Appendix A
Definition of Buerger-reduced cells

For reference, the definitions of the Buerger- and the Niggli-reduced cells are stated; a cell is *Buerger-reduced* if and only if its metric tensor belongs to the domain $D_{Buerger}$:

(Buerger-reduced domain)

$$\begin{aligned} D_{Buerger} &:= D_B^+ \cup D_B^-, && (61) \\ D_B^+ &:= \{(s_{ij})_{1 \le i,j \le 3} \in Sym^3(\mathbb{R}) : 0 < s_{11} \le s_{22} \le s_{33}, \\ & \qquad 0 \le s_{12}, s_{13} \le \frac{s_{11}}{2},\ 0 \le s_{23} \le \frac{s_{22}}{2}\}, && (62) \\ D_B^- &:= \{(s_{ij})_{1 \le i,j \le 3} \in Sym^3(\mathbb{R}) : 0 < s_{11} \le s_{22} \le s_{33}, \\ & \qquad 0 \le -s_{12}, -s_{13} \le \frac{s_{11}}{2},\ 0 \le -s_{23} \le \frac{s_{22}}{2}, \\ & \qquad -s_{12} - s_{13} - s_{23} \le \frac{s_{11} + s_{22}}{2}\}. && (63) \end{aligned}$$

It is well known that $D_{Buerger}[g_1]$ and $D_{Buerger}[g_2]$ share interior points only when $g_1 = \pm g_2$.

The Buerger-reduced cell is said to be *normalized* when it also satisfies the following boundary conditions:

$$(s_{ij}) \in D_B^+ \implies s_{12} > 0,\ s_{13} > 0,\ s_{23} > 0, \quad (64)$$

$$s_{11} = s_{22} \implies |s_{23}| \le |s_{13}|, \quad (65)$$

$$s_{22} = s_{33} \implies |s_{13}| \le |s_{12}|. \quad (66)$$

The following extra boundary conditions are added in the definition of the Niggli-reduced cell (Niggli(1928), Hahn (1983)).

1. (Case of $s_{12} > 0$, $s_{13} > 0$, $s_{23} > 0$)

$$s_{23} = \frac{s_{22}}{2} \quad \Rightarrow \quad s_{12} \le 2s_{13}, \tag{67}$$

$$s_{13} = \frac{s_{11}}{2} \quad \Rightarrow \quad s_{12} \le 2s_{23}, \tag{68}$$

$$s_{12} = \frac{s_{11}}{2} \quad \Rightarrow \quad s_{13} \le 2s_{23}. \tag{69}$$

2. (Case of $s_{12} \le 0$, $s_{13} \le 0$, $s_{23} \le 0$)

$$|s_{23}| = \frac{s_{22}}{2} \quad \Rightarrow \quad s_{12} = 0, \tag{70}$$

$$|s_{13}| = \frac{s_{11}}{2} \quad \Rightarrow \quad s_{12} = 0, \tag{71}$$

$$|s_{12}| = \frac{s_{11}}{2} \quad \Rightarrow \quad s_{13} = 0, \tag{72}$$

$$|s_{12} + s_{13} + s_{23}| = \frac{s_{11} + s_{22}}{2} \quad \Rightarrow \quad s_{11} \le |s_{12} + 2s_{13}|. \tag{73}$$

The Niggli-reduced cell is determined uniquely for any 3-dimensional lattices.

Appendix B
Domains containing nearly Buerger-reduced cells

All the facets and the extreme rays of $D_{Buerger}$ are presented in the following tables.

Table 1. *Facets of* $D_{Buerger}$.

Label	**Equation**
a	$s_{11} = s_{22}$
b	$s_{22} = s_{33}$
$c^{(\pm)}$	$\pm 2s_{12} = s_{11}$
$d^{(\pm)}$	$\pm 2s_{13} = s_{11}$
$e^{(\pm)}$	$\pm 2s_{23} = s_{22}$
$c^{(0)}$	$s_{12} = 0$
$d^{(0)}$	$s_{13} = 0$
$e^{(0)}$	$s_{23} = 0$
f	$s_{11} + s_{22} = -2s_{12} - 2s_{13} - 2s_{23}$

Table 2. *Extreme rays of $D_{Buerger}$.*

Label	Generating matrix	Rank	Active constraints (Facets)
D_B^+:			
3-1	$A_3 := \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$	3	a, b, $c^{(+)}$, $d^{(+)}$, $e^{(+)}$
3-2	$\begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(+)}$, $e^{(+)}$
3-3	$\begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$	3	a, b, $c^{(+)}$, $d^{(0)}$, $e^{(+)}$
3-4	$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(+)}$, $d^{(+)}$, $e^{(0)}$
3-5	$u_3 := \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(+)}$, $d^{(0)}$, $e^{(0)}$
3-6	$\begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(+)}$, $e^{(0)}$
3-7	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(0)}$, $e^{(+)}$
2-1	$A_2^+ := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$	2	b, $c^{(\pm)}$, $c^{(0)}$, $d^{(\pm)}$, $d^{(0)}$, $e^{(+)}$
D_B^-:			
3-8	$\begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(-)}$, $e^{(-)}$
3-9	$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$	3	a, b, $c^{(-)}$, $d^{(0)}$, $e^{(-)}$
3-10	$\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & 0 \\ -1 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(-)}$, $d^{(-)}$, $e^{(0)}$
3-11	$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(-)}$, $d^{(0)}$, $e^{(0)}$
3-12	$\begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(-)}$, $e^{(0)}$
3-13	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(0)}$, $e^{(-)}$
2-2	$A_2^- := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$	2	b, $c^{(\pm)}$, $c^{(0)}$, $d^{(\pm)}$, $d^{(0)}$, $e^{(-)}$, f
D_B^+ and D_B^-:			
3-14	$I_3 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3	a, b, $c^{(0)}$, $d^{(0)}$, $e^{(0)}$
2-3	$u_2 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2	b, $c^{(\pm)}$, $c^{(0)}$, $d^{(\pm)}$, $d^{(0)}$, $e^{(0)}$
1-1	$u_1 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	1	a, $c^{(\pm)}$, $c^{(0)}$, $d^{(\pm)}$, $d^{(0)}$, $e^{(\pm)}$, $e^{(0)}$, f

* Some extreme rays are not contained in $D_{Buerger}$, but in its boundary.

