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Delone lattice studies in $\mathbf{C^3}$, the space of three complex variables

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Abstract

The Delone (Selling) scalars, which are used in unit cell reduction and in lattice type determination, are studied in $\mathbf{C^3}$, the space of three complex variables. The three complex coordinate planes are composed of the six Delone scalars. The transformations at boundaries of the Selling reduced orthant are described as matrices of operators. A graphical representation as the projections onto the three coordinates is described.

Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. Introduction

The scalars used by Delaunay (1932) in his formulation of Selling reduction (Selling, 1874) are (in the conventional order) $b \cdot c$, $a \cdot c$, $a \cdot b$, $a \cdot d$, $b \cdot d$, $c \cdot d$, where $d = -a-b-c$.

(As a mnemonic device, observe that the first three terms use α, β, and γ, in that order, and the following terms use a, b, c, in that order.)

Andrews *et al.* (2019b) chose to represent the Selling scalars in the space $\mathbf{S^6}$, $\{s_1$, s_2, s_3, s_4, s_5, $s_6\}$ (defined in the order above), as a way to create a metric space for the measurement of the distance between lattices. They also considered the representation of this space as the space of three complex dimensions, $\mathbf{C^3}$ or $\{c_1$, c_2, $c_3\}$.

In $\mathbf{C^3}$, in terms of the Selling scalars, a vector is defined as $\{(s_1,s_4)$, (s_2,s_5),$(s_3,s_6)\}$, where the real and imaginary parts of each are the "opposite" scalars according to the definition of Delaunay (1932) (opposite in terms of the Bravais tetrahedron of scalars) (see Andrews *et al.* (2019a)). As a mnemonic device, note that the complex components involve (α, a), (β, b), and (γ, c). Additionally, each complex term uses all four three-space vectors; for example, c_1 is $(b \cdot c$, $a \cdot d)$.

Andrews *et al.* (2019b) considered the matrix representations of the reflections in $\mathbf{C^3}$ (and in $\mathbf{S^6}$). This paper describes the boundary transformations at the edges of the fundamental unit of $\mathbf{C^3}$ and also a graphical presentation. In $\mathbf{S^6}$, the fundamental unit is the all negative orthant, which contains only, and all of, the reduced cells. In $\mathbf{S^6}$ and $\mathbf{C^3}$, the boundaries located where any $\mathbf{S^6}$ scalar (or correspondingly in $\mathbf{C^3}$, a real or imaginary part) equals zero.

2. Notation

Complex numbers are represented in Cartesian format (x, y), where x is the real part and y is the imaginary part.

We represent a vector in $\mathbf{C^3}$ by $\{(x_1, y_1)$, (x_2, y_2), $(x_3, y_3)\}$ as an alternative to $\{(s_1,s_4)$, (s_2,s_5),$(s_3,s_6)\}$.

Next we define the operators in $\mathbf{C^3}$ that will be used in the matrix descriptions of the transformations at the boundaries of the fundamental unit, see Table 1.

Table 1. *The Result column values give the products of each operator as applied to* (x_j, y_j)

Operator	Usage	Result	Name
$\mathcal{M}_r$	$\mathcal{M}_r(c_j)$	$(-x_j, -x_j + y_j)$	Minus real
$\mathcal{M}_i$	$\mathcal{M}_i(c_j)$	$(x_j - y_j, -y_j)$	Minus imag
$\mathcal{P}_r$	$\mathcal{P}_r(c_j)$	(x_j, x_j)	Plus real
$\mathcal{P}_i$	$\mathcal{P}_i(c_j)$	(y_j, y_j)	Plus imag
$\mathcal{R}$	$\mathcal{R}(c_j)$	x_j or $(x_j, 0)$	Real
$\mathcal{I}$	$\mathcal{I}(c_j)$	y_j pr $(y_j, 0)$	Imaginary

3. Matrices of boundary transformations

Andrews *et al.* (2019b) listed the boundary transformations for each of the six $\mathbf{S^6}$ boundaries. For each, they only listed 2 transformations, following Delaunay (1932) and Delone *et al.* (1975). That list is incomplete in the sense that applying the 24 reflections gives 24 boundary transformation, four for each boundary, rather than 12.

The C3 vector transformations are represented as multiplication by a matrix of the operators defined in Table 1. When a complex vector component is 'multiplied' by an operator, the result is as defined in the table."

