FOUNDATIONS ADVANCES

ISSN 2053-2733

A table of geometrical ambiguities in powder indexing obtained by exhaustive search

R. Oishi-Tomiyasu*

JST PRESTO, Kawaguchi, Saitama, Japan, and Tohoku University, Sendai, Miyagi, Japan. *Correspondence e-mail: ryoko.tomiyasu.a5@tohoku.ac.jp

Received 4 September 2015
Accepted 16 November 2015

Edited by J.-G. Eon, Universidade Federal do Rio de Janeiro, Brazil

Keywords: powder indexing; geometrical ambiguity; derivative lattices; computer programs; multiple solutions.

Supporting information: this article has supporting information at journals.iucr.org/a

Geometrical ambiguity means the cases in which more than one powder indexing solution exists. Using a new function implemented in the powder indexing software *CONOGRAPH*, unit cells that involve geometrical ambiguity are exhaustively searched. As a result, many unknown cases are obtained, although the number of such unit cells is still rather limited. It is also proven that the number of solutions in powder auto-indexing is not always unique, but generally finite.

1. Introduction

It is known that crystal structures with distinct unit cells can have powder diffraction patterns with perfectly identical peak positions. This phenomenon known as geometrical ambiguity was initially studied by Mighell & Santoro (1975), since the phenomenon causes a problem in powder indexing.

A new function (for a generalized version, see Table 1) introduced in a previous paper (Oishi-Tomiyasu, 2014*a*) can output all unit-cell parameters with the same peak positions, if ambiguity occurs for the input unit cell. This is impossible for the functions proposed in previous studies by Santoro *et al.* (1980) and Kroll *et al.* (2011), because they assume that distinct unit cells with the same peak positions are derivative of each other.

The short computation time of this new function enables an exhaustive search for unit cells that involve geometrical ambiguity (Table 2 of §3; although our function can also search for unit cells with almost the same peak positions, such unit cells were excluded from the table). All of the metric tensors corresponding to the unit cells in the table have rather small determinants, compared to those contained in the searched region. Hence it is naturally expected that all the cases of geometrical ambiguity are given.

In §4, it is proved that the number of solutions in powder indexing is not unique, but generally finite. More precisely, for any $\Lambda \subset \mathbb{R}_{>0}$, the number of pairs $(L^*, (G, H))$ of a reciprocal lattice $L^* \subset \mathbb{R}$ and a type of systematic absence (G, H) that have Λ as the set of d spacings is finite. This does not hold for lattices of dimension greater than four. All proofs are included in the supporting information.

The new function is available on the *CONOGRAPH* graphic user interface (http://conograph.osdn.jp/ConographGUI/web_page.html).

1.1. Notation and symbols

The following positive-definite symmetric matrix S of size 3 determined from the unit-cell parameters $a, b, c, \alpha, \beta, \gamma$ (or

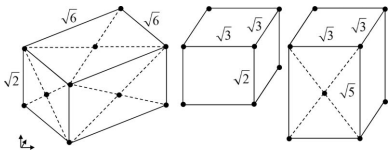

Table 1
A recursive function for lattice determination from $\Lambda \subset \mathbb{R}_{>0}$.

The asterisk symbol in line 19 signifies that the values of $p_{\min}$ and $p_{\max}$ are uniquely determined because equations (3) and (4) define a polyhedral convex cone.

void func$(\Lambda, M, N, S, m, n, q_{min}, q_{max}, Ans)$
(Input)
Λ : a sorted sequence $\langle q_1, \ldots, q_t \rangle$ of t positive numbers
M : a natural number
$1 \le N \le 4$: the dimension of lattices
S : an $N \times N$ metric tensor $(s_{ij})_{1 \le i,j \le N}$
m, n : integers $1 \le m \le n \le N$ indicating the algorithm is determining the (m,n)-entry of S
q_{min}, q_{max} : numbers indicating
$\begin{cases} \frac{q_{min}}{M^2} \le s_{nn} \le \frac{q_{max}}{M^2} & \text{if } m = n, \\ \frac{q_{min}}{M^2} \le s_{mm} + s_{nn} + 2s_{mn} \le \frac{q_{max}}{M^2} & \text{otherwise.} \end{cases}$
(Output)
Ans : an array of $N \times N$ Minkowski-reduced metric tensors $\tilde{S} := (\tilde{s}_{ij})$ that satisfy
$\begin{cases} \tilde{s}_{NN} \le q_t, \ \Lambda \cap [0, \tilde{s}_{NN}] \subset \Lambda(\tilde{S}), \\ \tilde{s}_{nn}, \tilde{s}_{mm} + \tilde{s}_{nn} + 2\tilde{s}_{mn} \in \frac{1}{M^2}\Lambda. \end{cases}$
(Start)
1: Take integers I and J such that $\Lambda \cap [q_{min}, q_{max}] = \langle q_I, \cdots, q_J \rangle$.
2: for $l = I$ to J do
3: if $m = n$ then
4: $s_{nn} := \frac{q_l}{M^2}$.
5: else
6: $s_{mn} := s_{nm} := \frac{1}{2}(\frac{q_l}{M^2} - s_{mm} - s_{nn})$.
7: end if
8: if $m = 1$ then
9: if $n \ge N$ then
10: Insert S in Ans.
11: else
12: $T := (s_{ij})_{1 \le i,j \le n}$. /* an $n \times n$ submatrix of S */.
13: $t_2 := \max\{1 \le i \le t : q_1, \ldots, q_{i-1} \in \Lambda(T)\}$.
14: func$(\Lambda, M, N, S, n+1, n+1, M^2 s_{nn}, M^2 q_{t_2}, Ans)$.
15: end if
16: else
17: Take p_{min}, p_{max} that satisfy the following:
18: $p_{min} \le s_{m-1m-1} + s_{nn} + 2s_{m-1n} \le p_{max}$
19 $\iff s_{m-1n}$ and the other entries of S satisfy (3) and (4)*.
20: func$(\Lambda, M, N, S, m-1, n, S, M^2 p_{min}, M^2 p_{max}, Ans)$.
21: end if
22: end for

the reciprocal unit-cell parameters $a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*$) is called a 3×3 *metric tensor*:

$$S := \begin{pmatrix} (a^*)^2 & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ a^*b^*\cos\gamma^* & (b^*)^2 & b^*c^*\cos\alpha^* \\ a^*c^*\cos\beta^* & b^*c^*\cos\alpha^* & (c^*)^2 \end{pmatrix} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}^{-1}. \quad (1)$$

If the positions of powder diffraction peaks are represented as q values ($d = q^{-1/2}$ is the d spacing), $\Lambda(S) := \{{}^t vSv : 0 \ne v \in \mathbb{Z}^3\}$ gives the set of all the q values. Hence, if two distinct unit cells have the same $\Lambda(S)$, their peak positions in powder diffraction patterns are perfectly identical. Such unit cells provide a case of geometrical ambiguity.

