Suppporting information for *Acta Cryst.* (2016). A**72**, doi:/10.1107/S2053273315021725

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

R. Oishi-Tomiyasu

Some terminologies in the theory of quadratic forms are used herein. In particular, the following symmetric matrix (also called the *metric tensor* in crystallography) is always identified with a ternary quadratic form $f(\mathbf{x}) = \sum_{1 \le i \le j \le 3} s_{ij} x_i x_j$:

$$S := \begin{pmatrix} s_{11} & s_{12}/2 & s_{13}/2 \\ s_{12}/2 & s_{22} & s_{23}/2 \\ s_{13}/2 & s_{23}/2 & s_{33} \end{pmatrix} \tag{A.1}$$

The above S is *singular* if the determinant equals zero, and *integral* if all the s_{ij} $(1 \le i, j \le 3)$ are integers. For any ring R such as $\mathbb{Z}$, $\mathbb{Z}_p$, $\mathbb{Q}_p$, two symmetric matrices S_1, S_2 are said to be *equivalent over* R, if there exists $w \in GL_3(R)$ such that $w S_1 {}^t w = S_2$. For any $0 \ne v \in R^3$, ${}^t v S v$ is called *a representation of* S *over* R.

A Proof of Proposition 1

Proof of Proposition 1. For the proof, it may be assumed that S, S_2 have rational entries, because S and S_2 are simultaneously represented as finite sums $\sum_j \lambda_j T_j$, $\sum_j \lambda_j T_{2j}$, where λ_j are linearly independent over $\mathbb{Q}$, and every T_j, T_{2j} is rational and positive-definite (Lemma A.1). In the rational case, the proposition is proved by Lemma A.2. □

Lemma A.1. *Let S_i $(1 \le i \le m)$ be N_i-by-N_i positive-definite symmetric matrices with real coefficients. There are $\lambda_1, \dots, \lambda_s \in \mathbb{R}_{>0}$ positive and linearly independent over $\mathbb{Q}$ and N_i-by-N_i rational positive-definite symmetric matrices T_{ij} $(1 \le i \le m,\ 1 \le j \le s)$ such that every S_i is represented as a finite sum $S_i = \sum_{j=1}^{s} \lambda_j T_{ij}$.*

Proof. Let v_{S_i} be the row vector of length $\frac{N_i(N_i+1)}{2}$ with the (k,l)-entry of S_i in the $(k + \frac{l(l-1)}{2})$-th entry. In this case, $v := {}^t(v_{S_1}, \cdots, v_{S_m})$ is a column vector of length $\sum_{i=1}^{m} \frac{N_i(N_i+1)}{2}$. Using this v, a set P is defined by:

$$P \ := \ \left\{ I \subset \left\{ v_j : 1 \le j \le \sum_{i=1}^{m} \tfrac{N_i(N_i+1)}{2} \right\} : v_j \in I \text{ are linearly independent over } \mathbb{Q} \right\}. \tag{A.2}$$

Let $\{t_1, \dots, t_s\}$ be one of the maximal elements of P under inclusive order. When vectors ${}^t(t_1, \dots, t_s)$ and ${}^t(1, \dots, 1)$ of length s are denoted by $\mathbf{t}$ and $\mathbf{1}_s$ respectively, there exists a $\sum_{i=1}^{m} \frac{N_i(N_i+1)}{2} \times s$ rational matrix C such that $v = C\mathbf{t}$. Furthermore, there exists $\epsilon > 0$ such that for any s-by-s matrix U with entries $|u_{kl}| < \epsilon$, every column ${}^t(v_{T_1}, \cdots, v_{T_m})$ of $C(\mathbf{t}\,{}^t\mathbf{1}_s - U)$ corresponds to m positive-definite symmetric matrices $T_1, \dots, T_m$ of size N_i $(1 \le i \le m)$.