From a geometrical point of view, it is seen that the number of operations to search for nearly Buerger-reduced cells in the sense of Andrews & Bernstein (1988) reaches its maximum when S^{obs} is close to one of the extreme rays of $D_{Buerger}$. Under the assumption (A_0) that is derived from the assumption (A), the generating matrix of the extreme ray close to S^{obs} must be positive definite:

(A_0) An observed metric tensor S^{obs} is sufficiently far from any 3-by-3 symmetric matrix that is not positive definite.

Therefore, the maximum is computed as the number of the change-of-basis matrices g such that $D_{Buerger}[g]$ contains a fixed extreme ray in $D_{Buerger}$ of rank 3. (Note that it is impossible to enumerate such g without assuming (A_0), because infinitely many $D_{Buerger}[g]$ share a singular matrix with $D_{Buerger}$.)

In Table 2, every generating matrix of rank 3 other than I_3 is equivalent to A_3 or u_3, *i.e.,* equals gA_3g^T, gu_3g^T for some change-of-basis matrix g. Such g is given as an element of $U_B^{(\pm)}$ when the matrix is equivalent to A_3, and of $W_B^{(\pm)}$, otherwise.

$$U_B^{(+)} := \left\{ I_3, \begin{pmatrix} -1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}, \tag{74}$$

$$U_B^{(-)} := \left\{ \begin{pmatrix} -1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}, \tag{75}$$

$$W_B^{(+)} := \left\{ I_3, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \right\}, \tag{76}$$

$$W_B^{(-)} := \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \right\}. \tag{77}$$

In this case, the following proposition is proved:

Proposition 3. *1. A_3 is contained in $D_{Buerger}[g^{-1}]$ if and only if g is an element of $\{g_1g_2 : g_1 \in U_B^{(\pm)},\ g_2 \in St(A_3)\}$.*

2. The matrix u_3 is contained in $D_{Buerger}[g^{-1}]$ if and only if g is an element of $\{g_1g_2 : g_1 \in W_B^{(\pm)},\ g_2 \in St(u_3)\}$, where $St(u_3)$ is the stabilizer subgroup of u_3 in $GL(3,\mathbb{Z})$.

3. I_3 is contained in $D_{Buerger}[g^{-1}]$ if and only if g belongs to $St(I_3)$.

The elements of $St(u_3)$ are presented in 3. Using proposition 3, the cardinalities of change-of-basis matrices g such that $D_{Buerger}[g]$ shares A_3, u_3 and I_3 with $D_{Buerger}$ are calculated. They equal 336, 144, and 48, respectively.

Now, $D_{Buerger}[g] = D_{Buerger}$ holds if and only if $g = \pm I_3$. Therefore, the number of operations necessary to obtain all nearly Buerger-reduced cells equals $\frac{336}{2} = 168$ at least in the worst case (Consequently, more than 168 matrices are required to be checked.). Since this always occurs if the metric tensor of a lattice is sufficiently close to A_3, the maximum is reached regardless of the magnitude of errors.

Table 3. *Elements of the stabilizer subgroup $St(u_3)$ in $GL(3, \mathbb{Z})$.*

$$
\pm\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}
\pm\begin{pmatrix}0&1&0\\1&0&0\\0&0&-1\end{pmatrix}
$$

$$
\pm\begin{pmatrix}-1&1&0\\0&1&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}1&-1&0\\1&0&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}-1&1&0\\0&1&0\\0&0&-1\end{pmatrix}
\pm\begin{pmatrix}1&-1&0\\1&0&0\\0&0&-1\end{pmatrix}
$$

$$
\pm\begin{pmatrix}0&1&0\\-1&1&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}1&0&0\\1&-1&0\\0&0&1\end{pmatrix}
\pm\begin{pmatrix}0&1&0\\-1&1&0\\0&0&-1\end{pmatrix}
\pm\begin{pmatrix}1&0&0\\1&-1&0\\0&0&-1\end{pmatrix}
$$

Using Proposition 3, it is also possible to enumerate all $g \in GL(3, \mathbb{Z})$ such that $D_{Buerger}[g]$ contains nearly Buerger-reduced cells; $D_{Buerger}[g]$ contains nearly Buerger-reduced cells if only if $D_{Buerger}[g]$ shares a positive definite matrix with $D_{Buerger}$. As a result, the number of such g (including $\pm I_3$) equals 1992. Among the 25 Gruber operations, 22 operations are contained in it. The remaining three operations are as follows (The number was given by Gruber(1973)):

$$
\begin{aligned}
12 &: (A, A+B+\zeta, B+C+\xi, 2B+\xi+\eta+\zeta, \eta+\zeta, 2A+\zeta),\\
21 &: (B, A+B-\zeta, A+C-\eta, 2A+\xi-\eta-\zeta, -\xi+\zeta, -2B+\zeta),\\
23 &: (C, A+B-\zeta, A+C-\eta, 2A+\xi-\eta-\zeta, -2C+\eta, -\xi+\eta).
\end{aligned}
$$

With regard to these operations, $D_{Buerger}$ and $D_{Buerger}[g]$ contain no positive definite matrix in common.