2. Algorithm

For simplicity, we assume that all values are exact and do not include errors. However, it is possible to extend the algorithm in Table 1 to the case of inaccurate values [see §2.2 of Oishi-Tomiyasu (2014*a*)].

Let S be an unknown $N \times N$ metric tensor with $N \le 4$. For a given input integer $M > 0$ and $\Lambda(S) := \{{}^t vSv : 0 \ne v \in \mathbb{Z}^N\}$, the algorithm returns a list containing all the $N \times N$ metric tensors S_2 that satisfy $\Lambda(S) \subset \Lambda(S_2) \subset M^{-2}\Lambda(S)$.

Recall that a set of vectors $v_1, \ldots, v_n$ of an N-dimensional lattice $L \subset \mathbb{R}^N$ is said to be *primitive* if it is a subset of some basis of L. An $N \times N$ metric tensor $S := (s_{ij})$ is *Minkowski-reduced* if the following holds for any $1 \le n \le N$:

$${}^t\mathbf{e}_n S \mathbf{e}_n = \min\left\{ {}^t vSv : \begin{array}{r} v \in \mathbb{Z}^N \text{ and } \langle \mathbf{e}_1, \ldots, \mathbf{e}_n, v \rangle \\ \text{is a primitive set of } \mathbb{Z}^N \end{array} \right\}, \quad (2)$$

where $\mathbf{e}_n$ is a vector with 1 in its nth component and 0 in the remaining components. For any $N \le 4$, S is Minkowski-reduced if and only if the following inequalities hold [*cf.* Lemma 1.2 of ch. 12, Cassels (1978)]:

$$\begin{cases} 0 < s_{11} \le \ldots \le s_{NN}, \\ s_{jj} \le {}^t vSv \text{ for any } 1 \le j \le N \text{ and vectors } v \text{ with} \\ v_i = -1, 0, 1 \ (1 \le i < j),\ v_j = 1,\ v_k = 0 \ (j < k \le N). \end{cases} \quad (3)$$

The following is frequently added to the definition of Minkowski reduction:

$$s_{ii+1} \le 0 \ (1 \le i < N). \quad (4)$$

Hereafter, equations (3) and (4) are adopted as the inequalities of the Minkowski reduction for $N \le 4$.

Table 1 presents a recursive function to generate $N \times N$ metric tensors from a set $\Lambda \subset \mathbb{R}_{>0}$. If the recursive procedure begins with arguments $m = n = 1, q_{\min} = q_1$ and $q_{\max} = M^2 q_1$, all the metric tensors that satisfy the following, in addition to (3) and (4), are enumerated in the output array:

$$\begin{cases} s_{NN} \le q_t, \ \Lambda \cap [0, s_{NN}] \subset \Lambda(S) := \{{}^t vSv : 0 \ne v \in \mathbb{Z}^N\}, \\ s_{nn}, s_{mm} + s_{nn} + 2s_{mn} \in M^{-2}\Lambda. \end{cases} \quad (5)$$

Hence, if a metric tensor S satisfies $\Lambda \subset \Lambda(S) \subset M^{-2}\Lambda$, S is output in the array when q_t is sufficiently large. After the algorithm terminates, it is possible to determine whether or not q_t was sufficiently large to ensure that all such S had been gained, by verifying if $t_2 < t$ holds in line 13 and the recursive function is always called with the argument $q_{\max} \le q_t$. If the inequalities always hold, all of the searched S are contained in the output. Otherwise, all such S may not have been obtained. The latter case may be considered to be caused by a similar reason to the dominant zone problem in powder indexing (*cf.* Shirley, 1980).

The algorithm is completed in a finite number of steps, even if $\Lambda(S_0)$ of an $N \times N$ metric tensor S_0 is used instead of a finite set Λ [this can be programmed by inputting S_0 instead of $\Lambda(S_0)$ and computing the elements of $\Lambda(S_0)$ in a finite interval $[a, b]$ when they are necessary]. Although $t = \infty$ in such cases, t_2 in line 13 of Table 1 is always finite. This is a consequence of

Proposition 1 (see Appendix *A* in the supporting information for the proof).

Proposition 1. Let S and S_2 be positive-definite metric tensors of sizes N and N_2. If $1 \le N_2 < \min\{4, N\}$, then $\Lambda(S) \not\subset \Lambda(S_2)$. Therefore, $\Lambda(S) \not\subset M^{-2}\Lambda(S_2)$ also holds for any integer $M > 0$.

The algorithm also relies on the fact that $s_{n+1n+1} \le q_{t_2}$ holds in line 13. This is proved as follows: $q_{t_2} \in \Lambda \subset \Lambda(S)$ does not belong to $\Lambda(T)$, where T is the matrix defined in line 12. Hence, there exists $v \in \mathbb{Z}^N$ such that $\mathbf{e}_1, \ldots, \mathbf{e}_n, v$ are linearly independent and ${}^t v S v = q_{t_2}$. Recall that the nth *successive minimum* of the Minkowski-reduced S is defined as follows:

$$\min\left\{ \max\{{}^t v_i S v_i : 1 \le i \le n\} : \begin{array}{c} v_1, \ldots, v_n \in \mathbb{Z}^N \\ \text{are linearly independent} \end{array} \right\}. \tag{6}$$

If $1 \le n \le N \le 4$, s_{nn} of a Minkowski-reduced $(s_{ij})_{1\le i,\, j\le N}$ equals its nth successive minimum (*cf.* van der Waerden, 1956). Therefore, $s_{n+1n+1} \le q_{t_2}$ holds in line 13 if $t_2 < t$.

