(0, 0, \tfrac{1}{\gamma}\right). \tag{2}$$

The generating matrices M and M^* of the lattices Λ and Λ^*, respectively,

$$M = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & \gamma \end{pmatrix}, \quad M^* = \begin{pmatrix} 1 & \frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\gamma} \end{pmatrix}, \tag{3}$$

are related by $M^* = \tilde{M}^{-1}$, where the tilde indicates transposition. The corresponding metric tensors are given by the Gram matrices:

$$g_h(\gamma) = M\tilde{M} = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & 0 & \gamma^2 \end{pmatrix}, \tag{4}$$

$$g_h^*(\gamma) = M^*\tilde{M}^* = \begin{pmatrix} \frac{4}{3} & \frac{2}{3} & 0 \\ \frac{2}{3} & \frac{4}{3} & 0 \\ 0 & 0 & \frac{1}{\gamma^2} \end{pmatrix}. \tag{5}$$

It follows that the axial ratio for the hexagonal lattice Λ^* is

$$\gamma^* = \frac{|a_3^*|}{|a_1^*|} = \frac{\sqrt{3}}{2\gamma}. \tag{6}$$

For γ^2 a rational number ($\gamma^2 \in \mathbb{Q}$), both Λ and Λ^* are integral lattices and commensurate. This means that there is a re-

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ciprocal-lattice vector in the direction of any direct lattice vector and conversely

$$v^* \sim S_{aa^*} v, \quad v \sim S_{a^*a} v^* \tag{7}$$

for $v \in \Lambda$ and $v^* \in \Lambda^*$ because the corresponding basis transformation matrices have rational entries. Indeed, one finds

$$S_{aa^*}(\gamma) = g_h(\gamma), \quad S_{a^*a}(\gamma) = g_h^*(\gamma). \tag{8}$$

It is, therefore, convenient to treat Λ^* as a direct hexagonal lattice with axial ratio γ^* and with a normalized metric tensor $g_h(\gamma^*)$:

$$g_h(\gamma^*) = \tilde{U}\tfrac{3}{4}g_h^*(\gamma)U = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & 0 & \frac{3}{4\gamma^2} \end{pmatrix} \tag{9}$$

with

$$U = \begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}. \tag{10}$$

In the case of a tetragonal lattice, the normalized metric tensor is

$$g_t(\gamma) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \gamma^2 \end{pmatrix}, \quad \gamma^2 \in \mathbb{Q}, \tag{11}$$

and the axial ratio of the reciprocal lattice is $\gamma^* = 1/\gamma$. The lattice vectors are given as $v = [n_1 n_2 n_3] \in \Lambda$ and $v^* = [h_1 h_2 h_3]_* \in \Lambda^*$ (written as row vectors for graphical reasons).

A *zone Z* is a set of direct lattice planes that intersect each other along parallel lines. The common direction of these lines is the zone axis. To each *zone plane* (hkl) there corresponds a reciprocal-lattice vector $[hkl]_*$, perpendicular to the zone axis, normally given in terms of a direct-lattice vector $[stu]$:

$$[stu][hkl]_* = 0 \longleftrightarrow (hkl) \in Z[stu], \tag{12}$$

where the zone Z is specified by its zone axis $[stu]$. Accordingly, a given zone defines a two-dimensional lattice of reciprocal vectors. The zone is hexagonal (or square) if this lattice is hexagonal (or square). In Singh *et al.* (1998) and Ranganathan *et al.* (2002), these zones are labeled by the letters F and G, respectively. As a consequence of (7), each of these lattices is proportional to a direct lattice of the same point symmetry, which together with the zone-axis vector generates a three-dimensional sublattice Σ of Λ. This sublattice is hexagonal (or tetragonal) if the zone is hexagonal (or square, respectively). The matrix S transforming the original hexagonal basis a to $s = (s_1, s_2, s_3)$ of the sublattice Σ has as third column vector the zone axis s_3, expressed in the basis a.

If the components s_{11}, s_{12}, s_{13}, s_{21}, s_{22}, s_{23} of s_1 and of s_2, respectively, or the components s_{31}, s_{32}, s_{33} of s_3, share a common factor, the basis s and the matrix S are *reducible*, otherwise they are *irreducible*. In the case of a hexagonal zone $Z[s_3] = F$, one has

$$\tilde{S}g_h(\gamma)S = \mu^2 g_h(\gamma'), \quad S \in GL(3, \mathbb{Q}), \tag{13}$$

where S has integral entries with column vectors s_1, s_2, s_3, the tilde indicates transposition and μ is the scaling factor. For μ a rational number, this scaling corresponds to a lattice–sublattice relation:

$$S : \gamma h \xrightarrow{\mu} \gamma' h, \quad \mu \in \mathbb{Q}, \tag{14}$$

where γh denotes an integral hexagonal lattice with axial ratio γ. The corresponding expressions for a square zone $Z[s_3] = G$ of γh are

$$\tilde{S}g_h(\gamma)S = \mu^2 g_t(\gamma'), \quad S \in GL(3, \mathbb{Q}), \tag{15}$$

$$S : \gamma h \xrightarrow{\mu} \gamma' t, \quad \mu \in \mathbb{Q}, \tag{16}$$

where $g_t(\gamma)$ is the metric tensor of the tetragonal sublattice γt with axial ratio γ.

Example: Frank's cubic hexagonal lattice Λ.
Axial ratio: $\gamma = \sqrt{\frac{3}{2}}$.
Reciprocal axial ratio: $\gamma^* = \frac{1}{\sqrt{2}}$.
(i) **Hexagonal zone *F*:** zone axis: $s_3 = [421]$; hexagonal zone lattice: $s_1^* = [\bar{1}20]_* = \frac{2}{3}[030]$, $s_2^* = [0\bar{1}2]_* = \frac{2}{3}[\bar{1}\bar{2}2]$.
Sublattice Σ*:* $s_1 = [030]$, $s_2 = [\bar{1}\bar{2}2]$, $s_3 = [421]$.
Scaling matrix:

$$S = \begin{pmatrix} 0 & -1 & 4 \\ 3 & -2 & 2 \\ 0 & 2 & 1 \end{pmatrix}.$$

Metric matrix: $\tilde{S}g_h(\sqrt{\frac{3}{2}})S = 9g_h(\sqrt{\frac{3}{2}})$.
Lattice–sublattice relation: $\Lambda = \sqrt{\frac{3}{2}}h \xrightarrow{3} S\Lambda = \sqrt{\frac{3}{2}}h$.
(ii) **Square zone *G*:** zone axis: $s_3 = [211]$; square zone lattice: $s_1^* = [\bar{1}20]_* = \frac{2}{3}[030]$, $s_2^* = [\bar{1}02]_* = \frac{2}{3}[\bar{2}\bar{1}2]$.
Sublattice Σ*:* $s_1 = [030]$, $s_2 = [\bar{2}\bar{1}2]$, $s_3 = [211]$.
Scaling matrix:

$$S = \begin{pmatrix} 0 & \bar{2} & 2 \\ 3 & \bar{1} & 1 \\ 0 & 2 & 1 \end{pmatrix}$$

Metric matrix: $\tilde{S}g_h(\sqrt{\frac{3}{2}})S = 9g_t(\frac{1}{\sqrt{2}})$.
Lattice–sublattice relation: $\Lambda = \sqrt{\frac{3}{2}}h \xrightarrow{3} S\Lambda = \frac{1}{\sqrt{2}}t$.