If ${}^t\mathbf{1}_s U^{-1}\mathbf{t} \neq 1$, we have the following equations (I_s is the identity matrix of size s):

$$(\mathbf{t}\,{}^t\mathbf{1}_s - U)^{-1} = U^{-1}(({}^t\mathbf{1}_s U^{-1}\mathbf{t} - 1)^{-1}\mathbf{t}\,{}^t\mathbf{1}_s U^{-1} - I_s), \tag{A.3}$$

$$(\mathbf{t}\,{}^t\mathbf{1}_s - U)^{-1}\mathbf{t} = ({}^t\mathbf{1}_s U^{-1}\mathbf{t} - 1)^{-1}U^{-1}\mathbf{t}. \tag{A.4}$$

If all the entries of $U^{-1}\mathbf{t}$ are negative, we have ${}^t\mathbf{1}_s U^{-1}\mathbf{t} < 0$, hence every entry of $(\mathbf{t}\,{}^t\mathbf{1}_s - U)^{-1}\mathbf{t}$ is positive. Fix $U := (u_{kl}) \in GL_s(\mathbb{R})$ from those having a rational $\mathbf{t}\,{}^t\mathbf{1}_s - U$ and $|u_{kl}| < \epsilon$. Let T_{ij} $(1 \le i \le m,\ 1 \le j \le s)$ be N_i-by-N_i symmetric matrices satisfying $C(\mathbf{t}\,{}^t\mathbf{1}_s - U) = (v_{T_{ij}})$. In this case, every T_{ij} is rational and positive definite by the choice of U. Owing to the following equation, S_i is represented as a linear sum of T_{ij} with positive coefficients:

$$v = C\mathbf{t} = (v_{T_{ij}})(\mathbf{t}\,{}^t\mathbf{1}_m - U)^{-1}\mathbf{t}. \tag{A.5}$$

Hence, the statement is proved. □

For any rings $R_2 \subseteq R$ and an N-by-N symmetric matrix S with entries in R_2, let $\Lambda_R(S)$ be the set $\{{}^t v S v : 0 \neq v \in R^N\}$ consisting of representations of S over R. If $0 \in \Lambda_R(S)$, S is said to be *isotropic* over R. Otherwise, S is *anisotropic* over R.

Lemma A.2. *Suppose that an N-by-N symmetric matrix S is rational and non-singular, and a symmetric matrix S_2 of size $1 \le N_2 < \min\{4, N\}$ is rational and anisotropic over $\mathbb{Q}$. In this case, $\Lambda_{\mathbb{Z}}(S) \not\subset \Lambda_{\mathbb{Z}}(S_2)$ holds.*

Proof. We assume $N_2 + 1 = N = 4$, because the other cases easily follow from this. Since S is not singular, it satisfies $\Lambda_{\mathbb{Q}_p}(S) \supset \mathbb{Q}_p^\times$ for any finite prime p. On the other hand, there exists a finite prime p such that $\Lambda_{\mathbb{Q}_p}(S_2) \not\supset \mathbb{Q}_p^\times$ (*cf.* Corollary 2 of Theorem 4.1 in Chapter 6, Cassels (1978)). If $\Lambda_{\mathbb{Z}}(S) \subset \Lambda_{\mathbb{Z}}(S_2)$, $\Lambda_{\mathbb{Q}_p}(S) \subset \Lambda_{\mathbb{Q}_p}(S_2)$ is required for any p. This is a contradiction. □

B Proof of Proposition 2

Two lattices in $\mathbb{R}^3$ are said to be *derivative* of each other if their metric tensors S_1, S_2 are equivalent over $\mathbb{Q}$:

Remaining proof of Proposition 2. The "if" part is proved herein; if there exists such an a, S_1 and S_2 are equivalent over $\mathbb{Q}_p$ for any $p \neq 2$ by Lemma B.1. They are also equivalent over $\mathbb{R}$, because they are positive-definite, hence they have the same Hasse-Minkowski symbols c_p for all primes p

including $2, \infty$ (Lemma 1.1, Chapter 6, Cassels(1978)). Therefore they are equivalent over $\mathbb{Q}$ by the weak Hasse principle (*cf.* Theorem 1.2, Chapter 6, Cassels(1978)). $\square$