After the algorithm finishes executing, it is possible to reduce the number of candidate solutions in *Ans* by (*a*) checking if $\Lambda \subset \Lambda(S) \cap [0, q_t]$ and $\Lambda(S) \cap [0, M^{-2}q_t] \subset M^{-2}\Lambda$ hold, (*b*) removing either of $S \ne S_2$, if they satisfy $S_2 = WS{}^tW$ for some $W \in GL_N(\mathbb{Z})$.

If the algorithm in Table 1 is used as a powder indexing method, it is not adversely affected by systematic absences as explained in §4. The dominant zone problem is also resolved theoretically as mentioned above. However, these advantageous properties are not exhibited if the Λ input as $\Lambda(S_0) \cap [0, q_t]$ includes errors and mistakes. Furthermore, its execution time diverges rapidly if M exceeds 1, while it is completed within 1 s if $M = 1$. For these reasons, another powder indexing method was adopted for *CONOGRAPH* (Oishi-Tomiyasu, 2014*b*).

3. Table of cases of geometrical ambiguity

For successful powder auto-indexing, it is important to know how often geometrical ambiguity occurs. In what follows, we discuss this problem. Geometrical ambiguity caused by a limited observed range is not considered herein, although the new function can also deal with such cases (*cf.* §3.1 Oishi-Tomiyasu, 2014*a*).

Firstly, it is known that geometrical ambiguity occurs for any hexagonal and rhombohedral cells; for any real numbers c and d, the following metric tensors have the same $\Lambda(S)$, although they are not equivalent over $\mathbb{Z}$:

(*a*) Hexagonal case

$$c\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & d \end{pmatrix}, c\begin{pmatrix} 2 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & d \end{pmatrix}.$$

(*b*) Rhombohedral case

$$c\begin{pmatrix} d & 1 & 1 \\ 1 & d & 1 \\ 1 & 1 & d \end{pmatrix}, c\begin{pmatrix} 2d+2 & 0 & 2 \\ 0 & 2d-2 & 0 \\ 2 & 0 & d \end{pmatrix}.$$

Consequently, even if S_1 and S_2 are not scalar multiples of rational matrices, $\Lambda(S_1) = \Lambda(S_2)$ may occur.

Conversely, if geometrical ambiguity occurs to metric tensors S_1 and S_2, and S_1 and S_2 are not scalar multiples of rational matrices, an infinite number of positive-definite rational metric tensors T_1, T_2 with $\Lambda(T_1) = \Lambda(T_2)$ are generated from $\Lambda(S_1) = \Lambda(S_2)$. We refer to Lemma A.1 of Appendix *A* for the proof.

Thus in order to see how often geometrical ambiguity occurs, it is sufficient to conduct an extensive search of metric tensors with rational entries. The algorithm in Table 1 was used with the argument $M = 1$ for the purpose. A metric tensor $S = (s_{ij})_{1\le i,\, j\le 3}$ is contained in the searched region if it satisfies the following:

(i) s_{11}, s_{22}, s_{33}, $2s_{12}$, $2s_{13}$, and $2s_{23}$ are integers, and their greatest common divisor is 1.

(ii) It is Niggli-reduced (*cf.* ch. 9.2.2, Hahn, 1983).

(iii) The obtained unit cells do not coincide with the above hexagonal and rhombohedral cases.

(iv) $s_{33} \le 115$.

If the upper bound in the last condition is increased, a scalar multiple of any metric tensors with rational entries is contained in the searched region.

The results of the exhaustive search are presented in Table 2. In this table, metric tensors are represented by their corresponding reciprocal unit-cell parameters, for application to powder indexing.

Overall, 53 cases consisting of 151 unit-cell parameters were obtained (Table 2). For example, No. 51 of Table 2 shows that metric tensors with orthorhombic (*I*, *C*), monoclinic (*B*) and triclinic symmetry can have perfectly identical peak positions. Since the number 151 is still small, it is not surprising that the actual examples of geometrical ambiguities are not known except for the high-symmetry cases in Mighell & Santoro (1975).

Considering that a perfect coincidence in peak positions is less likely to occur when the ratios of the entries of metric tensors are not represented by small integers, it is naturally expected that all the cases of geometrical ambiguity are included in the table or the above two families of rhombohedral and hexagonal cases. It is also expected that five is the maximum number of metric tensors that have identical peak positions. However, this conjecture might be a challenge even for modern mathematics, because it is not proved even that the unit cells in No. 35 have the same peak positions up to ∞ (see the footnote of Table 2). Note that all the unit cells in the table were only confirmed to have the same q values as peak positions up to $\max\{30\,000, 50D\}$, where D is the largest determinant among the cells in each group. This confirmation can be carried out computationally. The values of D are presented in the first column of Table 2.

Table 2
Reciprocal unit cells with perfectly identical peak positions.

The determinants of the metric tensors of the primitive cells are presented herein, not those of the conventional cells [*i.e.* det S of S in (1)]. As a result, the values provided are equal to multiplications of det S by 1 (primitive centring), 4 (base- or body-centred) or 16 (face-centred). This is in order to clarify the mysterious coincidence among the ratios of the determinants of the primitive cells. For example, the ratios computed for the cells in Nos. 51–53 are perfectly identical, although it is difficult to see this if the determinants of the conventional cells are used, owing to the difference in their centring types.

The Bravais types of the unit cells given by $a, b, c, \alpha, \beta, \gamma$ are presented for application to powder indexing solutions. The method in Oishi-Tomiyasu (2012) was used for the determination.