For the boundary at s_1: (the real component of c_1).

$$\begin{bmatrix}\mathcal{M}_r & 0 & 0\\ \mathcal{P}_r & \mathrm{i}\mathcal{R} & \mathcal{R}\\ \mathcal{P}_r & \mathrm{i}\mathcal{I} & \mathcal{I}\end{bmatrix}\begin{bmatrix}\mathcal{M}_r & 0 & 0\\ \mathcal{P}_r & \mathrm{i}\mathcal{I} & \mathcal{I}\\ \mathcal{P}_r & \mathrm{i}\mathcal{R} & \mathcal{R}\end{bmatrix}\begin{bmatrix}\mathcal{M}_r & 0 & 0\\ \mathcal{P}_r & \mathcal{R} & \mathrm{i}\mathcal{R}\\ \mathcal{P}_r & \mathcal{I} & \mathrm{i}\mathcal{I}\end{bmatrix}\begin{bmatrix}\mathcal{M}_r & 0 & 0\\ \mathcal{P}_r & \mathcal{I} & \mathrm{i}\mathcal{I}\\ \mathcal{P}_r & \mathcal{R} & \mathrm{i}\mathcal{R}\end{bmatrix}$$

For the boundary at s_4: (the imaginary component of c_1).

$$\begin{bmatrix}\mathcal{M}_i & 0 & 0\\ \mathcal{P}_i & \mathrm{i}\mathcal{R} & \mathcal{R}\\ \mathcal{P}_i & \mathrm{i}\mathcal{I} & \mathcal{I}\end{bmatrix}\begin{bmatrix}\mathcal{M}_i & 0 & 0\\ \mathcal{P}_i & \mathrm{i}\mathcal{I} & \mathcal{I}\\ \mathcal{P}_i & \mathrm{i}\mathcal{R} & \mathcal{R}\end{bmatrix}\begin{bmatrix}\mathcal{M}_i & 0 & 0\\ \mathcal{P}_i & \mathcal{R} & \mathrm{i}\mathcal{R}\\ \mathcal{P}_i & \mathcal{I} & \mathrm{i}\mathcal{I}\end{bmatrix}\begin{bmatrix}\mathcal{M}_i & 0 & 0\\ \mathcal{P}_i & \mathcal{I} & \mathrm{i}\mathcal{I}\\ \mathcal{P}_i & \mathcal{R} & \mathrm{i}\mathcal{R}\end{bmatrix}$$

For the boundary at s_2 (the real component of c_2):

$$\begin{bmatrix}\mathrm{i}\mathcal{R} & \mathcal{P}_r & \mathcal{R}\\ 0 & \mathcal{M}_r & 0\\ \mathrm{i}\mathcal{I} & \mathcal{P}_r & \mathcal{I}\end{bmatrix}\begin{bmatrix}\mathrm{i}\mathcal{I} & \mathcal{P}_r & \mathcal{I}\\ 0 & \mathcal{M}_r & 0\\ \mathrm{i}\mathcal{R} & \mathcal{P}_r & \mathcal{R}\end{bmatrix}\begin{bmatrix}\mathcal{R} & \mathcal{P}_r & \mathrm{i}\mathcal{R}\\ 0 & \mathcal{M}_r & 0\\ \mathcal{I} & \mathcal{P}_r & \mathrm{i}\mathcal{I}\end{bmatrix}\begin{bmatrix}\mathcal{I} & \mathcal{P}_r & \mathrm{i}\mathcal{I}\\ 0 & \mathcal{M}_r & 0\\ \mathcal{R} & \mathcal{P}_r & \mathrm{i}\mathcal{R}\end{bmatrix}$$

For the boundary at s_5: (the imaginary component of c_2).

$$\begin{bmatrix} \mathrm{i}\mathcal{R} & \mathcal{P}_i & \mathcal{R} \\ 0 & \mathcal{M}_i & 0 \\ \mathrm{i}\mathcal{I} & \mathcal{P}_i & \mathcal{I} \end{bmatrix} \begin{bmatrix} \mathrm{i}\mathcal{I} & \mathcal{P}_i & \mathcal{I} \\ 0 & \mathcal{M}_i & 0 \\ \mathrm{i}\mathcal{R} & \mathcal{P}_i & \mathcal{R} \end{bmatrix} \begin{bmatrix} \mathcal{R} & \mathcal{P}_i & \mathrm{i}\mathcal{R} \\ 0 & \mathcal{M}_i & 0 \\ \mathcal{I} & \mathcal{P}_i & \mathrm{i}\mathcal{I} \end{bmatrix} \begin{bmatrix} \mathcal{I} & \mathcal{P}_i & \mathrm{i}\mathcal{I} \\ 0 & \mathcal{M}_i & 0 \\ \mathcal{R} & \mathcal{P}_i & \mathrm{i}\mathcal{R} \end{bmatrix}$$