Lemma B.1. *Suppose that p is an odd prime and S_1 and S_2 are 3-by-3 non-singular symmetric matrices with $\mathbb{Q}_p$ entries and $\det S_1 = a^2 \det S_2$ holds for some $a \in \mathbb{Q}_p$. If S_1 and S_2 have the same representations over $\mathbb{Z}_p$, they are equivalent over $\mathbb{Q}_p$.*

Proof. By replacing S_1, S_2 with cS_1, cS_2 for some $c \in \mathbb{Q}_p$, we may assume that all their entries belong to $\mathbb{Z}_p$, and 1 is represented by both of S_1 and S_2 over $\mathbb{Z}_p$. Take $n_1, n_2 \in \mathbb{Z}$ and $u_1, u_2 \in \mathbb{Z}_p^\times$ so that $\det S_i = p^{n_i} u_i \neq 0$ is satisfied for both $i = 1, 2$.

In this case, for each $i = 1, 2$, there exists $t_i \in \mathbb{Z}_p^\times$ and $0 \leq l_i \leq \frac{n_i}{2}$ such that S_i is equivalent over $\mathbb{Z}_p$ to the following:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & p^{l_i} t_i & 0 \\ 0 & 0 & p^{n_i - l_i} t_i^{-1} u_i \end{pmatrix} \tag{A.6}$$

We shall show that we can choose the same l, t as l_1, l_2 and t_1, t_2. If so, each S_i is equivalent over $\mathbb{Z}_p$ to the following:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & p^{l} t & 0 \\ 0 & 0 & (p^l t)^{-1} \det S_i \end{pmatrix}, \tag{A.7}$$

From the assumption on $\det S_i$, S_1 and S_2 are equivalent over $\mathbb{Q}_p$ as a result.

If $l_1 < n_1 - l_1$, then $l_1 = l_2$ and $\left(\frac{t_1}{p}\right) = \left(\frac{t_2}{p}\right)$ are obtained immediately. Hence, t_1, t_2 can be set to a common value $t \in \mathbb{Z}_p^\times$. Otherwise, $l_1 = n_1 - l_1$, hence S_1 is equivalent to $\begin{pmatrix} 1 & 0 & 0 \\ 0 & p^{l_1} s & 0 \\ 0 & 0 & p^{l_1} s^{-1} u_1 \end{pmatrix}$ for any $s \in \mathbb{Z}^\times$ (*cf.* Lemma 3.4, Chapter8, Cassels (1978)). As a result, $l_1 = l_2$ and $t_1 = t_2$ may be assumed even in this case. $\square$

C Proof of Proposition 3

What follows, coordinates in the real and reciprocal space are represented as a row vector and a column vector respectively. Furthermore, group actions on the spaces are represented as a right and left action respectively.

Any congruent transformation of the real space $\mathbb{R}^N$ ($N = 3$ is not necessary in this section) is represented as a composition of the orthogonal group $O(N)$ and a translation; if σ is a congruent transformation of $\mathbb{R}^N$, there exist $\tau \in O(N)$ and $\nu \in \mathbb{R}^N$ such that:

$$x^\sigma = x^\tau + \nu \text{ for any } x \in \mathbb{R}^N. \tag{A.8}$$

Such a σ is denoted by $\{\tau|\nu\}$.