No.	Determinant (Ratio of determinants)	a^*	b^*	c^*	$\cos\alpha^*$	$\cos\beta^*$	$\cos\gamma^*$	Bravais type in real space
1	† 13824 (8)	$2\sqrt{11}$	$4\sqrt{2}$	$\sqrt{11}$	$-\frac{1}{\sqrt{22}}$	$-\frac{1}{11}$	$-\frac{1}{\sqrt{22}}$	Triclinic
	† 19008 (11)	$\sqrt{59}$	$4\sqrt{2}$	$\sqrt{11}$	$\frac{1}{\sqrt{22}}$	$\frac{5}{\sqrt{649}}$	$\frac{1}{\sqrt{118}}$	Triclinic
2	† 4608 (8)	$2\sqrt{5}$	$4\sqrt{3}$	$\sqrt{5}$	0	$\frac{1}{5}$	0	Monoclinic (P)
	† 6336 (11)	$2\sqrt{17}$	$2\sqrt{5}$	$\sqrt{5}$	$-\frac{1}{5}$	$-\frac{1}{\sqrt{85}}$	$-\frac{1}{\sqrt{85}}$	Triclinic
3	† 4608 (8)	$\sqrt{5}$	$2\sqrt{3}$	$2\sqrt{5}$	0	$\frac{1}{5}$	0	Monoclinic (B)
	† 6336 (11)	$2\sqrt{2}$	$2\sqrt{3}$	$\sqrt{17}$	0	$\frac{1}{\sqrt{34}}$	0	Monoclinic (B)
4	† 1536 (8)	$\sqrt{15}$	4	$\sqrt{7}$	0	$\frac{3}{\sqrt{105}}$	0	Monoclinic (P)
	† 2112 (11)	$\sqrt{23}$	$\sqrt{15}$	$\sqrt{7}$	$-\frac{3}{\sqrt{105}}$	$-\frac{1}{\sqrt{161}}$	$-\frac{3}{\sqrt{345}}$	Triclinic
5	† 1536 (8)	$\sqrt{7}$	2	4	0	$\frac{1}{\sqrt{7}}$	0	Monoclinic (B)
	† 2112 (11)	$\sqrt{7}$	2	$\sqrt{19}$	0	$\frac{1}{\sqrt{133}}$	0	Monoclinic (B)
6	† 864 (8)	$\sqrt{5}$	$\sqrt{6}$	$2\sqrt{2}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (B)
	† 1188 (11)	$\sqrt{15}$	$\sqrt{11}$	$2\sqrt{2}$	$-\frac{1}{\sqrt{22}}$	0	$-\frac{3}{\sqrt{165}}$	Triclinic
7	† 288 (8)	$\sqrt{3}$	$\sqrt{2}$	$2\sqrt{3}$	0	0	0	Orthorhombic (C)
	† 396 (11)	$\sqrt{2}$	$\sqrt{3}$	$\sqrt{17}$	0	$\frac{1}{\sqrt{34}}$	0	Monoclinic (B)
8	† 96 (8)	$\sqrt{6}$	1	2	0	0	0	Orthorhombic (C)
	† 132 (11)	$\sqrt{6}$	1	$\sqrt{7}$	0	$\frac{3}{\sqrt{42}}$	0	Monoclinic (B)
9	† 540 (5)	$\sqrt{2}$	$\sqrt{15}$	$\sqrt{5}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (B)
	† 864 (8)	$2\sqrt{2}$	$2\sqrt{6}$	$\sqrt{5}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (P)
10	† 180 (5)	$\sqrt{5}$	$\sqrt{3}$	$\sqrt{3}$	0	0	0	Orthorhombic (C)
	† 288 (8)	$2\sqrt{3}$	$2\sqrt{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (P)
11	† 60 (5)	$\sqrt{15}$	1	1	0	0	0	Orthorhombic (C)
	† 96 (8)	$2\sqrt{6}$	2	1	0	0	0	Orthorhombic (P)
12	675/4 (25)	$2\sqrt{2}$	$\sqrt{5}$	$\sqrt{5}$	$-\frac{1}{5}$	$-\frac{1}{\sqrt{10}}$	$-\frac{1}{4\sqrt{10}}$	Triclinic
	999/4 (37)	$2\sqrt{2}$	$2\sqrt{2}$	$\sqrt{5}$	$-\frac{1}{\sqrt{10}}$	$-\frac{1}{4\sqrt{10}}$	$-\frac{5}{16}$	Triclinic
13	225/4 (25)	$\frac{\sqrt{13}}{2}$	$\frac{\sqrt{3}}{2}$	$\sqrt{7}$	0	$\frac{4}{\sqrt{91}}$	0	Monoclinic (B)
	333/4 (37)	$\sqrt{7}$	$\sqrt{3}$	2	0	$\frac{1}{4\sqrt{7}}$	0	Monoclinic (P)
14	75/4 (25)	$\frac{\sqrt{19}}{2}$	$\frac{1}{2}$	2	0	$\frac{1}{2\sqrt{19}}$	0	Monoclinic (B)
	111/4 (37)	$\sqrt{7}$	1	2	0	$\frac{1}{4\sqrt{7}}$	0	Monoclinic (P)
15	162 (1)	$\frac{\sqrt{19}}{2}$	$\frac{3}{2}$	2	0	$\frac{1}{\sqrt{19}}$	0	Monoclinic (B)
	648 (4)	5	$\sqrt{7}$	2	$-\frac{1}{2\sqrt{7}}$	$-\frac{1}{10}$	$-\frac{2}{5\sqrt{7}}$	Triclinic
16	243/2 (1)	$\frac{9\sqrt{2}}{2}$	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{2}}{2}$	0	0	0	Orthorhombic (I)
	486 (4)	$\sqrt{41}$	$\sqrt{6}$	$\sqrt{2}$	0	$-\frac{1}{2\sqrt{82}}$	$-\frac{3}{2\sqrt{246}}$	Triclinic
17	81/2 (1)	$\frac{3\sqrt{6}}{2}$	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{2}}{2}$	0	0	0	Orthorhombic (I)
	162 (4)	$\sqrt{14}$	$\sqrt{6}$	$\sqrt{2}$	0	$-\frac{1}{4\sqrt{7}}$	$-\frac{3}{4\sqrt{21}}$	Triclinic
18	27/2 (1)	$\frac{\sqrt{14}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{2}$	0	$\frac{1}{2\sqrt{7}}$	0	Monoclinic (B)
	54 (4)	$2\sqrt{2}$	2	$\sqrt{2}$	$\frac{1}{4\sqrt{2}}$	$\frac{1}{8}$	$\frac{1}{2\sqrt{2}}$	Triclinic
19	162 (1)	$\sqrt{7}$	$\sqrt{7}$	$\sqrt{5}$	$-\frac{5}{2\sqrt{35}}$	$\frac{1}{2\sqrt{35}}$	$-\frac{3}{7}$	Triclinic
	162 (1)	$2\sqrt{2}$	$\sqrt{5}$	$\sqrt{5}$	$-\frac{3}{10}$	$-\frac{1}{\sqrt{10}}$	0	Triclinic

Table 2 (continued)