For the boundary at s_3 (the real component of c_3):

$$\begin{bmatrix} \mathrm{i}\mathcal{R} & \mathcal{R} & \mathcal{P}_r \\ \mathrm{i}\mathcal{I} & \mathcal{I} & \mathcal{P}_r \\ 0 & 0 & \mathcal{M}_r \end{bmatrix} \begin{bmatrix} \mathrm{i}\mathcal{I} & \mathcal{I} & \mathcal{P}_r \\ \mathrm{i}\mathcal{R} & \mathcal{R} & \mathcal{P}_r \\ 0 & 0 & \mathcal{M}_r \end{bmatrix} \begin{bmatrix} \mathcal{R} & \mathrm{i}\mathcal{R} & \mathcal{P}_r \\ \mathcal{I} & \mathrm{i}\mathcal{I} & \mathcal{P}_r \\ 0 & 0 & \mathcal{M}_r \end{bmatrix} \begin{bmatrix} \mathcal{I} & \mathrm{i}\mathcal{I} & \mathcal{P}_r \\ \mathcal{R} & \mathrm{i}\mathcal{R} & \mathcal{P}_r \\ 0 & 0 & \mathcal{M}_r \end{bmatrix}$$

For the boundary at s_6 (the imaginary component of c_3):

$$\begin{bmatrix} \mathrm{i}\mathcal{R} & \mathcal{R} & \mathcal{P}_i \\ \mathrm{i}\mathcal{I} & \mathcal{I} & \mathcal{P}_i \\ 0 & 0 & \mathcal{M}_i \end{bmatrix} \begin{bmatrix} \mathrm{i}\mathcal{I} & \mathcal{I} & \mathcal{P}_i \\ \mathrm{i}\mathcal{R} & \mathcal{R} & \mathcal{P}_i \\ 0 & 0 & \mathcal{M}_i \end{bmatrix} \begin{bmatrix} \mathcal{R} & \mathrm{i}\mathcal{R} & \mathcal{P}_i \\ \mathcal{I} & \mathrm{i}\mathcal{I} & \mathcal{P}_i \\ 0 & 0 & \mathcal{M}_i \end{bmatrix} \begin{bmatrix} \mathcal{I} & \mathrm{i}\mathcal{I} & \mathcal{P}_i \\ \mathcal{R} & \mathrm{i}\mathcal{R} & \mathcal{P}_i \\ 0 & 0 & \mathcal{M}_i \end{bmatrix}$$

3.1. Derivation

Consider the $\mathbf{S^6}$ vector $\{(x_1, y_1), (x_2, y_2), (x_3, y_3)\}$; in $\mathbf{C^3}$ that vector is: $\{(s_1,s_4), (s_2,s_5),(s_3,s_6)\}$. Stated in $\mathbf{C^3}$, the problem is to find a matrix that converts a $\mathbf{C^3}$ vector to a more reduced one. Take the case of $s_1$positive and the other scalars negative.

$$\begin{aligned} & \{(\text{-}s_1,\ s_4\text{-}s_1),\ (s_3{+}s_1,\ s_2{+}s_1),\ (s_6{+}s_1,\ s_5{+}s_1)\} \\ = \quad & \mathrm{RedMat} \begin{Bmatrix} (s_1,s_4) \\ (s_2,s_5) \\ (s_3,s_6) \end{Bmatrix} \end{aligned}$$

We need to solve for RedMat. Here, one of the four possible result vectors has been chosen (arbitrarily).

Element 1 of result vector is (-s_1, s_4-s_1), and it is created by multiplying the beginning $\mathbf{C^3}$ vector by the first row of the transformation matrix. In this case, we see that $c_1$of the result only contains scalars from $c_1$of the input, so the first row must contain some operator to be multiplied times input c_1, and the second and third elements of the matrix row must be zero. We create an operator (*Minus real*) to transform the input $c_1$to the output c_1; so the first row of the reduction matrix is: $\mathcal{M}_i00$.

Element 2 of the result vector is (s_3+s_1, s_2+s_1), and it is created by multiplying the beginning $\mathbf{C^3}$ vector by the second row of the transformation matrix. The result $c_2$contains $s_1$in both the real and imaginary parts. So the first matrix element in that row must insert s_1, the real part of the input c_1, into both the real and imaginary parts. An operator to produce that is created (Plus real). Next we see that the result contains $s_2$and s_3. $s_3$appears in the real part of the result element and in the third part of the input vector. So the third element of the second matrix row must extract the s_3, the real part of $c_3$of the input. So the second row now contains the Plus real operator and the element to put the real part of $c_3$of the input. The final matrix element of the second row (the second element) must extract the real part of input $c_2$and place it in the imaginary part of the output vector. The resulting second row of the matrix is $\mathcal{P}_r$ $\mathcal{R}$ $i\mathcal{R}$.

Using similar logic, the third row of the matrix is: $\mathcal{P}_r$ $\mathcal{I}$ $i\mathcal{I}$.