Appendix C
Proofs of theorems

Proof of Theorem 1. Let g be an element of $GL_3(\mathbb{Z})$ such that $S \in \tilde{D}_{min}[g]$. Then, $S[g^{-1}]$ belongs to $V_{mono,p} \cap \tilde{D}_{min}$. By replacing g with gg_0 for some $g_0 \in St(I_3)$, it may be supposed that $S[g^{-1}]$ is also contained in the following subset of $V_{mono,p,b}$.

$$\begin{aligned} U_{mono,p,b} \quad := \quad & \{(s_{ij})_{1 \le i,j \le 3} \in V_{mono,p,b} : \\ & \qquad s_{11} \le s_{33},\ -s_{11} \le 2s_{13} \le 0\}. \end{aligned} \tag{78}$$

The (i,j)-entries of S and $g^T g$ are denoted by s_{ij} and a_{ij}, respectively. The following inequality is obtained from $S[g^{-1}] \in U_{mono,p,b}$:

$$\begin{aligned} & \langle S, I_3 \rangle - \langle S[g^{-1}], I_3 \rangle \\ = \quad & \left\langle \begin{pmatrix} s_{11} & 0 & s_{13} \\ 0 & s_{22} & 0 \\ s_{13} & 0 & s_{33} \end{pmatrix}, g^T g - I_3 \right\rangle \\ = \quad & (a_{11} - 1)s_{11} + 2a_{13}s_{13} + (a_{22} - 1)s_{22} + (a_{33} - 1)s_{33} \\ \ge \quad & (a_{11} + a_{33} - 2 - |a_{13}|)s_{11} + (a_{22} - 1)s_{22} \\ \ge \quad & \frac{1}{2}(a_{11} + a_{33} - 2)s_{11} + (a_{22} - 1)s_{22}. \end{aligned} \tag{79}$$

For the last inequality, $a_{11} + a_{33} \ge 2|a_{13}| + 1$ is used. Since $g^T g$ is an integer-valued positive definite symmetric matrix, a_{11}, a_{22}, and a_{33} are positive integers. Hence, the coefficients of s_{11} and s_{22} are not negative in the last line of (79).

On the other hand, $\langle S^{obs}, I_3 \rangle - \langle S^{obs}[g^{-1}], I_3 \rangle \le 0$ also holds because $S^{obs} \in \tilde{D}_{min}$. Therefore, the coefficients of s_{11} and s_{22} must be less than $\frac{1}{2}$ from the assumption (A). Hence, we have

$$a_{11} = a_{22} = a_{33} = 1. \tag{80}$$

Thus, it is proved that g belongs to $U_{mono,p,b}$. From the assumption, $S[g^{-1}] \in U_{mono,p,b}$, therefore S is an element of $V_{mono,p}$. □

Proof of Theorem 2. Let g be an element of $GL_3(\mathbb{Z})$ with $\tilde{S} \in \tilde{D}_{del}[g]$. Then, $\tilde{S}[g^{-1}]$ belongs to $\tilde{V}_F \cap \tilde{D}_{del}$. By replacing g with gg_0 for some $g_0 \in St(A_3)$, it may also be supposed that $\tilde{S}[g^{-1}]$ belongs to the subset of $\tilde{V}_{F,1,2} \cap \tilde{D}_{del}$.

The (i,j)-entry of $g^T A_3 g$ is denoted by a_{ij} and the entries of $\tilde{S}$ are denoted by

$$\begin{pmatrix} -\tilde{s}_{12} - 2\tilde{s}_{13} & \tilde{s}_{12} & \tilde{s}_{13} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\tilde{s}_{12} - 2\tilde{s}_{13} & \tilde{s}_{13} & \tilde{s}_{13} \\ \tilde{s}_{13} & \tilde{s}_{13} & -2\tilde{s}_{13} - \tilde{s}_{34} & \tilde{s}_{34} \\ \tilde{s}_{13} & \tilde{s}_{13} & \tilde{s}_{34} & -2\tilde{s}_{13} - \tilde{s}_{34} \end{pmatrix}. \tag{81}$$

Then,

$$\begin{aligned} & \langle \tilde{S}[g^{-1}], I_4 \rangle - \langle \tilde{S}, I_4 \rangle \\ = & \left\langle \begin{pmatrix} -\tilde{s}_{12} - 2\tilde{s}_{13} & \tilde{s}_{12} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\tilde{s}_{12} - 2\tilde{s}_{13} & \tilde{s}_{13} \\ \tilde{s}_{13} & \tilde{s}_{13} & -2\tilde{s}_{13} - \tilde{s}_{34} \end{pmatrix}, g^T A_3 g - A_3 \right\rangle \\ = & -(a_{11} + a_{22} - 2a_{12} - 2)\tilde{s}_{12} \\ & -2(a_{11} + a_{22} + a_{33} - a_{13} - a_{23} - 4)\tilde{s}_{13} - (a_{33} - 2)\tilde{s}_{34} \\ \geq & -2(a_{11} + a_{22} + a_{33} - a_{13} - a_{23} - 4)\tilde{s}_{13}. \end{aligned} \tag{82}$$

For the last inequality, $a_{11} + a_{22} - 2a_{12} \geq 2$ and $a_{33} \geq 2$ are utilized. They follow from the fact that

$$0 \neq u \in \mathbb{Z}^3 \Longrightarrow u^T A_3 u \text{ is positive and even.} \tag{83}$$

On the other hand, $\langle \tilde{S}^{obs}[g^{-1}], I_4 \rangle - \langle \tilde{S}^{obs}, I_4 \rangle \leq 0$ follows from $\tilde{S}^{obs} \in \tilde{D}_{del}$. Furthermore, from $-4\tilde{s}_{13} = (1,1,0,0)\tilde{S}(1,1,0,0)^T$ and the assumption (A), the following inequality is obtained:

$$a_{11} + a_{22} + a_{33} - a_{13} - a_{23} < 5. \tag{84}$$

Therefore, using (83),

$$a_{11} = a_{22} = a_{11} + a_{33} - 2a_{13} = a_{22} + a_{33} - 2a_{23} = 2. \tag{85}$$