A *crystallographic group* G is defined as a discrete and cocompact subgroup of the congruence transformation group. The translation group L and the point group R_G and of G are defined by:

$$R_G := \{\sigma \in O(N) : \{\sigma|\nu\} \text{ for some } \nu \in \mathbb{R}^N\}, \tag{A.9}$$
$$L := \{\nu \in \mathbb{R}^N : \{1_N|\nu\} \in G\}. \tag{A.10}$$

In general, G is a group extension of L by R_G (*i.e.,* L is the kernel of the natural onto map $G \twoheadrightarrow R_G$: $\{\sigma|\nu\} \mapsto \sigma$). From the definition of L, for any $\{\sigma|\nu_\sigma\} \in G$, the class $\nu_\sigma + L \in \mathbb{R}^N/L$ is uniquely determined. Furthermore, the map $R_G \to \mathbb{R}^N/L$: $\sigma \mapsto \nu_\sigma + L$ satisfies

$$\nu_{\sigma\tau} \equiv \nu_\sigma^\tau + \nu_\tau \bmod L. \tag{A.11}$$

Such a map is called a 1-cocycle in the theory of group cohomology, and corresponds to a cohomology class in $[\nu_\sigma] \in H^1(R_G, \mathbb{R}^N/L)$.

For any crystallographic group G and a finite subgroup $H \subset G$, the following $\Gamma_{ext}(G,H)$ defines the set of systematic absences:

$$\Gamma_{ext}(G,H) := \left\{ 0 \neq l^* \in L^* : \begin{array}{c} \sum_{\sigma \in H\backslash G/L} e^{2\pi i x^\sigma \cdot l^*} = 0 \\ \text{for any } x \in \mathbb{R}^N \text{ stabilized by } H \end{array} \right\}, \tag{A.12}$$

The following lemma provides a method to compute $\Gamma_{ext}(G,H)$ listed in the International Tables Vol. A (Hahn(1983)):

Lemma C.1. *Let R_H be the image of H by the natural onto map $G \to R_G : \{\sigma|\nu_\sigma\} \mapsto \sigma$. For fixed $l^* \in L^*$, the equivalence relation among the right cosets $R_H\backslash R_G$ is defined by:*

$$R_H\sigma_1 \overset{l^*}{\sim} R_H\sigma_2 \underset{def}{\Longleftrightarrow} \sum_{\sigma \in R_H\sigma_1} \sigma l^* = \sum_{\sigma \in R_H\sigma_2} \sigma l^*. \tag{A.13}$$

For any $x \in \mathbb{R}^N$ stabilized by H, $l^* \in L^*$ belongs to $\Gamma_{ext}(G,H)$ if and only if for every $R_H\sigma_1 \in R_H\backslash R$, we have

$$\sum_{R_H\sigma_2 \overset{l^*}{\sim} R_H\sigma_1} e^{2\pi i x^{\{\sigma_2|\nu_{\sigma_2}\}} \cdot l^*} = 0. \tag{A.14}$$

Proof. For any $x \in \mathbb{R}^N$ stabilized by H, $l^* \in \Gamma_{ext}(G,H)$ holds if and only if

$$\sum_{R_H\sigma_1 \in R_H\backslash R} e^{2\pi i((x+\delta x)^{\sigma_1} + \nu_{\sigma_1}) \cdot l^*} = 0 \text{ for any } \delta x \in \mathbb{R}^N \text{ stabilized by } R_H. \tag{A.15}$$

Furthermore,

$$\begin{aligned}
&\delta x^{\sigma_1}\cdot l^* = \delta x^{\sigma_2}\cdot l^* \text{ for any } \delta x\in\mathbb{R}^N \text{ stabilized by } R_H\\
\iff& \sum_{\tau\in R_H}(\delta\tilde{x}^{\tau\sigma_1}-\delta\tilde{x}^{\tau\sigma_2})\cdot l^*=0 \text{ for any } \delta\tilde{x}\in\mathbb{R}^N\\
\iff& \sum_{\tau\in R_H}\delta\tilde{x}\cdot(\tau\sigma_1 l^*-\tau\sigma_2 l^*)=0 \text{ for any } \delta\tilde{x}\in\mathbb{R}^N\\
\iff& \sum_{\tau\in R_H}\tau(\sigma_1 l^*-\sigma_2 l^*)=0 \iff R_H\sigma_1\overset{l^*}{\sim}R_H\sigma_2. \qquad (A.16)
\end{aligned}$$