3. γ_0 families

From a given lattice–sublattice transformation S_0 of a lattice with axial ratio $\gamma_0 = \sqrt{m_0/n_0}$, with relatively prime and square-free integers m_0 and n_0, one easily derives the transformation S for a lattice with axial ratio $\gamma = (m/n)\gamma_0$ for $m/n \in \mathbb{Q}$. All such integral lattices belong to the same γ_0 *family*. One simply has

$$S_0 = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{pmatrix} \xrightarrow{m/n} S = \begin{pmatrix} ms_{11} & ms_{12} & ms_{13} \\ ms_{21} & ms_{22} & ms_{23} \\ ns_{31} & ns_{32} & ns_{33} \end{pmatrix}. \tag{17}$$

Depending on the integers m and n (supposed to be relatively prime), the S matrix can be reduced in the way indicated

Table 1
Lattice–sublattice relations for the same zone (the matrices S_i are given in Tables 2 to 5).

Integral lattice	Zone	$[z_1 z_2]$	Lattice sublattice
$\frac{m}{n}\sqrt{\frac{3}{2}}h$	$Z[4m\ 2m\ n]$	$[1\bar{1}]$	$S_1 \xrightarrow{3} S_2$
$\frac{m}{n}\sqrt{3}h$	$Z[120]$	$[1\bar{1}]$	$S_6 \xrightarrow{3} S_7$
		$[21]$	$S_6 \xrightarrow{3} S_8$
$\frac{m}{n}\sqrt{3}t$	$Z[100]$	$[1\bar{1}]$	$S_{10} \xrightarrow{3} S_{11}$
$\frac{m}{n}\sqrt{2}h$	$Z[4m\ 0\ n]$	$[1\bar{1}]$	$S_{13} \xrightarrow{3} S_{14}$
$\frac{m}{n}\sqrt{2}t$	$Z[2m\ 0\ n]$	$[\bar{1}\bar{1}]$	$S_{18} \xrightarrow{1} S_{19}$
		$[1\bar{1}]$	$S_{18} \xrightarrow{3} S_{20}$
$\frac{m}{n}h$	$Z[100]$	$[1\bar{1}]$	$S_{22} \xrightarrow{3} S_{23}$

above. So, for example, for the $\sqrt{\frac{3}{2}}$ family, one finds the hexagonal zones $Z[4m\,2m\,n]$ and the lattice–sublattice transformation:

$$S = \begin{pmatrix} 0 & -m & 4m \\ 3m & -2m & 2m \\ 0 & 2n & n \end{pmatrix}: \quad \frac{m}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3m} \sqrt{\frac{3}{2}}h. \tag{18}$$

This relation is irreducible for m and n odd. For $m = 2p$ even (and thus n odd), the transformation can be reduced and one finds

$$S = \begin{pmatrix} 0 & -p & 8p \\ 3p & -2p & 4p \\ 0 & n & n \end{pmatrix}: \quad \frac{2p}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3p} 2\sqrt{\frac{3}{2}}h. \tag{19}$$

In a similar way for $n = 2q$ even (and m odd), one derives a corresponding reduced transformation:

$$S = \begin{pmatrix} 0 & -m & 2m \\ 3m & -2m & m \\ 0 & 4q & q \end{pmatrix}: \quad \frac{m}{2q}\sqrt{\frac{3}{2}}h \xrightarrow{3m} \frac{1}{2}\sqrt{\frac{3}{2}}h. \tag{20}$$

In the present note, rational scalings and lattice–sublattice relations are derived for the four hexagonal families $\sqrt{\frac{3}{2}}H$, $\sqrt{3}H$, $\sqrt{2}H$ and $1H$ with $\gamma_0 = \sqrt{\frac{3}{2}}$, $\sqrt{3}$, $\sqrt{2}$ and 1, respectively (corresponding to molecular form lattices observed in axial-symmetric proteins). Using the methods explained below, one also gets similar relations for the two tetragonal families $\sqrt{2}T$ and $\sqrt{3}T$ with $\gamma_0 = \sqrt{2}$ and $\sqrt{3}$, respectively. The lattice–sublattice relations for the same zone are listed in Table 1 and the matrices S_i are indicated in Tables 2 to 5 for the hexagonal and the square zones, some of which are given for Frank's lattice in Singh *et al.* (1998) and in Ranganathan *et al.* (2002).

4. Reciprocal transformation

Given a zone Z with zone axis s_3 and the two-dimensional zone lattice spanned by s_1^*, s_2^*, instead of transforming these two into the direct lattice vectors s_1, s_2 as in equation (7), leading to the three-dimensional sublattice Σ of Λ, one can transform the zone-axis vector into a reciprocal one by $s_3^* \sim S_{aa^*}s_3$ and consider the sublattice Σ^* of Λ^* spanned by s_1^*, s_2^*, s_3^*. The lattice–sublattice relation for the reciprocal lattice Λ^* is then given by the matrix $S^* = (s_1^*, s_2^*, s_3^*)$ with column vectors s_i^*. This corresponds to a zone $Z[s_3^*] = Z[hkl]_*$.

But the lattices Λ^* and Σ^* are also hexagonal and can be treated as such, after expressing the reciprocal basis as a normalized hexagonal basis (1).

To the hexagonal lattices Λ with axial ratios $\sqrt{\frac{3}{2}}$, $\sqrt{3}$, $\sqrt{2}$, 1, there correspond the reciprocal lattices Λ^* with axial ratio $\frac{1}{2}\sqrt{2}$, $\frac{1}{2}$, $\frac{1}{2}\sqrt{\frac{3}{2}}$, $\frac{1}{2}\sqrt{3}$, respectively. This implies that the set of families $\sqrt{\frac{3}{2}}H$, $\sqrt{2}H$ and $\sqrt{3}H$, $1H$, respectively, is left invariant by reciprocity, not however the individual families.

In the tetragonal case, each of the families $\sqrt{2}T$, $\sqrt{3}T$ is invariant with respect to reciprocity.