No.	Determinant (Ratio of determinants)	a^*	b^*	c^*	$\cos\alpha^*$	$\cos\beta^*$	$\cos\gamma^*$	Bravais type in real space
20	58 (1)	$\sqrt{5}$	$\sqrt{5}$	$\sqrt{3}$	$\frac{3}{2\sqrt{15}}$	$\frac{1}{2\sqrt{15}}$	$\frac{3}{10}$	Triclinic
	58 (1)	$\sqrt{7}$	$\sqrt{3}$	$\sqrt{3}$	$\frac{1}{6}$	$\frac{1}{\sqrt{21}}$	$\frac{1}{2\sqrt{21}}$	Triclinic
21	† 27 (1)	$\frac{3\sqrt{3}}{2}$	$\frac{1}{2}$	2	0	0	0	Orthorhombic (*C*)
	† 27 (1)	$\frac{\sqrt{19}}{2}$	$\frac{1}{2}$	$\sqrt{7}$	0	$\frac{5}{\sqrt{133}}$	0	Monoclinic (*B*)
22	† 27/4 (1)	$\frac{3\sqrt{3}}{2}$	$\frac{1}{2}$	1	0	0	0	Orthorhombic (*C*)
	† 27/4 (1)	$\frac{\sqrt{7}}{2}$	$\frac{1}{2}$	2	0	$\frac{1}{2\sqrt{7}}$	0	Monoclinic (*B*)
23	531/4 (59)	$\sqrt{6}$	$\sqrt{5}$	$\sqrt{5}$	$-\frac{1}{5}$	$-\frac{3}{2\sqrt{30}}$	0	Triclinic
	639/4 (71)	$2\sqrt{2}$	$\sqrt{5}$	$\sqrt{5}$	$-\frac{2}{5}$	$-\frac{1}{2\sqrt{10}}$	$-\frac{1}{4\sqrt{10}}$	Triclinic
24	177/4 (59)	$\sqrt{7}$	2	$\sqrt{2}$	$\frac{1}{4\sqrt{2}}$	$\frac{1}{\sqrt{14}}$	$\frac{1}{\sqrt{7}}$	Triclinic
	213/4 (71)	$\sqrt{7}$	2	$\sqrt{2}$	$-\frac{1}{4\sqrt{2}}$	$-\frac{1}{2\sqrt{14}}$	0	Triclinic
25	81 (4)	$\sqrt{6}$	2	2	$-\frac{1}{4}$	$-\frac{3}{4\sqrt{6}}$	0	Triclinic
	567/4 (7)	$\sqrt{7}$	$\sqrt{6}$	2	$\frac{3}{4\sqrt{6}}$	$\frac{1}{2\sqrt{7}}$	$\frac{3}{2\sqrt{42}}$	Triclinic
26	† 135 (5)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{15}}{2}$	$2\sqrt{2}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (*B*)
	† 216 (8)	$\sqrt{2}$	$\sqrt{6}$	$\sqrt{5}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (*B*)
	† 297 (11)	3	$2\sqrt{2}$	$\sqrt{5}$	$\frac{1}{2\sqrt{10}}$	$\frac{1}{2\sqrt{5}}$	$\frac{1}{2\sqrt{2}}$	Triclinic
27	† 45 (5)	$\sqrt{3}$	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{3}}{2}$	0	0	0	Orthorhombic (*F*)
	† 72 (8)	$\sqrt{3}$	$\sqrt{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (*C*)
	† 99 (11)	$\frac{\sqrt{17}}{2}$	$\frac{\sqrt{3}}{2}$	$2\sqrt{2}$	0	$\frac{1}{\sqrt{34}}$	0	Monoclinic (*B*)
28	† 15 (5)	$\frac{\sqrt{15}}{2}$	1	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 24 (8)	$\sqrt{6}$	1	1	0	0	0	Orthorhombic (*C*)
	† 33 (11)	$\frac{\sqrt{19}}{2}$	$\frac{1}{2}$	$\sqrt{7}$	0	$\frac{1}{\sqrt{133}}$	0	Monoclinic (*B*)
29	† 48 (3)	$2\sqrt{2}$	$2\sqrt{2}$	1	0	0	$\frac{1}{2}$	Hexagonal
	† 176 (11)	$\sqrt{22}$	$\sqrt{2}$	1	0	0	0	Orthorhombic (*C*)
	† 192 (12)	$2\sqrt{6}$	$2\sqrt{2}$	1	0	0	0	Orthorhombic (*P*)
30	† 3 (3)	$\sqrt{2}$	$\sqrt{2}$	1	0	0	$\frac{1}{2}$	Hexagonal
	† 11 (11)	$\frac{\sqrt{22}}{2}$	$\frac{\sqrt{2}}{2}$	1	0	0	0	Orthorhombic (*C*)
	† 12 (12)	$\sqrt{6}$	$\sqrt{2}$	1	0	0	0	Orthorhombic (*P*)
31	† 3/2 (3)	1	1	$\sqrt{2}$	0	0	$\frac{1}{2}$	Hexagonal
	† 11/2 (11)	$\frac{\sqrt{11}}{2}$	$\frac{1}{2}$	$\sqrt{2}$	0	0	0	Orthorhombic (*C*)
	† 6 (12)	$\sqrt{3}$	$\sqrt{2}$	1	0	0	0	Orthorhombic (*P*)
32	† 16 (1)	1	1	1	0	0	0	Cubic (*F*)
	† 64 (4)	$\sqrt{2}$	1	$2\sqrt{2}$	0	0	0	Orthorhombic (*C*)
	† 144 (9)	$3\sqrt{2}$	$\sqrt{2}$	1	0	0	0	Orthorhombic (*I*)
33	† 2 (1)	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$\frac{5}{6}$	$\frac{5}{6}$	$\frac{5}{6}$	Rhombohedral
	† 8 (4)	$\sqrt{2}$	1	1	0	0	0	Orthorhombic (*C*)
	† 18 (9)	$\frac{\sqrt{11}}{2}$	$\frac{1}{2}$	$2\sqrt{2}$	0	$\frac{2}{\sqrt{22}}$	0	Monoclinic (*B*)
34	† 1 (1)	1	1	1	0	0	0	Cubic (*P*)
	† 4 (4)	$\sqrt{2}$	$\sqrt{2}$	1	0	0	0	Tetragonal (*P*)
	† 9 (9)	$\frac{3\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	1	0	0	0	Orthorhombic (*C*)
35	† 27/2 (2)	$\frac{3}{2}$	$\frac{\sqrt{6}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	†54 (8)	3	$\sqrt{6}$	1	0	0	0	Orthorhombic (*P*)
	†! 297/4 (11)	$\frac{\sqrt{51}}{2}$	$\frac{1}{2}$	$\sqrt{6}$	0	$\frac{1}{\sqrt{34}}$	0	Monoclinic (*B*)
36	† 25/2 (2)	$\frac{\sqrt{10}}{2}$	$\frac{\sqrt{5}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 75/4 (3)	$\frac{\sqrt{15}}{2}$	$\frac{1}{2}$	$\sqrt{5}$	0	0	0	Orthorhombic (*C*)
	† 50 (8)	$\sqrt{10}$	$\sqrt{5}$	1	0	0	0	Orthorhombic (*P*)