Hence, (A.15) holds if and only if the following does for all δx stabilized by H:

$$\sum_{[\sigma_1]\in(R_H\backslash R)/\overset{l^*}{\sim}} e^{2\pi i\delta x^{\sigma_1}\cdot l^*}\sum_{R_H\sigma_2\overset{l^*}{\sim}R_H\sigma_1} e^{2\pi i(x^{\sigma_2}+\nu_{\sigma_2})\cdot l^*}=0, \qquad (A.17)$$

which leads to the statement. □

Proof of Proposition 3. If x is stabilized by H, $\nu_\tau\equiv x-x^\tau \bmod L$ holds for any $\tau\in R_H$. Hence, the cohomology class $[\nu_\sigma]\in H^1(R_G,\mathbb{R}^N/L)$ of the 1-cocycle $\sigma\mapsto\nu_\sigma$ is mapped to 0 by the natural map $H^1(R_G,\mathbb{R}^N/L)\longrightarrow H^1(R_H,\mathbb{R}^N/L)$. As a result, $[\nu_\tau]$ is also mapped to 0 by $H^1(R_G,\mathbb{R}^N/L)\overset{\times M/m}{\longrightarrow} H^1(R_G,\mathbb{R}^N/L)$, where m is the order of R_H (*cf.* Proposition 6 in Chap. VII of Serre (1980)). Thus, for any $\sigma\in R_G$, there exist $y\in\mathbb{R}^N$ and $\mu_\sigma\in(M/m)^{-1}L$ such that $\nu_\sigma\equiv y-y^\sigma+\mu_\sigma \bmod L$. Hence, $x-y\equiv(x-y)^\tau+\mu_\tau \bmod L$ for any $\tau\in R_H$, therefore $m(x-y)-\sum_{\tau\in R_H}(x-y)^\tau\in(M/m)^{-1}L$ is obtained. If $u\in\mathbb{R}^N$ with $mu=x-y$ is fixed, we have $(x-y)-\sum_{\tau\in R_H}u^\tau\in M^{-1}L$. As a result, for any $\sigma\in R_G$, there exists $\xi_\sigma\in M^{-1}L$ such that ν_σ is represented as follows:

$$\nu_\sigma\equiv x-x^\sigma-\sum_{\tau\in R_H}u^\tau+\sum_{\tau\in R_H}u^{\tau\sigma}+\xi_\sigma. \qquad (A.18)$$

From Lemma C.1, $l^*\in L^*$ belongs to $\Gamma_{ext}(G,H)$ if and only if the following holds for any $R_H\sigma_1\in R_H\backslash R_G$:

$$\begin{aligned}
\sum_{R_H\sigma_2\overset{l^*}{\sim}R_H\sigma_1} e^{2\pi i(x^{\sigma_2}+\nu_{\sigma_2})\cdot l^*} &= \sum_{R_H\sigma_2\overset{l^*}{\sim}R_H\sigma_1} e^{2\pi i(x-\sum_{\tau\in R_H}u^\tau+\sum_{\tau\in R_H}u^{\tau\sigma_2}+\xi_{\sigma_2})\cdot l^*}\\
&= e^{2\pi i(x-\sum_{\tau\in R_H}u^\tau)\cdot l^*}e^{2\pi i u\cdot\sum_{\tau\in R_H}\tau\sigma_1 l^*}\sum_{R_H\sigma_2\overset{l^*}{\sim}R_H\sigma_1} e^{2\pi i\xi_{\sigma_2}\cdot l^*}=0 \qquad (A.19)
\end{aligned}$$

This is impossible if l^* belongs to ML^*. □