That is, the column vectors of $g := \begin{pmatrix} g_1 & g_2 & g_3 \end{pmatrix}$ satisfy

$$\begin{aligned} g_1^T A_3 g_1 &= g_2^T A_3 g_2 = (g_1 - g_3)^T A_3 (g_1 - g_3) \\ &= (g_2 - g_3)^T A_3 (g_2 - g_3) = 2. \end{aligned} \tag{86}$$

Because g is a matrix of determinant ± 1, $g_1, g_2, g_1 - g_3, g_2 - g_3$ are the elements of the following set and they differ from one another:

$$\left\{ \pm \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \right\}. \tag{87}$$

Hence, $h_{del}g_1, h_{del}g_2, h_{del}(g_1 - g_3), h_{del}(g_2 - g_3)$ are different elements of the set

$$\left\{ \pm\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}, \pm\begin{pmatrix}0\\1\\0\\-1\end{pmatrix}, \pm\begin{pmatrix}0\\0\\1\\-1\end{pmatrix}, \pm\begin{pmatrix}1\\-1\\0\\0\end{pmatrix}, \pm\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \pm\begin{pmatrix}0\\1\\-1\\0\end{pmatrix} \right\}. \tag{88}$$

Then, by direct computation, it is confirmed that $h_{del}\begin{pmatrix}g_1 & g_2 & g_3\end{pmatrix} = \pm p_0 h$ for a 4-by-4 permutation matrix p_0 and h equals one of the matrices:

$$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\\-1&-1&-1\end{pmatrix}, \begin{pmatrix}-1&0&0\\0&1&0\\1&0&1\\0&-1&-1\end{pmatrix}, \begin{pmatrix}1&0&1\\0&1&1\\0&0&-1\\-1&-1&-1\end{pmatrix}. \tag{89}$$

Therefore, g is one of the following matrices:

$$g_0,\ g_0\begin{pmatrix}-1&0&0\\0&1&0\\1&0&1\end{pmatrix},\ g_0\begin{pmatrix}1&0&1\\0&1&1\\0&0&-1\end{pmatrix}\quad (g_0 \in St(A_3)). \tag{90}$$

As a result, it is proved that at least one g in (90) satisfies $\tilde{S}[g^{-1}] \in \tilde{V}_{F,1,2} \cap \tilde{D}_{del}$. Now, $\tilde{V}_{F,1,2}[g_0]$ is contained in $\tilde{V}_F$ for any $g_0 \in St(A_3)$. Furthermore, it is checked by direct calculation that the following equations are true:

$$\tilde{V}_{F,1,2}\left[\begin{pmatrix}-1&0&0\\0&1&0\\1&0&1\end{pmatrix}\right] = \tilde{V}_{F,1,2}, \tag{91}$$

$$\tilde{V}_{F,1,2}\left[\begin{pmatrix}1&0&1\\0&1&1\\0&0&-1\end{pmatrix}\right] = \tilde{V}_{F,1,2}. \tag{92}$$

Therefore, $\tilde{S}$ belongs to $\tilde{V}_F$. □

Proof of Theorem 3. Let g be an element of $GL_3(\mathbb{Z})$ with $\tilde{S} \in \tilde{D}_{del}[g]$. Then, $\tilde{S}[g^{-1}]$ belongs to $\tilde{V}_R \cap \tilde{D}_{del}$. By replacing g with gg_0 for some $g_0 \in St(A_3)$, it may be supposed that $\tilde{S}[g^{-1}]$ belongs to $(\tilde{V}^{-}_{R,1,2,3} \cup \tilde{V}^{+}_{R,3,4,1}) \cap \tilde{D}_{del}$.

Subsequently, the (i,j)-entry of $g^T A_3 g$ is denoted by a_{ij}.

(a) (Case of $\tilde{S}[g^{-1}] \in \tilde{V}^{-}_{R,1,2,3}$)

The entries $\tilde{S}[g^{-1}] \in \tilde{V}^{-}_{R,1,2,3}$ are denoted by

$$\begin{pmatrix} -2\tilde{s}_{12} - \tilde{s}_{14} & \tilde{s}_{12} & \tilde{s}_{12} & \tilde{s}_{14} \\ \tilde{s}_{12} & -2\tilde{s}_{12} - \tilde{s}_{14} & \tilde{s}_{12} & \tilde{s}_{14} \\ \tilde{s}_{12} & \tilde{s}_{12} & -2\tilde{s}_{12} - \tilde{s}_{14} & \tilde{s}_{14} \\ \tilde{s}_{14} & \tilde{s}_{14} & \tilde{s}_{14} & -3\tilde{s}_{14} \end{pmatrix}. \tag{93}$$

Then,

$$\begin{aligned} & \langle \tilde{S}[g^{-1}], I_4 \rangle - \langle \tilde{S}, I_4 \rangle \\ = & \left\langle \begin{pmatrix} -2\tilde{s}_{12} - \tilde{s}_{14} & \tilde{s}_{12} & \tilde{s}_{12} \\ \tilde{s}_{12} & -2\tilde{s}_{12} - \tilde{s}_{14} & \tilde{s}_{12} \\ \tilde{s}_{12} & \tilde{s}_{12} & -2\tilde{s}_{12} - \tilde{s}_{14} \end{pmatrix}, g^T A_3 g - A_3 \right\rangle \\ = & -2(a_{11} + a_{22} + a_{33} - a_{12} - a_{13} - a_{33} - 3)\tilde{s}_{12} \\ & -(a_{11} + a_{22} + a_{33} - 6)\tilde{s}_{14} \\ \geq & -(a_{11} + a_{22} + a_{33} - 6)\tilde{s}_{14}. \end{aligned} \tag{94}$$

For the last inequality, $a_{ii} + a_{jj} - 2a_{ij} \geq 2$ obtained from (83).