Table 2 (continued)

No.	Determinant (Ratio of determinants)	a^*	b^*	c^*	$\cos\alpha^*$	$\cos\beta^*$	$\cos\gamma^*$	Bravais type in real space
37	† 5/2 (2)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 15/4 (3)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{3}}{2}$	1	0	0	0	Orthorhombic (*C*)
	† 10 (8)	$\sqrt{5}$	$\sqrt{2}$	1	0	0	0	Orthorhombic (*P*)
38	† 25/4 (1)	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	Rhombohedral
	† 25 (4)	$\frac{\sqrt{10}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{5}$	0	0	0	Orthorhombic (*C*)
	† 25 (4)	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{5}}{2}$	$\sqrt{7}$	0	$\frac{1}{\sqrt{21}}$	0	Monoclinic (*B*)
39	† 5/4 (1)	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	Rhombohedral
	† 5 (4)	$\frac{\sqrt{10}}{2}$	$\frac{\sqrt{2}}{2}$	1	0	0	0	Orthorhombic (*C*)
	† 5 (4)	$\frac{\sqrt{7}}{2}$	$\frac{1}{2}$	$\sqrt{3}$	0	$\frac{1}{\sqrt{21}}$	0	Monoclinic (*B*)
40	624 (39)	$\sqrt{6}$	$\sqrt{6}$	$\sqrt{5}$	0	$\frac{2}{\sqrt{30}}$	0	Monoclinic (*B*)
	1136 (71)	$\sqrt{21}$	$2\sqrt{3}$	$\sqrt{5}$	$-\frac{1}{\sqrt{15}}$	$-\frac{1}{\sqrt{105}}$	$-\frac{1}{3\sqrt{7}}$	Triclinic
	1264 (79)	$2\sqrt{6}$	$2\sqrt{3}$	$\sqrt{5}$	$-\frac{1}{\sqrt{15}}$	0	$-\frac{1}{3\sqrt{2}}$	Triclinic
	1520 (95)	$2\sqrt{7}$	$2\sqrt{3}$	$\sqrt{5}$	$-\frac{1}{\sqrt{15}}$	$-\frac{1}{\sqrt{35}}$	0	Triclinic
41	39 (39)	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{6}}{2}$	$\sqrt{5}$	0	$\frac{2}{\sqrt{30}}$	0	Monoclinic (*B*)
	71 (71)	$\sqrt{6}$	$\sqrt{5}$	$\sqrt{3}$	$\frac{1}{\sqrt{15}}$	$\frac{1}{3\sqrt{2}}$	$\frac{2}{\sqrt{30}}$	Triclinic
	79 (79)	$\sqrt{6}$	$\sqrt{5}$	$\sqrt{3}$	$-\frac{1}{\sqrt{15}}$	$-\frac{1}{3\sqrt{2}}$	0	Triclinic
	95 (95)	$\sqrt{7}$	$\sqrt{5}$	$\sqrt{3}$	$-\frac{1}{\sqrt{15}}$	0	$-\frac{1}{\sqrt{35}}$	Triclinic
42	39/2 (39)	$\frac{3}{2}$	$\frac{\sqrt{3}}{2}$	$\sqrt{3}$	0	$\frac{1}{3\sqrt{3}}$	0	Monoclinic (*B*)
	71/2 (71)	$\sqrt{5}$	$\sqrt{3}$	$\sqrt{3}$	$\frac{1}{6}$	$\frac{3}{2\sqrt{15}}$	$\frac{1}{\sqrt{15}}$	Triclinic
	79/2 (79)	$\sqrt{5}$	$\sqrt{3}$	$\sqrt{3}$	$-\frac{1}{6}$	$-\frac{1}{\sqrt{15}}$	$-\frac{1}{2\sqrt{15}}$	Triclinic
	95/2 (95)	$\sqrt{5}$	$\sqrt{5}$	$\sqrt{3}$	$\frac{3}{2\sqrt{15}}$	$\frac{1}{\sqrt{15}}$	$\frac{1}{2}$	Triclinic
43	† 112 (7)	$\sqrt{5}$	$\sqrt{5}$	$\sqrt{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	Rhombohedral
	† 240 (15)	$\sqrt{10}$	$\sqrt{3}$	$\sqrt{2}$	0	0	0	Orthorhombic (*I*)
	† 368 (23)	$\sqrt{10}$	$\sqrt{2}$	$\sqrt{5}$	0	$\frac{2}{5\sqrt{2}}$	0	Monoclinic (*B*)
	† 448 (28)	$2\sqrt{3}$	$2\sqrt{2}$	$\sqrt{5}$	0	$\frac{1}{\sqrt{15}}$	0	Monoclinic (*P*)
44	† 7 (7)	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	Rhombohedral
	† 15 (15)	$\frac{\sqrt{10}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (*C*)
	† 23 (23)	$\frac{\sqrt{10}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{5}$	0	$\frac{2}{5\sqrt{2}}$	0	Monoclinic (*B*)
	† 28 (28)	$\sqrt{5}$	$\sqrt{2}$	$\sqrt{3}$	0	$\frac{1}{\sqrt{15}}$	0	Monoclinic (*P*)
45	† 7/2 (7)	$\sqrt{5}$	$\sqrt{5}$	$\sqrt{5}$	$\frac{9}{10}$	$\frac{9}{10}$	$\frac{9}{10}$	Rhombohedral
	† 15/2 (15)	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{5}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 23/2 (23)	$\frac{\sqrt{11}}{2}$	$\frac{1}{2}$	$\sqrt{5}$	0	$\frac{3}{\sqrt{55}}$	0	Monoclinic (*B*)
	† 14 (28)	$\sqrt{5}$	1	$\sqrt{3}$	0	$\frac{1}{\sqrt{15}}$	0	Monoclinic (*P*)
46	† 27/4 (1)	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	Rhombohedral
	† 27 (4)	$\frac{3\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (*C*)
	† 27 (4)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{3}}{2}$	$2\sqrt{2}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (*B*)
	† 189/4 (7)	$2\sqrt{2}$	$\sqrt{3}$	$\sqrt{2}$	0	$\frac{1}{8}$	0	Monoclinic (*P*)
47	† 9/4 (1)	1	1	$\sqrt{3}$	0	0	$\frac{1}{2}$	Hexagonal
	† 9 (4)	$\sqrt{3}$	$\sqrt{3}$	1	0	0	0	Tetragonal (*P*)
	† 9 (4)	$\sqrt{3}$	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 63/4 (7)	$\frac{\sqrt{21}}{2}$	$\frac{\sqrt{3}}{2}$	1	0	0	0	Orthorhombic (*C*)
48	† 3/4 (1)	1	1	1	0	0	$\frac{1}{2}$	Hexagonal
	† 3 (4)	1	1	$\sqrt{3}$	0	0	0	Tetragonal (*P*)
	† 3 (4)	1	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 21/4 (7)	$\frac{\sqrt{7}}{2}$	$\frac{1}{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (*C*)
49	† 27/4 (1)	1	1	3	0	0	$\frac{1}{2}$	Hexagonal
	† 27/4 (1)	$\sqrt{3}$	$\sqrt{3}$	1	0	0	$\frac{1}{2}$	Hexagonal
	† 27 (4)	3	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 27 (4)	3	$\sqrt{3}$	1	0	0	0	Orthorhombic (*P*)