Given a lattice–sublattice transformation S for Λ, the corresponding one S^* for Λ^* is obtained by

$$S^* = U^{-1}S_{aa^*}(\gamma)S, \quad U^{-1} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{21}$$

up to constant factors ensuring that S^* is integral and irreducible. Indeed, using the identity $S_{aa^*}(\gamma) = g_h(\gamma)$, one finds

$$\tilde{S}^* g_h(\gamma^*) S^* \sim \tilde{S} g_h(\gamma) S \sim g_h(\gamma'). \tag{22}$$

Example for $\gamma = (m/n)\sqrt{\frac{3}{2}}$.
The reciprocal axial ratio is $\gamma^* = n/(m\sqrt{2})$. To the hexagonal zone $Z[4m\,2m\,n]$ corresponds the matrix

$$S = \begin{pmatrix} 0 & -m & 4m \\ 3m & -2m & 2m \\ 0 & 2n & n \end{pmatrix}$$

(see Table 2). One then has

$$\begin{aligned} U^{-1}g_h\left(\sqrt{\frac{3}{2}}\right)S &\sim \begin{pmatrix} 3mn & -3mn & 6mn \\ 6mn & -3mn & 0 \\ 0 & 6m^2 & 3m^2 \end{pmatrix} \\ &\sim \begin{pmatrix} n & -n & 2n \\ 2n & -n & 0 \\ 0 & 2m & m \end{pmatrix} = S^*, \end{aligned} \tag{23}$$

which is irreducible for m, n odd and relatively prime. One verifies that

$$\tilde{S}^* g_h\left(\frac{n}{m}\frac{1}{\sqrt{2}}\right) S^* = 3n^2 g_h\left(\sqrt{\frac{3}{2}}\right) \tag{24}$$

for the zone $Z[2n\,0\,m]$. It is then easy to derive a corresponding transformation of $g_h[(m/n)\sqrt{2}]$ and the zone $Z[4m\,0\,n]$, which in fact is the one indicated in Table 4 for the $\sqrt{2}H$ family, in terms of Λ, Σ and S.

5. Inverse transformation

The inverse of S is a rational matrix proportional to an integral one, denoted by T, having corresponding properties:

$$S^{-1} \sim T, \quad \text{integral } T \in GL(3, \mathbb{Q}). \tag{25}$$

One then gets the inverse hexagonal lattice–sublattice relation:

Table 2
$\sqrt{\frac{3}{2}}$-hexagonal family.

Family	γ	Zone	Transformation	Scaling relation
$\sqrt{\frac{3}{2}}H$	$\frac{m}{n}\sqrt{\frac{3}{2}}$	$Z[4m\ 2m\ n] = F$ $[\bar{n}\,2n\,0]_*\quad [0\,\bar{n}\,2m]_*$	$S_1 = \begin{pmatrix} 0 & -m & 4m \\ 3m & -2m & 2m \\ 0 & 2n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3m} \sqrt{\frac{3}{2}}h$
		$Z[4m\ 2m\ n]$ $[\bar{n}\,3n\,2\bar{m}]_*\quad [\bar{n}\,0\,4m]_*$	$S_2 = \begin{pmatrix} m & -2m & 4m \\ 5m & -m & 2m \\ -2n & 4n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3\sqrt{3}m} \frac{1}{2}\sqrt{2}h$
		$Z[2m\ m\ n] = G$ $[\bar{n}\,2n\,0]_*\quad [n\,0\,2\bar{m}]_*$	$S_3 = \begin{pmatrix} 0 & 2m & 2m \\ 3m & m & m \\ 0 & -2n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3m} \frac{1}{2}\sqrt{2}t$
	$\frac{2m}{n}\sqrt{\frac{3}{2}}$	$Z[8m\ 4m\ n]$ $[\bar{n}\,2n\,0]_*\quad [0\,\bar{n}\,4m]_*$	$S_4 = \begin{pmatrix} 0 & -m & 8m \\ 3m & -2m & 4m \\ 0 & n & n \end{pmatrix}$	$\frac{2m}{n}\sqrt{\frac{3}{2}}h \xrightarrow{3m} 2\sqrt{\frac{3}{2}}h$
	$\frac{m}{2n}\sqrt{\frac{3}{2}}$	$Z[2m\ m\ n]$ $[\bar{n}\,2n\,0]_*\quad [0\,\bar{n}\,m]_*$	$S_5 = \begin{pmatrix} 0 & -m & 2m \\ 3m & -2m & m \\ 0 & 4n & n \end{pmatrix}$	$\frac{m}{2n}\sqrt{\frac{3}{2}}h \xrightarrow{3m} \frac{1}{2}\sqrt{\frac{3}{2}}h$

$$\tilde{T}g_h(\gamma')T = \nu^2 g_h(\gamma) \quad \text{for} \quad \tilde{S}g_h S = \mu^2 g_h(\gamma') \tag{26}$$

and correspondingly for a square zone:

$$\tilde{T}g_t(\gamma')T = \nu^2 g_h(\gamma) \quad \text{for} \quad \tilde{S}g_h S = \mu^2 g_t(\gamma'), \tag{27}$$

implying the product $ST = \mu^2\nu^2\mathbb{I}$, where $\mathbb{I}$ denotes the unit matrix. In this way, one obtains hexagonal sublattice and scaling relations for tetragonal lattices belonging to the two families $\sqrt{3}T$, $\sqrt{2}T$, as indicated in Tables 3 and 4.

6. Sublattices of a given zone

By applying the various procedures indicated so far, a number of sublattices have been found, which share the same zone. One has, first of all, to realise that, in general, a zone of an integral lattice depends not only on the zone axis but also on the axial ratio. So, for example, the zone $Z[2m\,m\,n]$ for $\gamma = \frac{m}{n}\sqrt{\frac{3}{2}}$ is square, whereas it is hexagonal for $\gamma = \frac{m}{2n}\sqrt{\frac{3}{2}}$ (see Table 2). Of course, the zone $Z[001]$ with zone plane perpendicular to the rotational axis has a hexagonal symmetry, which does not depend on the axial ratio.

For a given zone, different sublattice transformations correspond to either a different choice of the basis (setting) of the same lattice (and are, therefore, equivalent) or to a sublattice of the two-dimensional zone lattice Σ_0. An example of the first case is given by S_{18} and S_{19} of Table 4 and S_1, S_2 of Table 2 represent examples of the second case.