On the other hand, $\langle \tilde{S}^{obs}[g^{-1}], I_4 \rangle - \langle \tilde{S}^{obs}, I_4 \rangle \leq 0$ follows from $\tilde{S}^{obs} \in \tilde{D}_{del}$. Furthermore, $a_{11} + a_{22} + a_{33} - 6 < \frac{3}{2}$ is required because $-3\tilde{s}_{14}$ is the square of the length of a lattice vector. As a result, $a_{ii} = 2$ $(1 \leq i \leq 3)$ is obtained from (83).

As in the proof of Theorem 2, the column vectors of $h_{del} g$ belong to

$$\left\{ \pm \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \pm \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \right\}. \tag{95}$$

Hence, $h_{del} g$ equals one of the matrices:

$$\pm p_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & -1 & -1 \end{pmatrix} h_0 q_0, \pm p_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \end{pmatrix} h_1 q_0, \tag{96}$$

where p_0 is a 4-by-4 permutation matrix, q_0 is a 3-by-3 permutation matrix, $h_0 = I_3, t_{001}$, and $h_1 = I_3, t_{010}, t_{001}$.

Therefore, g equals one of the following matrices for some $g_0 \in St(A_3)$:

$$g_0 h_0 q_0, \ g_0 T_R^{+} h_1 q_0. \tag{97}$$

From the assumption that $\tilde{S}$ belongs to $V^{-}_{R,1,2,3}[g]$, $\tilde{S}$ is an element of the set:

$$\bigcup_{g_0 \in St(A_3)} \tilde{V}^{-}_{R,1,2,3}[g_0] \cup \bigcup_{g_0 \in St(A_3)} \tilde{V}^{-}_{R,1,2,3}[g_0 T^{+}_{R}] \cup \bigcup_{g_0 \in St(A_3)} \tilde{V}^{-}_{R,1,2,3}[g_0 t_{001}] \cup \bigcup_{\substack{g_0 \in St(A_3),\\ h = t_{010}, t_{001}}} \tilde{V}^{-}_{R,1,2,3}[g_0 T^{+}_{R} h]. \tag{98}$$

Now, $\tilde{V}^{-}_{R,1,2,3}[T^{+}_{R}] = \tilde{V}^{+}_{R,3,4,1}$ is obtained by the equation:

$$\begin{aligned} & h_{del} T^{+}_{R} \begin{pmatrix} -\tilde{s}_{12} - r & -\tilde{s}_{12} & -\tilde{s}_{12} \\ -\tilde{s}_{12} & -\tilde{s}_{12} - r & -\tilde{s}_{12} \\ -\tilde{s}_{12} & -\tilde{s}_{12} & -\tilde{s}_{12} - r \end{pmatrix} (h_{del} T^{+}_{R})^{T} \\ = & \begin{pmatrix} -\tilde{s}_{12} - r & \tilde{s}_{12} & r & 0 \\ \tilde{s}_{12} & -\tilde{s}_{12} - r & 0 & r \\ r & 0 & -2r & r \\ 0 & r & r & -2r \end{pmatrix}. \end{aligned} \tag{99}$$

Therefore, the statement of the theorem is true in this case.

(b) (Case of $\tilde{S}[g^{-1}] \in \tilde{V}^{+}_{R,3,4,1}$)

The entries of $\tilde{S}[g^{-1}] \in \tilde{V}^{-}_{R,1,2,3}$ are denoted by

$$\begin{pmatrix} -\tilde{s}_{12} - \tilde{s}_{13} & \tilde{s}_{12} & \tilde{s}_{13} & 0 \\ \tilde{s}_{12} & -\tilde{s}_{12} - \tilde{s}_{13} & 0 & \tilde{s}_{13} \\ \tilde{s}_{13} & 0 & -2\tilde{s}_{13} & \tilde{s}_{13} \\ 0 & \tilde{s}_{13} & \tilde{s}_{13} & -2\tilde{s}_{13} \end{pmatrix}. \tag{100}$$

Then,

$$\begin{aligned} & \langle \tilde{S}[g^{-1}], I_4 \rangle - \langle \tilde{S}, I_4 \rangle \\ = & \left\langle \begin{pmatrix} -\tilde{s}_{12} - \tilde{s}_{13} & \tilde{s}_{12} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\tilde{s}_{12} - \tilde{s}_{13} & 0 \\ \tilde{s}_{13} & 0 & -2\tilde{s}_{13} \end{pmatrix}, g^{T} A_3 g - A_3 \right\rangle \\ = & -(a_{11} + a_{22} - 2a_{12} - 2)\tilde{s}_{12} \\ & -(a_{11} + a_{22} + 2a_{33} - 2a_{13} - 6)\tilde{s}_{13} \\ \geq & -(a_{11} + a_{22} + 2a_{33} - 2a_{13} - 6)\tilde{s}_{13}. \end{aligned} \tag{101}$$

For the last inequality, $a_{11} + a_{22} - 2a_{12} \geq 2$ is utilized. Now, $-2\tilde{s}_{13}$ is the square of the length of a lattice vector. As a result, $a_{11} + a_{33} - 2a_{13} = a_{22} = a_{33} = 2$ is obtained from $\langle \tilde{S}^{obs}[g^{-1}], I_4 \rangle - \langle \tilde{S}^{obs}, I_4 \rangle \leq 0$ and the assumption (A).