Table 2 (continued)

No.	Determinant (Ratio of determinants)	a^*	b^*	c^*	$\cos\alpha^*$	$\cos\beta^*$	$\cos\gamma^*$	Bravais type in real space
50	† 1/2 (1)	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	0	0	0	Cubic (*I*)
	† 2 (4)	1	1	$\sqrt{2}$	0	0	0	Tetragonal (*P*)
	† 9/2 (9)	$\frac{3}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$	0	0	0	Orthorhombic (*F*)
	† 8 (16)	2	$\sqrt{2}$	1	0	0	0	Orthorhombic (*P*)
51	† 27/2 (2)	$\frac{3\sqrt{2}}{2}$	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{2}}{2}$	0	0	0	Orthorhombic (*I*)
	† 135/4 (5)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{15}}{2}$	$\sqrt{2}$	0	$\frac{1}{\sqrt{10}}$	0	Monoclinic (*B*)
	† 54 (8)	$\frac{3\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	$\sqrt{6}$	0	0	0	Orthorhombic (*C*)
	† 54 (8)	$\sqrt{6}$	$\sqrt{5}$	$\sqrt{2}$	$-\frac{1}{2\sqrt{10}}$	0	$-\frac{3}{2\sqrt{30}}$	Triclinic
	† 297/4 (11)	$2\sqrt{2}$	$\sqrt{5}$	$\sqrt{2}$	$-\frac{1}{2\sqrt{10}}$	$-\frac{1}{8}$	$-\frac{1}{2\sqrt{10}}$	Triclinic
52	† 9/2 (2)	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{6}}{2}$	$\frac{\sqrt{2}}{2}$	0	0	0	Tetragonal (*I*)
	† 45/4 (5)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{3}}{2}$	$\sqrt{3}$	0	0	0	Orthorhombic (*C*)
	† 18 (8)	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{2}$	0	0	0	Tetragonal (*P*)
	† 18 (8)	$\frac{\sqrt{5}}{2}$	$\frac{\sqrt{3}}{2}$	$\sqrt{5}$	0	$\frac{1}{5}$	0	Monoclinic (*B*)
	† 99/4 (11)	$\frac{\sqrt{17}}{2}$	$\frac{\sqrt{3}}{2}$	$\sqrt{2}$	0	$\frac{1}{\sqrt{34}}$	0	Monoclinic (*B*)
53	† 3/2 (2)	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{6}}{2}$	0	0	0	Tetragonal (*I*)
	† 15/4 (5)	$\frac{\sqrt{15}}{2}$	$\frac{1}{2}$	1	0	0	0	Orthorhombic (*C*)
	† 6 (8)	1	1	$\sqrt{6}$	0	0	0	Tetragonal (*P*)
	† 6 (8)	$\frac{\sqrt{7}}{2}$	$\frac{1}{2}$	2	0	$\frac{1}{\sqrt{7}}$	0	Monoclinic (*B*)
	† 33/4 (11)	$\frac{\sqrt{7}}{2}$	$\frac{1}{2}$	$\sqrt{6}$	0	$\frac{3}{\sqrt{42}}$	0	Monoclinic (*B*)

† This signifies that the quadratic form is regular. The symbol ! signifies that it is one of the 14 quadratic forms that might be regular, although the regularity has been proved only under the generalized Riemann hypothesis (Oliver, 2014).

In Table 2, information about the *regularity* of each quadratic form is provided using the results of Jagy *et al.* (1997) and Oh (2011). If a set in Table 2 consists of regular quadratic forms, *i.e.* they are marked with †, it is possible to prove that they have perfectly identical peak positions up to ∞ as a consequence of theorems known about genus representations.

In the table, 38 of the 53 cases are given by regular quadratic forms. In more than half of the cases, the cells are not derivative of each other. This can be verified by applying the following proposition.

Proposition 2. Two 3×3 positive-definite S_1, S_2 with $\Lambda(S_1)=\Lambda(S_2)$ are derivative of each other if and only if the ratio of their determinants equals a^2 for some rational number a.

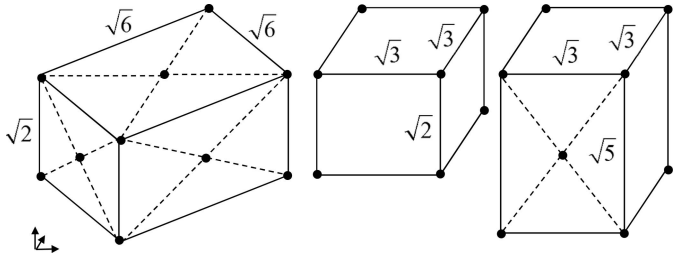

Figure 1
The reciprocal unit cells of the tetragonal (*P*, *I*) and orthorhombic (*C*) cells with perfectly identical *d* spacings (see No. 52); from this figure, it is not difficult to see that the two left-hand tetragonal cells are derivative of each other, and the rightmost orthorhombic cell has a number of two-dimensional sublattices common to the other two. However, the orthorhombic cell is not derivative of the other two, which is also easily proved because the ratio of the cell volumes is irrational.