In order to characterize these situations, consider two hexagonal lattice–sublattice relations for a given zone axis s_3:

$$\begin{aligned} S(s_1, s_2, s_3):&\quad \Lambda \longrightarrow \Sigma \\ S'(s_1', s_2', s_3):&\quad \Lambda \longrightarrow \Sigma', \quad \Sigma' \subseteq \Sigma, \end{aligned} \tag{28}$$

with s_1, s_2 a hexagonal basis of Σ_0. Then,

$$s_1' = z_1 s_1 + z_2 s_2, \quad s_2' = z_1' s_1 + z_2' s_2 = R s_1', \quad z_1, z_2, z_1', z_2' \in \mathbb{Z} \tag{29}$$

with $R \in GL(2, \mathbb{Z})$ a sixfold integral transformation, which can be chosen to be

$$R = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

Accordingly, the vector $[z_1 z_2]$ characterizes the relation between S and S' or Σ and Σ', respectively. The determinant of the matrix

$$\begin{pmatrix} z_1 & z_1' \\ z_2 & z_2' \end{pmatrix}$$

is the *index* σ of Σ' in Σ:

$$[z_1 z_2] : S \xrightarrow{\sigma} S'. \tag{30}$$

Example: Zone $\frac{m}{n}\sqrt{3}$, $\quad Z[120]$: S_6, S_7, S_8 of Table 3

$$S_6 = S(s_1, s_2, s_3) : s_1 = [2m\,0\,0], \quad s_2 = [\bar{m}0n], \quad s_3 = [120]$$

with s_1, s_2 a hexagonal basis of Σ_0.

For $S_7 = S'(s_1', s_2', s_3)$, one has

$$s_1' = [3m\,0\,\bar{n}] = s_1 - s_2, \quad s_2' = [0\,0\,2n] = s_1 + 2s_2$$

and one verifies the relation:

$$R[z_1 z_2] = R[1\bar{1}] = [z_1' z_2'] = [12].$$

In a similar way, one finds for S_8: $[z_1 z_2] = [21]$ and $[z_1' z_2'] = R[21] = [\bar{1}1]$.

These relations for the transformations indicated in Tables 2 to 5 sharing the same zone are summarized in Table 1.

7. Composition

Another way to get additional lattice–sublattice relations is by *composition*, combining successively transformations already derived:

$$\Lambda \xrightarrow{S_1} \Sigma_1 \xrightarrow{S_2} \Sigma \quad \rightarrow \quad \Lambda \xrightarrow{S_1 S_2} \Sigma. \tag{31}$$

In Tables 2 to 5, the transformations given imply the following integral scaling relations for the hexagonal and tetragonal families:

Table 3
$\sqrt{3}$-hexagonal and $\sqrt{3}$-tetragonal families.

Family	γ	Zone	Transformation	Scaling relation
$\sqrt{3}\,H$	$\frac{m}{n}\sqrt{3}$	$Z[1\ 2\ 0] = F$ $[4n\,2\bar{n}\,0]_*$ $[2\bar{n}\,n\,6m]_*$	$S_6 = \begin{pmatrix} 2m & -m & 1 \\ 0 & 0 & 2 \\ 0 & n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}h \xrightarrow{2m} \frac{1}{2m}\sqrt{3}h$
		$[2n\,\bar{n}\,2m]_*$ $[0\,0\,4m]_*$	$S_7 = \begin{pmatrix} 3m & 0 & 1 \\ 0 & 0 & 2 \\ -n & 2n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}h \xrightarrow{2\sqrt{3}m} \frac{1}{2m}h$
		$[2n\,\bar{n}\,2m]_*$ $[2\bar{n}\,n\,2m]_*$	$S_8 = \begin{pmatrix} 3m & -3m & 1 \\ 0 & 0 & 2 \\ n & n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}h \xrightarrow{2\sqrt{3}m} \frac{1}{2m}h$
		$Z[1\ 0\ 0] = G$ $[4n\,3n\,0]_*$ $[0\,0\,6m]_*$	$S_9 = \begin{pmatrix} m & 0 & 1 \\ 2m & 0 & 0 \\ 0 & n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}h \xrightarrow{\sqrt{3}m} \frac{1}{3m}\sqrt{3}t$
$\sqrt{3}\,T$	$\frac{m}{n}\sqrt{3}$	$Z[1\ 0\ 0]$ $[0\,2n\,0]_*$ $[0\,\bar{n}\,3m]_*$	$S_{10} = \begin{pmatrix} 0 & 0 & 1 \\ 2m & -m & 0 \\ 0 & n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}\,t \xrightarrow{2m} \frac{1}{2m}\,h$
		$[0\,n\,\bar{m}]_*$ $[0\,0\,2m]_*$	$S_{11} = \begin{pmatrix} 0 & 0 & 1 \\ 3m & 0 & 0 \\ -n & 2n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{3}t \xrightarrow{2\sqrt{3}m} \frac{1}{6m}\sqrt{3}h$
		$Z[3m\ 0\ n]$ $[0\,2n\,0]_*$ $[\bar{n}\,0\,3m]_*$	$S_{12} = \begin{pmatrix} 0 & -m & 3m \\ 2m & 0 & 0 \\ 0 & n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{3}t \xrightarrow{2m} \sqrt{3}t$

$$\begin{aligned} \sqrt{\tfrac{3}{2}}H &\longrightarrow \sqrt{\tfrac{3}{2}}H,\, \sqrt{2}H,\, \sqrt{2}T \\ \sqrt{2}H &\longrightarrow \sqrt{\tfrac{3}{2}}H,\, \sqrt{2}H,\, \sqrt{2}T \\ \sqrt{2}T &\longrightarrow \sqrt{\tfrac{3}{2}}H,\, \sqrt{2}T \end{aligned} \tag{32}$$

so that the set of families $\sqrt{\frac{3}{2}}H$, $\sqrt{2}H$ and $\sqrt{2}T$ is closed under composition. In a similar way, from

$$\begin{aligned} \sqrt{3}H &\longrightarrow \sqrt{3}H,\, 1H,\, \sqrt{3}T \\ 1H &\longrightarrow \sqrt{3}H,\, 1H,\, \sqrt{3}T \\ \sqrt{3}T &\longrightarrow \sqrt{3}H,\, 1H,\, \sqrt{3}T \end{aligned} \tag{33}$$

follows the other closed set $\sqrt{3}H$, $1H$, $\sqrt{3}T$.

Example: $\frac{m}{n}\sqrt{2}h$.

From the transformations S_{15} and S_{20}, one deduces the composed transformation S: $\sqrt{2}h \longrightarrow \sqrt{2}t \longrightarrow \sqrt{2}h = \sqrt{2}h \longrightarrow \sqrt{2}h$:

$$\begin{aligned} S &= \begin{pmatrix} 1 & 1 & 2 \\ 2 & 0 & 0 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} -1 & 2 & 2 \\ 3 & 0 & 0 \\ -1 & 2 & -1 \end{pmatrix} \\ &\sim \begin{pmatrix} 0 & 3 & 0 \\ -1 & 2 & 4 \\ -2 & 1 & -1 \end{pmatrix} \sim \begin{pmatrix} 2 & -1 & 4 \\ 3 & 0 & 0 \\ -1 & 2 & 1 \end{pmatrix}. \end{aligned} \tag{34}$$

It then follows that

$$S \sim \begin{pmatrix} 2m & -m & 4m \\ 3m & 0 & 0 \\ -n & 2n & n \end{pmatrix} = S_{14}, \quad \frac{m}{n}\sqrt{2}h \xrightarrow{3m} \sqrt{2}h, \tag{35}$$

as indicated in Table 4.