The equalities hold if and only if

$$(\tilde{a}_{ij})_{1\le i,j\le 3} := (gT_R^+)^T A_3 g T_R^+ \text{ satisfies } \tilde{a}_{11} = \tilde{a}_{22} = \tilde{a}_{33} = 2$$
$$\iff gT_R^+ \text{ equals one of the matrices in (97).}$$

Since we have $\tilde{S} \in \tilde{V}^+_{R,3,4,1}[g] = \tilde{V}^-_{R,1,2,3}[gT_R^+]$, the statement is proved as in the case of (a).

□

Proof of Theorem 4. Let g be an element of $GL_3(\mathbb{Z})$ with $\tilde{S} \in \tilde{D}_{del}[g]$. Then, $\tilde{S}[g^{-1}]$ belongs to $\tilde{V}_B \cap \tilde{D}_{del}$. By replacing g with gg_0 for some $g_0 \in St(A_3)$, it may be supposed that $\tilde{S}[g^{-1}]$ belongs to $(\tilde{V}^{(1)}_{B,1,2} \cup \tilde{V}^{(2)}_{B,1,2} \cup \tilde{V}^{(3)}_{B,3,2}) \cap \tilde{D}_{del}$. Furthermore, it may be assumed that $\tilde{S}[g^{-1}]$ belongs to $(\tilde{U}^{(1)}_{B,1,2} \cup \tilde{U}^{(2)}_{B,1,2} \cup \tilde{U}^{(3)}_{B,3,2}) \cap \tilde{D}_{del}$, where $\tilde{U}^{(1)}_{B,1,2}$, $\tilde{U}^{(2)}_{B,1,2}$, $\tilde{U}^{(3)}_{B,3,2}$ are defined by

$$\tilde{U}^{(1)}_{B,1,2} := \{\tilde{s}_{ij} \in \tilde{V}^{(1)}_{B,1,2} : \tilde{s}_{14} \le \tilde{s}_{13}\}, \tag{102}$$
$$\tilde{U}^{(2)}_{B,1,2} := \{\tilde{s}_{ij} \in \tilde{V}^{(2)}_{B,1,2} : \tilde{s}_{13} \le \tilde{s}_{14},\ \tilde{s}_{34} \le \tilde{s}_{12}\}, \tag{103}$$
$$\tilde{U}^{(3)}_{B,3,2} := \{\tilde{s}_{ij} \in \tilde{V}^{(3)}_{B,3,2} : \tilde{s}_{24} \le \tilde{s}_{12}\}. \tag{104}$$

These domains consist of elements that are transformed into the standard form of base-centered cells (*i.e.,* $0 \le -d \le \min\{\frac{a}{2}, c\}$) by the transforms in (38)–(40).

Subsequently, the (i,j)-entry of $g^T A_3 g$ is denoted by a_{ij}.

(a) (Case of $\tilde{S}[g^{-1}] \in \tilde{U}^{(1)}_{B,1,2}$)

The entries of $\tilde{S}[g^{-1}] \in \tilde{U}^{(1)}_{B,1,2}$ are denoted by

$$\begin{pmatrix} -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} & \tilde{s}_{14} \\ \tilde{s}_{12} & -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{13} & \tilde{s}_{14} \\ \tilde{s}_{13} & \tilde{s}_{13} & -2\tilde{s}_{13} - \tilde{s}_{34} & \tilde{s}_{34} \\ \tilde{s}_{14} & \tilde{s}_{14} & \tilde{s}_{34} & -2\tilde{s}_{14} - \tilde{s}_{34} \end{pmatrix}. \tag{105}$$

Then

$$\begin{aligned}
&\langle \tilde{S}[g^{-1}], I_4\rangle - \langle \tilde{S}, I_4\rangle \\
= &\left\langle \begin{pmatrix} -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{13} \\ \tilde{s}_{13} & \tilde{s}_{13} & -2\tilde{s}_{13} - \tilde{s}_{34} \end{pmatrix}, g^T A_3 g - A_3 \right\rangle \\
= & -(a_{11} + a_{22} - 2a_{12} - 2)\tilde{s}_{12} \\
& -(a_{11} + a_{22} + 2a_{33} - 2a_{13} - 2a_{23} - 4)\tilde{s}_{13} \\
& -(a_{11} + a_{22} - 4)\tilde{s}_{14} - (a_{33} - 2)\tilde{s}_{34}.
\end{aligned} \tag{106}$$

From $\tilde{S}[g^{-1}] \in \tilde{U}^{(1)}_{B,1,2}$, we have $-4s_{14} \geq -2(s_{13} + s_{14}) = (1,1,0,0)\tilde{S}(1,1,0,0)^T$, and $-2s_{13} - s_{34}$ is also the square of the length of a lattice vector. Therefore, the following equations are obtained from (83) and the assumption (A):

$$\text{(i)} \quad a_{11} = a_{22} = 2, \tag{107}$$

$$\text{(ii)} \quad a_{11} + a_{33} - 2a_{13} = a_{22} + a_{33} - 2a_{23} = 2,$$

$$\text{or } a_{33} = 2. \tag{108}$$

From the discussion in the proof of Theorem 2, g is one of the matrices in (90) if $a_{11} = a_{22} = a_{11} + a_{33} - 2a_{13} = a_{22} + a_{33} - 2a_{23} = 2$. On the other hand, as shown in the proof of Theorem 3, g is one of the matrices in (97) if $a_{11} = a_{22} = a_{33} = 2$.
Let h_B be the matrix defined by (40). $\tilde{V}^{(1)}_{B,1,2}[g] = \tilde{V}^{(1)}_{B,1,2}$ holds if and only if $g \in GL(3,\mathbb{Z})$ belongs to the group:

$$St(\tilde{V}^{(1)}_{B,1,2}) := \left\{ g : h_B^{-1} g h_B = \begin{pmatrix} c_{11} & 0 & c_{13} \\ 0 & c_{22} & 0 \\ c_{13} & 0 & c_{33} \end{pmatrix} \ (c_{ij} \in \mathbb{R}) \right\}. \tag{109}$$