Proof. The part 'only if' is proved. See Appendix *B* for the proof of the 'if' part; 'derivative' means that there exists $w\in GL_3(\mathbb{Q})$ such that $wS_1{}^{\rm t}w=S_2$. Hence if we put $a=\det w$, $a^2\det S_1=\det S_2$ is obtained. □

For example, Nos. 15–22 correspond to derivative lattices, while Nos. 1–14 do not. Fig. 1 explains the situation in a more intuitive way, by using unit cells in No. 52.

4. Finiteness theorem of powder indexing solutions under systematic absences

In what follows, the lattice dimension N is no longer fixed to $N=3$; instead, the case when $1\le N\le 4$ is considered. As in the *International Tables* Volume *A* (Hahn, 1983), systematic absences are classified by: (*a*) the isomorphism class of a crystallographic group G, (*b*) the conjugacy class of the site symmetry group H in G.

Let $L\subset\mathbb{R}^N$ be the abelian group consisting of all translations in G. In this case, $H\cap L=\emptyset$, because H is a finite subgroup of G. For a fixed (G,H), let $\Gamma_{\rm ext}(G,H)$ be the subset of the reciprocal lattice L^* of L consisting of all the $l^*\in L^*$ that correspond to systematic absences of type (G,H). The following general property of systematic absences seems to be unknown [however, it was used for the theorems in Oishi-Tomiyasu (2013) without being proved].

Proposition 3. Let M be the index $[G:L]$ and ML^* be the set $\{Ml^*: l^*\in L^*\}$. Then $ML^*\cap\Gamma_{\rm ext}(G,H)=\emptyset$ holds regardless of the choice of (G,H).

See Appendix *C* for the proof, where the theory of group cohomology is applied [see Serre (1980) for terminology].

Note that Proposition 3 holds even if M is replaced by $M^{\rm com}$, the least common multiple of the indices $[G : L]$ of all the crystallographic groups G with dim $L = N$. For $N = 2, 3$ and 4, $M^{\rm com}$ equals 24, 48 and 11 520, respectively. When $N = 4$, this is seen, for example, using the orders 240 and 2304 of the groups [[3,3,3]] and [[3,4,3]], respectively.

For a fixed crystallographic group G with the translation group $L \cong \mathbb{Z}^N$, assume that S is a metric tensor of L^*, and that (G, H) is a type of systematic absence. Define $\Lambda(S, G, H) \subset \Lambda(S)$ to be the subset consisting of all ${}^t\nu S\nu\,(0 \neq \nu \in \mathbb{Z}^N)$ that do not correspond to systematic absences of the type (G, H).

In §2, we proved that the algorithm of Table 1 is completed in a finite number of steps, even if $\Lambda(S_0)$ of an N-by-N positive-definite metric tensor S_0 is input instead of Λ. Therefore, only a finite number of S satisfy $\Lambda(S_0) \subset \Lambda(S) \subset M^{-2}\Lambda(S_0)$ for any integer $M > 0$. By setting the M to $M^{\rm com}$, the following result is obtained.

Theorem 1. For any $2 \leq N \leq 4$ and a subset $\Lambda \subset \mathbb{R}_{>0}$, only a finite number of triplets (S, G, H) of the following satisfy $\Lambda(S, G, H) = \Lambda$: (i) the equivalent class of $N \times N$ positive-definite S over $\mathbb{Z}$, (ii) an isomorphism class of a crystallographic group G, (iii) the conjugacy class of a site symmetry group H in G.

If $N = 1$, S is uniquely determined from $\Lambda(S)$. As a result of Lagrange's four-square theorem, infinitely many (S, G, H) can have the same $\Lambda(S, G, H)$ if $N > 4$. Theorem 1 claims that an intermediate result holds for $2 \leq N \leq 4$, even under systematic absences. This indicates that only finitely many solutions exist in powder indexing.

5. Conclusion

Unit cells that involve geometrical ambiguity were exhaustively searched using a function implemented in *CONOGRAPH*. A table containing all of the detected unit cells is presented. The result indicates that geometrical ambiguity rarely occurs if high-symmetry cases are excluded. Furthermore, a finiteness theorem on the number of powder indexing solutions was proved using the algorithm.

References

Cassels, J. W. S. (1978). *Rational Quadratic Forms.* London, New York: Academic Press.

Hahn, T. (1983). *International Tables for Crystallography*, Vol. *A*. Dordrecht: Kluwer.

Jagy, W. C., Kaplansky, I. & Schiemann, A. (1997). *Mathematika*, **44**, 332–341.

Kroll, H., Stöckelmann, D. & Heinemann, R. (2011). *J. Appl. Cryst.* **44**, 812–819.

Mighell, A. D. & Santoro, A. (1975). *J. Appl. Cryst.* **8**, 372–374.

Oh, B.-K. (2011). *Acta Arith.* **147**, 233–243.

Oishi-Tomiyasu, R. (2012). *Acta Cryst.* A**68**, 525–535.

Oishi-Tomiyasu, R. (2013). *Acta Cryst.* A**69**, 603–610.

Oishi-Tomiyasu, R. (2014*a*). *J. Appl. Cryst.* **47**, 2055–2059.

Oishi-Tomiyasu, R. (2014*b*). *J. Appl. Cryst.* **47**, 593–598.

Oliver, R. J. L. (2014). *Bull. London Math. Soc.* **46**, 1237–1247.

Santoro, A., Mighell, A. D. & Rodgers, J. R. (1980). *Acta Cryst.* A**36**, 796–800.

Serre, J. P. (1980). *Local Fields.* Berlin, New York: Springer-Verlag.

Shirley, R. (1980). *Accuracy in Powder Diffraction*, edited by S. Block & C. R. Hubbard. National Bureau of Standards (US) Special Publication, No. 567, pp. 361–382.

Waerden, B. L. van der (1956). *Acta Math.* **96**, 265–3309.