Not all these scaling transformations correspond to a lattice–sublattice relation. So, for example for S_9: $\sqrt{3}h \xrightarrow{\sqrt{3}} \sqrt{3}t$, the scaling factor is $\sqrt{3}$. This implies that, starting from a hexagonal lattice with a and c parameters given by 1 and $\sqrt{3}$, respectively, one finds that the corresponding lattice parameters for the tetragonal sublattice are $a = \sqrt{3}$, $c = 3$ and not 1 and $\sqrt{3}$, as indicated in the scaling relation. This is because the choice of a unit of length leading to a normalized metric tensor for a given lattice cannot be repeated for its sublattices.

8. Rational equivalence of integral lattices

Let us denote by $\Lambda(a)$ the lattice spanned by a basis $a = (a_1, a_2, a_3)$, by $g(a)$ the corresponding metric tensor with entries $g_{ik} = a_i a_k$ and a crystallographic point group $K(a)$ of orthogonal transformations, expressed in the basis a, leaving the lattice Λ invariant. Therefore, the point-group elements $A(a)$ of $K(a)$ are invertible integral matrices that leave the metric tensor $g(a)$ invariant:

$$\tilde{A}(a)g(a)A(a) = g(a), \quad A(a) \in K(a) \subseteq GL(3, \mathbb{Z}). \tag{36}$$

$K(a)$ is a finite subgroup of $GL(3, \mathbb{Z})$. The *holohedry* of Λ is the largest point group leaving Λ invariant.

The *real linear transformation* S of the basis $a \to s = Sa = (Sa_1, Sa_2, Sa_3) = (s_1, s_2, s_3)$ transforms lattice, metric tensor and point group accordingly and defines an affine equivalence:

Table 4
$\sqrt{2}$-hexagonal and $\sqrt{2}$-tetragonal families.

Family	γ	Zone	Transformation	Scaling relation
$\sqrt{2}\,H$	$\frac{m}{n}\sqrt{2}$	$Z[4m\ 0\ n] = F$ $[0\,3n\,0]_*\quad[\bar{n}\,\bar{n}\,4m]_*$	$S_{13} = \begin{pmatrix} m & -m & 4m \\ 2m & -m & 0 \\ 0 & n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}h \xrightarrow{\sqrt{3}m} 2\sqrt{\frac{3}{2}}h$
		$[n\,4n\,4\bar{m}]_*\quad[2\bar{n}\,n\,8m]_*$	$S_{14} = \begin{pmatrix} 2m & -m & 4m \\ 3m & 0 & 0 \\ -n & 2n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}h \xrightarrow{3m} \sqrt{2}h$
		$Z[2m\ 0\ n]$ $[0\,3n\,0]_*\quad[2n\,\bar{n}\,4\bar{m}]_*$	$S_{15} = \begin{pmatrix} m & m & 2m \\ 2m & 0 & 0 \\ 0 & -n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}h \xrightarrow{\sqrt{3}m} \sqrt{2}t$
	$\frac{m}{2n}\sqrt{2}$	$Z[2m\ 0\ n]$ $[0\,3n\,0]_*\quad[\bar{n}\,\bar{n}\,2m]_*$	$S_{16} = \begin{pmatrix} m & -m & 2m \\ 2m & -m & 0 \\ 0 & 2n & n \end{pmatrix}$	$\frac{m}{2n}\sqrt{2}h \xrightarrow{\sqrt{3}m} \sqrt{\frac{3}{2}}h$
		$Z[m\ 0\ n]$ $[0\,3n\,0]_*\quad[2n\,\bar{n}\,2\bar{m}]_*$	$S_{17} = \begin{pmatrix} m & m & m \\ 2m & 0 & 0 \\ 0 & -2n & n \end{pmatrix}$	$\frac{m}{2n}\sqrt{2}h \xrightarrow{\sqrt{3}m} \frac{1}{2}\sqrt{2}t$
$\sqrt{2}\,T$	$\frac{m}{n}\sqrt{2}$	$Z[2m\ 0\ n]$ $[0\,2n\,0]_*\quad[n\,\bar{n}\,2\bar{m}]_*$	$S_{18} = \begin{pmatrix} 0 & m & 2m \\ 2m & -m & 0 \\ 0 & -n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}t \xrightarrow{2m} \sqrt{\frac{3}{2}}h$
		$[\bar{n}\,\bar{n}\,2m]_*\quad[0\,2n\,0]_*$	$S_{19} = \begin{pmatrix} -m & 0 & 2m \\ -m & 2m & 0 \\ n & 0 & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}t \xrightarrow{2m} \sqrt{\frac{3}{2}}h$
		$[\bar{n}\,3n\,2m]_*\quad[2n\,0\,4\bar{m}]_*$	$S_{20} = \begin{pmatrix} -m & 2m & 2m \\ 3m & 0 & 0 \\ n & -2n & n \end{pmatrix}$	$\frac{m}{n}\sqrt{2}t \xrightarrow{2\sqrt{3}m} \frac{1}{2}\sqrt{2}h$
		$Z[1\ 1\ 0]$ $[n\,\bar{n}\,2m]_*\quad[\bar{n}\,n\,2m]_*$	$S_{21} = \begin{pmatrix} m & -m & 1 \\ -m & m & 1 \\ n & n & 0 \end{pmatrix}$	$\frac{m}{n}\sqrt{2}t \xrightarrow{2m} \frac{1}{2m}\sqrt{2}t$

$$\begin{aligned} \Lambda(a) &\xrightarrow{\mathbb{R}} \Sigma(s) = \Sigma(Sa) = S\Lambda(a), \\ g(a) &\xrightarrow{\mathbb{R}} g(s) = g(Sa) = \tilde{S}g(a)S, \\ K(a) &\xrightarrow{\mathbb{R}} K(Sa) = SK(a)S^{-1}, \quad S \in GL(3,\mathbb{R}). \end{aligned} \tag{37}$$

An *integral transformation* $S \in GL(3,\mathbb{Z})$ leaves the lattice invariant, whereas metric tensor and point group are transformed into *arithmetic* equivalent ones

$$\Lambda(Sa) = \Lambda(a), \quad g(Sa) = \tilde{S}g(a)S \overset{\mathbb{Z}}{\sim} g(a), \quad SK(a)S^{-1} \overset{\mathbb{Z}}{\sim} K(a) \tag{38}$$

with $S \in GL(3,\mathbb{Z})$. There are 73 arithmetic classes of the three-dimensional point groups.