For example, the following matrices are contained in $St(\tilde{V}^{(1)}_{B,1,2})$.

$$-I_3,\ t_{110},\ t_{001},\ \sigma_{12} := \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & -1 \end{pmatrix}. \tag{110}$$

Furthermore, $T_R^+ = T_B^{(2)} t_{001} = T_B^{(3)} \sigma_{23} t_{010}$. Thus, g is one of the following matrices for some

$g_0 \in St(A_3)$ and $q_0 \in St(\tilde{V}^{(1)}_{B,1,2})$:

$$g_0 q_0,\ g_0 T^{(2)}_B q_0,\ g_0 T^{(3)}_B q_0,\ g_0 t_{001}\sigma_{13} q_0,\ g_0 t_{001}\sigma_{23} q_0,$$
$$g_0 T^{(2)}_B t_{001}\sigma_{13} q_0,\ g_0 T^{(2)}_B t_{001}\sigma_{23} q_0, \tag{111}$$
$$g_0 T^{(3)}_B \sigma_{23} q_0,\ g_0 T^{(2)}_B t_{011}\sigma_{13} q_0,\ g_0 T^{(2)}_B \sigma_{13} q_0,\ g_0 T^{(2)}_B \sigma_{23} q_0,$$

where

$$\sigma_{13} := \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{112}$$

In addition, we have

$$\tilde{V}^{(1)}_{B,1,2}[T^{(i)}_B] = \tilde{V}^{(i)}_{B,1,2}\ (i = 2, 3), \tag{113}$$

$$\begin{aligned} t_{010} &= \sigma_{13} t_{001} \sigma_{13} t_{110} \in St(A_3) t_{001} \sigma_{13} St(\tilde{V}^{(1)}_{B,1,2}), \\ &= \sigma_{23} t_{001} \sigma_{23} \in St(A_3) t_{001} \sigma_{23} St(\tilde{V}^{(1)}_{B,1,2}), \end{aligned} \tag{114}$$

$$\begin{aligned} T^{(2)}_B t_{001}\sigma_{13} &= h T^{(2)}_B t_{001} \sigma_{23}\sigma_{12} \in St(A_3) T^{(2)}_B t_{001}\sigma_{23} St(\tilde{V}^{(1)}_{B,1,2}) \\ &= h T^{(3)}_B t_{001}\sigma_{12} \in St(A_3) T^{(3)}_B St(\tilde{V}^{(1)}_{B,1,2}), \end{aligned} \tag{115}$$

$$\begin{aligned} T^{(2)}_B t_{011}\sigma_{13} &= T^{(2)}_B \sigma_{13} t_{110} \in St(A_3) T^{(2)}_B \sigma_{13} St(\tilde{V}^{(1)}_{B,1,2}) \\ &= h T^{(2)}_B \sigma_{23}\sigma_{12} t_{110} \in St(A_3) T^{(2)}_B \sigma_{23} St(\tilde{V}^{(1)}_{B,1,2}), \end{aligned} \tag{116}$$

where

$$h := T^{(2)}_B \sigma_{12} (T^{(2)}_B)^{-1} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix} \in St(A_3). \tag{117}$$

From all these equations, the assertion of the theorem is obtained.

(b) (Case of $\tilde{S}[g^{-1}] \in \tilde{U}^{(2)}_{B,1,2}$)
The entries of $\tilde{S}[g^{-1}] \in \tilde{U}^{(1)}_{B,1,2}$ are denoted by

$$\begin{pmatrix} -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} & \tilde{s}_{14} \\ \tilde{s}_{12} & -\sum_{i=2}^4 \tilde{s}_{1i} & \tilde{s}_{14} & \tilde{s}_{13} \\ \tilde{s}_{13} & \tilde{s}_{14} & -\tilde{s}_{13} - \tilde{s}_{14} - \tilde{s}_{34} & \tilde{s}_{34} \\ \tilde{s}_{14} & \tilde{s}_{13} & \tilde{s}_{34} & -\tilde{s}_{13} - \tilde{s}_{14} - \tilde{s}_{34} \end{pmatrix}. \tag{118}$$

Hence,

$$\begin{aligned}
&\langle \tilde{S}[g^{-1}], I_4\rangle - \langle \tilde{S}, I_4\rangle \\
&= \left\langle \begin{pmatrix} -\sum_{i=2}^{4}\tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\sum_{i=2}^{4}\tilde{s}_{1i} & \tilde{s}_{14} \\ \tilde{s}_{13} & \tilde{s}_{14} & -\tilde{s}_{13}-\tilde{s}_{14}-\tilde{s}_{34} \end{pmatrix}, g^T A_3 g - A_3 \right\rangle \\
&= -(a_{11}+a_{22}-2a_{12}-2)\tilde{s}_{12} - (a_{11}+a_{22}+a_{33}-2a_{13}-4)\tilde{s}_{13} \\
&\quad -(a_{11}+a_{22}+a_{33}-2a_{23}-4)\tilde{s}_{14} - (a_{33}-2)\tilde{s}_{34}. \qquad (119)
\end{aligned}$$

Since $-4s_{13} \geq -2(s_{13}+s_{14}) = (1,1,0,0)\tilde{S}(1,1,0,0)^T$ and $-2(\tilde{s}_{14}+\tilde{s}_{34}) \geq -(\tilde{s}_{12}+2\tilde{s}_{14}+\tilde{s}_{34}) = (1,0,1,0)\tilde{S}(1,0,1,0)^T$, the following are required by (83) and the assumption (A):

$$\text{(iii)} \quad a_{11}+a_{33}-2a_{13} = a_{22} = 2, \qquad (120)$$

$$\text{(iv)} \quad a_{11} = a_{22}+a_{33}-2a_{23} = 2 \text{ or } a_{33} = 2. \qquad (121)$$