The *rational transformations* $S \in GL(3,\mathbb{Q})$ lead in a similar way to *geometric* equivalence classes:

$$\begin{aligned} \Lambda(a) &\overset{\mathbb{Q}}{\sim} S\Lambda(a), \quad g(Sa) = \tilde{S}g(a)S \overset{\mathbb{Q}}{\sim} g(a), \\ SK(a)S^{-1} &\overset{\mathbb{Q}}{\sim} K(a), \qquad S \in GL(3,\mathbb{Q}). \end{aligned} \tag{39}$$

There are 32 geometric classes of the three-dimensional point groups, which are called *crystal classes*. Geometric equivalent lattices have the property to be in a lattice–sublattice relation, as considered in the previous sections:

$$\Lambda \overset{\mathbb{Q}}{\sim} \Sigma \quad \leftrightarrow \quad \Lambda \subseteq \Sigma \quad \text{or} \quad \Sigma \subseteq \Lambda. \tag{40}$$

In crystallography, affine equivalence is considered for isomorphic space groups, for point groups it is replaced by group isomorphism, whereas all lattices of a given dimension are affine equivalent. As for lattices, the arithmetic equivalence means identity, the arithmetic class of their holohedry is considered instead, leading to the *Bravais classes*. The geometric classes of the holohedries define, in a similar way, the *crystal systems*. What have been considered in the previous sections are in fact the geometric classes of the lattices themselves, with equivalence indicated by a $\sim$ symbol. The rational equivalence of integral lattices is presented first in the general case and then for two and three dimensions.

8.1. General case

The problem of the classification of integral lattices according to geometric equivalence classes has been solved by Minkowski, Hasse and Witt (see ch. 15 in Conway & Sloane, 1988, and references therein). The full theory requires notions that go beyond the aim of the present work, like *p-adic* invariants for integral forms. Here, only three basic and elementary properties are considered, which help to find the rational equivalence in most of the relevant crystallographic cases.

I. An integral symmetric matrix is rational equivalent to a diagonal matrix:

Table 5
1-hexagonal family (isometric).

Family	γ	Zone	Transformation	Scaling relation
$1H$	$\frac{m}{n}$	$Z[1\ 0\ 0] = F$ $[0\,0\,4m]_*$ $[0\,3n\,2\bar{m}]_*$	$S_{22} = \begin{pmatrix} 0 & m & 1 \\ 0 & 2m & 0 \\ 2n & -n & 0 \end{pmatrix}$	$\frac{m}{n}h \xrightarrow{2m} \frac{1}{2m}h$
		$[0\,\bar{n}\,2m]_*$ $[0\,2n\,0]_*$	$S_{23} = \begin{pmatrix} -m & 2m & 1 \\ -2m & 4m & 0 \\ 3n & 0 & 0 \end{pmatrix}$	$\frac{m}{n}h \xrightarrow{2\sqrt{3}m} \frac{1}{6m}\sqrt{3}h$
		$Z[2\ 1\ 0] = G$ $[\bar{n}\,2n\,0]_*$ $[0\,0\,2m]_*$	$S_{24} = \begin{pmatrix} 0 & 0 & 2 \\ m & 0 & 1 \\ 0 & n & 0 \end{pmatrix}$	$\frac{m}{n}h \xrightarrow{m} \frac{1}{m}\sqrt{3}t$

$$\tilde{S}g'S = \mathrm{diag}\{a, b, c, \ldots\} = g\{a, b, c, \ldots\}, \quad S \in GL(n, \mathbb{Q}). \tag{41}$$

Different sequences of the diagonal elements are arithmetically equivalent. From the crystallographic point of view, (I) implies that any integral lattice is rational equivalent to an orthorhombic one and, therefore, for any given integral lattice there are always super- and sublattices that are orthorhombic.

II. The elements $\{a, b, c, d, \ldots\}$ of the diagonal matrix can be assumed to be square free integers.

It is sufficient to consider the first diagonal element and to suppose $a = n^2a_0$ for n integer. Then by $S = \mathrm{diag}(1/n, 1, \ldots, 1)$, one gets

$$g\{n^2a_0, b, c, d, \ldots\} \overset{\mathbb{Q}}{\sim} g\{a_0, b, c, d, \ldots\}. \tag{42}$$

III. Witt's cancellation theorem:

$$\text{If} \quad g\{a, b, c, d, \ldots\} \overset{\mathbb{Q}}{\sim} g\{a, b', c', d', \ldots\} \quad \text{and} \quad a \neq 0,$$

$$\text{then} \quad g\{b, c, d, \ldots\} \overset{\mathbb{Q}}{\sim} g\{b', c', d' \ldots\}. \tag{43}$$

This means that two rationally equivalent n-dimensional orthorhombic lattices that share one lattice parameter imply the equivalence of their $(n-1)$-dimensional orthorhombic sublattice having the remaining lattice parameters.

While one can always assume $a = 1$, by choosing the unit of length, this cannot be done for the two lattices independently. This is the reason why the families with members that are correspondingly related by an integral scaling transformation (as indicated in Tables 2 to 5) need not be rational equivalent.

Using this theorem, a number of three-dimensional cases can be reduced to the two-dimensional equivalence problem, without making explicit use of *p-adic* invariants.

8.2. Two-dimensional case

In two dimensions, there are four lattice systems: oblique, rectangular, square and hexagonal. According to the property (I), all integral ones can be transformed to a rectangular lattice by $S \in GL(2, \mathbb{Q})$. One may suppose $g_{11} = 1$, by choosing the appropriate unit of length:

$$\tilde{S}\begin{pmatrix} 1 & t \\ t & q \end{pmatrix}S = \begin{pmatrix} 1 & 0 \\ 0 & q - t^2 \end{pmatrix} = g_r(\gamma), \quad S = \begin{pmatrix} 1 & -t \\ 0 & 1 \end{pmatrix} \tag{44}$$

with $\gamma = \sqrt{q - t^2}$. Note that one always has $t^2 < q$. For g integral, $t \in \mathbb{Q}$, $S \in GL(2, \mathbb{Q})$. The axial ratio γ of the rectangular lattice $\Lambda(a) = \gamma r$, generated by the normalized basis $a = (a_1, a_2)$, is given by

$$\gamma = \sqrt{q - t^2} = \frac{m}{n}\gamma_0 = \frac{m}{n}\sqrt{\frac{m_0}{n_0}}$$

with m_0 and n_0 square free. According to property (II), $\gamma r \overset{\mathbb{Q}}{\longrightarrow} \gamma_0 r$.

Consider now a rectangular sublattice $\Sigma(s)$ of $\Lambda(a) = \gamma_0 r$, with basis vectors s_1, s_2 and axial ratio $\gamma_1 = \sqrt{m_1/n_1}$. Then,

$$s_1 = x_1a_1 + x_2a_2, \quad s_2 = y_1a_1 + y_2a_2, \quad x_1, x_2, y_1, y_2 \in \mathbb{Z}$$

$$s_1^2 = \frac{m_1}{n_1}s_2^2, \quad s_1s_2 = 0, \quad S = \begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix} \in GL(2, \mathbb{Q}). \tag{45}$$

Solving the equations leads to the relations $y_1 = -(m_0/n_0)(x_2/x_1)y_2$ and $x_1 = \sqrt{m_0n_1/n_0m_1}y_2$, *i.e.* to the condition

$$\gamma_1 = \frac{m}{n}\gamma_0, \quad \frac{m}{n} \in \mathbb{Q}. \tag{46}$$

The solution is then given by

$$x_1 = \frac{m}{n}y_2, \quad y_1 = -\frac{m_0}{n_0}\frac{n}{m}x_1. \tag{47}$$

Therefore, in two dimensions the geometric class of an integral lattice is fixed by the rectangular axial ratio γ_0.

8.3. Three-dimensional case

Let us first consider the rational diagonalization of integral metric tensors of the three-dimensional crystal systems. This yields an orthorhombic integral lattice with metric

$$g_{or}(pqr) = \begin{pmatrix} p & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & r \end{pmatrix}, \quad p, q, r \in \mathbb{Z}. \tag{48}$$

Triclinic:

$$g_{tr}(a) = \begin{pmatrix} p & t & u \\ t & q & v \\ u & v & r \end{pmatrix} = g_{tr}(pqr, tuv).$$

By

$$S_1 = \begin{pmatrix} q & 0 & 0 \\ -t & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

one gets $\tilde{S}_1 g_{tr}(pqr, tuv) S_1 = g_{tr}(p'q'r', 0u'v')$.

By

$$S_2 = \begin{pmatrix} v & qu & qu \\ -u & pv & pv \\ 0 & 0 & 1 \end{pmatrix},$$

one gets $\tilde{S}_2 g_{tr}(pqr, 0uv) S_2 = g_{tr}(p'q'r', 00v')$.

By

$$S_3 = \begin{pmatrix} 0 & 0 & 1 \\ r & 0 & 0 \\ -v & 1 & 0 \end{pmatrix},$$

one gets $\tilde{S}_3 g_{tr}(pqr, 00v) S_3 = g_{tr}(p'q'r', 000)$.

A combination of these transformations allows one to diagonalize triclinic and monoclinic metric tensors.

Monoclinic:

$$g_m(pqr, v) = g_{tr}(pqr, 00v).$$

Tetragonal:

$$g_t(pr) = g_{or}(ppr) = g_{tr}(ppr, 000).$$

Hexagonal:

$$g_h(pr) = g_{or}(p3pr) = g_{tr}(p3pr, 000).$$

After these preliminary results, let us look at the rational equivalence of the hexagonal families $\sqrt{\frac{3}{2}}H$, $\sqrt{3}H$, $\sqrt{2}H$, $1H$ and of the tetragonal ones $\sqrt{2}T$, $\sqrt{3}T$, considered in the previous sections. For all these families, one can choose a normalized metric tensor so that they all share the lattice parameter $a = 1$. In the above parametrization, $p = a^2$ is also 1. One can, therefore, apply Witt's cancellation theorem (III) and reduce the problem to the two-dimensional rectangular case. The two-dimensional axial ratio is not the same as the three-dimensional one. So, for example for $\sqrt{\frac{3}{2}}H$ with $a = 1$ and $c = \sqrt{\frac{3}{2}}$:

$$g_h(1\tfrac{3}{2}) \overset{\mathbb{Q}}{\sim} g_{or}(13\tfrac{3}{2}) \longrightarrow g_r(3\tfrac{3}{2}) \longrightarrow \gamma = \tfrac{1}{\sqrt{2}} \sim \gamma_0 = \sqrt{2},$$

yielding

$$\sqrt{\tfrac{3}{2}}H \longrightarrow \sqrt{2}r. \tag{49}$$

In a similar way, one finds the correspondences

$$\begin{aligned} &\sqrt{2}H \longrightarrow \sqrt{\tfrac{3}{2}}r, \quad \sqrt{3}H \longrightarrow 1r, \quad 1H \longrightarrow \sqrt{3}r, \\ &\sqrt{2}T \longrightarrow \sqrt{2}r, \quad \sqrt{3}T \longrightarrow \sqrt{3}r. \end{aligned} \tag{50}$$

Accordingly, one finds

$$1H \overset{\mathbb{Q}}{\sim} \sqrt{3}T, \quad \sqrt{\tfrac{3}{2}}H \overset{\mathbb{Q}}{\sim} \sqrt{2}T. \tag{51}$$

All the other families, indicated above, are rationally inequivalent.

This result is consistent with the integral scaling relations reported in Tables 2 to 5. So, for example, the integral scaling relation between $\sqrt{\frac{3}{2}}H$ and $\sqrt{2}H$ implied by the transformation S_2 of Table 2 does not imply rational equivalence because the scaling factor $\mu = 3\sqrt{3}m$ is not rational.

9. Extended rational equivalence

The equivalence relation to be adopted for classifying lattices depends on the properties considered. Geometric equivalence is applicable for lattice–sublattice relations or if one considers the frequency distribution of crystals as a function of a single lattice parameter, as done by Constant & Shlichta (2003) for cubic crystals.

There are other lattice properties that are also invariant with respect to a scalar multiplication of their metric tensor, like the point-group symmetry or the axial ratio for hexagonal and tetragonal integral lattices. In these cases, it is appropriate to extend the rational equivalence with the additional equivalence:

IV. Extended rational equivalence:

Two integral metric tensors that differ by a non-zero integral factor z are equivalent:

$$g(a) \sim zg(a) = g(\sqrt{z}a), \quad z \in \mathbb{Z}, z \neq 0. \tag{52}$$

This equivalence relation can be expressed in a way similar to the rational equivalence by considering the set of matrices $\sqrt{z}S$, with $z \in \mathbb{Z}$ and $S \in GL(n, \mathbb{Q})$. These matrices form a subgroup of $GL(n, \mathbb{R})$. In particular, $(\sqrt{z}S)^{-1} = \sqrt{z}(zS^{-1})$. A possible notation for this group is $\sqrt{\mathbb{Z}}GL(n, \mathbb{Q})$. Actually, as remarked by Souvignier to the author, by transitivity, this group also consists of matrices of $GL(n, \mathbb{Q})$ multiplied by the square root of a non-zero rational number, so that a better notation is $\sqrt{\mathbb{Q}}GL(n, \mathbb{Q})$:

$$\sqrt{\mathbb{Q}}GL(n, \mathbb{Q}) = \left\{ \sqrt{\frac{m}{n}}S \,\middle|\, \frac{m}{n} \neq 0, \frac{m}{n} \in \mathbb{Q}, S \in GL(n, \mathbb{Q}) \right\}. \tag{53}$$

One can then reformulate the property (IV).