These equations hold if and only if

$$(\tilde{a}_{ij})_{1\leq i,j\leq 3} := (gT_B^{(2)})^T A_3 g T_B^{(2)} \text{ satisfies (i), (ii) in } (a),$$

$$\Longleftrightarrow gT_B^{(2)} \text{ equals one of the matrices in (111).}$$

It has been already shown that the statement of the theorem holds in the case of (a). Therefore, the statement is also true in this case because $\tilde{S}$ is assumed to belong to $\tilde{V}^{(2)}_{B,1,2}[g] = \tilde{V}^{(1)}_{B,1,2}[gT_B^{(2)}]$.

(c) (Case of $\tilde{S}[g^{-1}] \in \tilde{U}^{(3)}_{B,3,2}$)
The entries of $\tilde{S}[g^{-1}] \in \tilde{U}^{(1)}_{B,1,2}$ are denoted by

$$\begin{pmatrix} -\sum_{i=2}^{4}\tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} & \tilde{s}_{14} \\ \tilde{s}_{12} & -\tilde{s}_{12}-\tilde{s}_{24} & 0 & \tilde{s}_{24} \\ \tilde{s}_{13} & 0 & -2\tilde{s}_{13} & \tilde{s}_{13} \\ \tilde{s}_{14} & \tilde{s}_{24} & \tilde{s}_{13} & -\tilde{s}_{13}-\tilde{s}_{14}-\tilde{s}_{24} \end{pmatrix}. \qquad (122)$$

Then,

$$\begin{aligned}
&\langle \tilde{S}[g^{-1}], I_4\rangle - \langle \tilde{S}, I_4\rangle \\
&= \left\langle \begin{pmatrix} -\sum_{i=2}^{4}\tilde{s}_{1i} & \tilde{s}_{12} & \tilde{s}_{13} \\ \tilde{s}_{12} & -\tilde{s}_{12}-\tilde{s}_{24} & 0 \\ \tilde{s}_{13} & 0 & -2\tilde{s}_{13} \end{pmatrix}, g^T A_3 g - A_3 \right\rangle \\
&= -(a_{11}+a_{22}-2a_{12}-2)\tilde{s}_{12} - (a_{11}+2a_{33}-2a_{13}-4)\tilde{s}_{13} \\
&\quad -(a_{11}-2)\tilde{s}_{14} - (a_{22}-2)\tilde{s}_{24}. \qquad (123)
\end{aligned}$$

Now, $-2\tilde{s}_{13}$ and $-2\tilde{s}_{24} \geq -\tilde{s}_{12} - \tilde{s}_{24}$ are not smaller than the square of the length of a lattice vector. From the assumption (A), it follows that $a_{11} + 2a_{33} - 2a_{13} = 4$ and $a_{22} = 2$. From these equations, $(\tilde{a}_{ij})_{1 \leq i,j \leq 3} := (gT_B^{(3)})^T A_3 g T_B^{(3)}$ satisfies (i), (ii) in (a). Therefore, $gT_B^{(3)}$ equals one of the matrices in (111). Hence, the statement of the theorem follows from $\tilde{S} \in \tilde{V}_{B,3,2}^{(3)}[g] = \tilde{V}_{B,1,2}^{(1)}[gT_B^{(3)}]$ as in the case of (b).

□

Appendix D
Proofs of propositions

Proof of Proposition 1. For any 3-by-3 symmetric matrix S^{obs} and $g \in St(A_3)$, $h_{del} S^{obs}[g] h^T{}_{del} \in \tilde{D}_{del}$ if and only if $h_{del} S^{obs} h^T{}_{del} \in \tilde{D}_{del}$. Therefore, it is enough if the inequalities are proved when g is an identity matrix. Now, the (i,j)-entry s_{ij} of $h_{del} S^{obs} h_{del}^T$ is not negative. Hence, the assertion follows from the following formulas obtained by direct calculation:

$$\delta_R(S^{obs}[t_{001}^{-1}]) - \delta_R(S^{obs}) = \frac{4rs_{12}(s_{13}+s_{23})}{9}, \tag{124}$$

$$\delta_R(S^{obs}[(T_R^+ t_{001})^{-1}]) - \delta_R(S^{obs}[(T_R^+)^{-1}]) = \frac{4rs_{12}(2s_{12}+s_{14}+s_{23})}{3}, \tag{125}$$

$$\delta_R(S^{obs}[(T_R^+ t_{010})^{-1}]) - \delta_R(S^{obs}[(T_R^+ t_{001})^{-1}]) = \frac{4r(s_{12}+s_{23})s_{14}}{3}. \tag{126}$$

□

Proof of Proposition 2. By the same reason described in the proof of Proposition 1, it may be assumed that g is an identity matrix. The assertion follows from the following formulas:

$$\delta_B(S^{obs}[t_{010}^{-1}]) - \delta_B(S^{obs}) = 2rs_{13}s_{23}, \tag{127}$$

$$\delta_B(S^{obs}[(T_B^{(3)}\sigma_{23})^{-1}]) - \delta_B(S^{obs}[(T_B^{(2)})^{-1}]) = 2rs_{12}(s_{12}+s_{14}+s_{23}) + 2rs_{14}s_{23}, \tag{128}$$

$$\delta_B(S^{obs}[(T_B^{(2)}\sigma_{23})^{-1}]) - \delta_B(S^{obs}[(T_B^{(3)})^{-1}]) = 2rs_{12}(s_{12}+s_{23}). \tag{129}$$

□