IV′. Integral lattices Λ and Λ', with metric tensors g and g', respectively, such that

$$g' = \tilde{S}gS, \quad S \in \sqrt{\mathbb{Q}}GL(n, \mathbb{Q}), \tag{54}$$

are extended rationally equivalent:

$$g \overset{\sqrt{z}\mathbb{Q}}{\sim} g', \quad \Lambda \overset{\sqrt{z}\mathbb{Q}}{\sim} \Lambda', \quad z \in \mathbb{Z}. \tag{55}$$

This equivalence relation implies rational equivalence and an extended equivalence class consists of one or more rationally equivalent classes.

One can now reformulate the property (II).

V. The diagonal elements $\{a, b, c, d, \ldots\}$ of the metric tensor of an orthorhombic integral lattice can be assumed to be pair-wise relatively prime.

If a pair has a common factor z, one has

$$g_{or}(za_0, zb_0, c, d, \ldots) \overset{\sqrt{z}\mathbb{Q}}{\sim} g_{or}(a_0, b_0, zc, zd, \ldots). \tag{56}$$

Indeed,

$$g_{or}(za_0, zb_0, c, d, \ldots) = zg_{or}(a_0, b_0, \tfrac{c}{z}, \tfrac{d}{z}, \ldots) \overset{\mathbb{Q}}{\sim} z\, g_{or}(a_0, b_0, zc, zd, \ldots).$$

This same equivalence has been considered by Fricke & Klein (1897) for ternary indefinite integral quadratic forms.

9.1. Application

It is now possible to discuss this extended equivalence for the six three-dimensional families $\sqrt{3/2}H$, $\sqrt{3}H$, $\sqrt{2}H$, $1H$, $\sqrt{2}T$, $\sqrt{3}T$. The rational equivalences $\sqrt{3/2}H \sim \sqrt{2}T$ and $1H \sim \sqrt{3}T$ have already been derived. In addition, one now has

$$\sqrt{\tfrac{3}{2}}H = g_{or}(13\tfrac{3}{2}) \sim g_{or}(263) \sim g_{or}(136) \sim g_{or}(312),$$
$$\sqrt{2}H = g_{or}(132),$$

implying

$$\sqrt{\tfrac{3}{2}}H \overset{\sqrt{z}\mathbb{Q}}{\sim} \sqrt{2}H \overset{\sqrt{z}\mathbb{Q}}{\sim} \sqrt{2}T, \quad z \in \mathbb{Z}. \tag{57}$$

In a similar way,

$$\sqrt{3}H = g_{or}(133) \sim g_{or}(311),$$
$$\sqrt{3}T = g_{or}(113),$$

thus

$$\sqrt{3}H \overset{\sqrt{z}\mathbb{Q}}{\sim} 1H \overset{\sqrt{z}\mathbb{Q}}{\sim} \sqrt{3}T, \quad z \in \mathbb{Z}. \tag{58}$$

Moreover, $\sqrt{2}T$ is not equivalent with $\sqrt{3}T$, so that these six families of axial lattices split into two inequivalent extended rational classes.

10. Conclusions

There are three empirical roots of the present work.

1. The existence of molecular forms of a number of axial-symmetric biomacromolecules characterized by integral lattices, like those explicitly considered here (Janner, 2004).

2. The occurrence of sharp peaks in the distribution of crystals at integral lattice positions (Constant & Shlichta, 2003; Janner, 2004).

3. The peculiar symmetry of zones in Frank's cubic hexagonal structures, and related ones, with Bragg peaks at points of a square lattice, and of tetragonal crystals having zones with hexagonal lattice symmetry (Frank, 1965; Singh *et al.*, 1998; Ranganathan *et al.*, 2002).

The explanation of all these observations is still missing, despite partial interpretations. Some of these facts can be considered to be accidental but not all of them. There is certainly an interplay between composition and geometry. One way to attack this difficult problem involving a non-negligible number of crystal structures is to restrict the consideration to the geometry only and to learn more about the properties of integral lattices. This is what has been attempted in this paper, starting from a few concrete cases towards an appropriate mathematical characterization. The other way round, from mathematics to crystallography, is much more difficult. One has to be aware that the field involved, that of integral quadratic forms and quadratic spaces, has been intensively studied by the greatest mathematicians over more than two centuries. The knowledge required is beyond the range of crystallography.

The results reached in this note in a fairly elementary way appear to fit the general mathematical theory: moreover, the rational equivalence of integral quadratic forms (describing the metric of the lattices) is a completely solved problem that goes beyond the rational equivalence of the point-group symmetry of the lattices classified accordingly in crystal systems. Both equivalence relations are based on transformations by the same geometric linear group $GL(n, \mathbb{Q})$, which occurs for properties like zones and lattice–sublattice relations. One is, however, surprised to find out that for other properties like axial ratio or point-group symmetry it is another linear group that is relevant for the appropriate extended rational equivalence: the group denoted here as $\sqrt{\mathbb{Q}}GL(n, \mathbb{Q})$ of invertible rational matrices multiplied by the square root of non-zero rationals. The lack in the literature of a specific notation for this group is probably because mathematicians are primarily interested in quadratic forms and less in the corresponding lattices.

The practical utility of these concepts for the problems raised by the empirical observations mentioned in the *Introduction* and in this section seems at first to be very limited and to suggest only some ways of approach. For example, instead of considering the frequency distribution of monoclinic crystals as a function of their lattice parameters, it could be more convenient to convert their lattices to rationally equivalent orthorhombic ones, which are characterized by fewer lattice parameters. This appears indeed to be the case (de Gelder & Janner, 2004*b*). Also, the hexagonal and tetragonal crystals could be considered as special cases of the orthorhombic ones, allowing for a comparison with the non-axial lattices.

In fact, the crystallographic importance of the zones derived is possibly greater than one would think. Indeed, the property of a crystal to appear within a given γ peak of integral lattices can be accidental or due to structural relations, leading to additional (hidden) symmetries. It is important to be able to find out to which of these two cases a given crystal belongs. The geometric properties of an integral lattice are essentially different from those of a generic lattice case (as usually considered). The position of the Bragg peaks only depends on the lattice geometry, quite independently of whether the metrical relations are accidental or not. This is not the case for the intensity of the Bragg peaks. If one considers, in particular, the diffraction pattern of a hexagonal or square zone, it is unlikely that a symmetric intensity distribution will occur when the metrical relations observed are purely accidental. For the integral lattices discussed, the present work can help to identify the zones one should look at, in order to identify the crystals deserving to be analyzed further.

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