Having derived the first matrix, the other 23 can be derived by the same process. However because all the $\mathbf{S^6}$boundaries are related by the 24 reflection, the other 23 matrices can be generated simply by multiplying by each of the reflection matrices.

3.2. Example C++ implementation

```
static std::complex<double> c3_Minus_Real(std::complex<double>& a) {
   const std::complex<double> c = { -a.real(), -a.real() + a.imag() };
   return c;
}

C3 C3::c3_s1(const C3& a) {
   C3 c;
   c[0] = c3_Minus_Real(a[0]);
   c[1] = c3_Plus_Real(a[0]) + c3_Real(a[1]) +
   c3_I_Times_Real(a[2]);
   c[2] = c3_Plus_Real(a[0]) + c3_Imag(a[1]) +
   c3_I_Times_Imag(a[2]);
   return c;
}
```

3.3. Example of use

To demonstrate the application of the above matrices, example C++ code was written to create matrices of operators; see the supplementary material for the code or the complete library reference in the Availability of Code below.

Create a $\mathbf{C^3}$ vector c3 with the values {(1,2),(3,4),(5,6)} (which does not correspond to a valid unit cell). Multiply it by the matrix of operators derived above.

The matrix multiplication can be implemented as follows (including only one example of the functions for operators (c3_Minus_Real))"

Therefore, RedMat =

$$\begin{bmatrix} \mathcal{M}_r & 0 & 0 \\ \mathcal{P}_r & \mathrm{i}\mathcal{R} & \mathcal{R} \\ \mathcal{P}_r & \mathrm{i}\mathcal{I} & \mathcal{I} \end{bmatrix}$$

For example:

$$\{(\text{-}1.000,1.000)\ (4.000,6.000)\ (5.000,7.000)\} = \begin{bmatrix} \mathcal{M}_r & 0 & 0 \\ \mathcal{P}_r & \mathrm{i}\mathcal{R} & \mathcal{R} \\ \mathcal{P}_r & \mathrm{i}\mathcal{I} & \mathcal{I} \end{bmatrix} \begin{Bmatrix} (1,2) \\ (3,4) \\ (5,6) \end{Bmatrix}$$

which can be verified by hand.

4. Basics

The standard representation of the identity operation is

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{c}.$$

The identity in $\mathbf{C^3}$ could also be written:

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \mathcal{R}+\mathrm{i}\mathcal{I} & 0 \\ 0 & 0 & \mathcal{R}+\mathrm{i}\mathcal{I} \end{bmatrix} \mathbf{c}.$$

which is simply replacement of the value one with an equivalent representation as operators.

Delaunay (1932) does not consider the boundary transformations in detail. However, he uses them to define the process of Selling reduction. For example in $\mathbf{S^6}$, he lists the following as one of the possible results for a transformation on s_1, translated to $\mathbf{S^6}$: $\{-s_1, -s_1+s_2, s_1+s_3, s_1+s_5, s_1+s_4, s_1+s_6\}$. The third boundary transform for s_1 above implements this operation and interchanges the real part of c_3 and the imaginary part of c_2:

$$\begin{bmatrix} \mathcal{M}_r & 0 & 0 \\ \mathcal{P}_r & \mathcal{R} & \mathrm{i}\mathcal{R} \\ \mathcal{P}_r & \mathcal{I} & \mathrm{i}\mathcal{I} \end{bmatrix}$$

Considered in $\mathbf{C^3}$, Delone's alternate transformation for the s_1 boundary would exchange the real of c_2 with the imaginary part of c_3. That is the fourth matrix above in the list for s_1. The other two transformations for s_1 can be generated from the two we have just mentioned by the "exchange operation" (Andrews *et al.*, 2019b) applied to the second and third $\mathbf{C^3}$ coordinates. Delone did not describe the latter two transformations, perhaps because even a single transformation was adequate to implement reduction. He had already listed two.

5. Graphical display of projections

The two-dimensional nature of the three coordinates of $\mathbf{C^3}$ suggests their use for graphical display.

As an example, we use Phospholipase A2 (**PLA2**) (retrieved from the Protein Data Bank (Bernstein *et al.*, 1977)), which has had several similar or identical structures determined (Le Trong & Stenkamp, 2007). Andrews *et al.* (2019b) found additional cases (see Table 2)

PDB id	Centering	a	b	c	α	β	γ
1DPY & 1FE5	hR	57.98	57.98	57.98	92.02	92.02	92.02
1G0Z & 1U4J	hP	80.36	80.36	99.44	90	90	120
1G2X	mC	80.95	80.57	57.1	90	90.35	90
2OSN	hR	57.10	57.10	57.10	89.75	89.75	89.75

Table 2. *Phospholipase A2 unit cells*

Below, Figure 1 shows the unit cells as reported (the centering of lattices has not been removed). The following figures (Figures 2 to 3) show various transformations and embellishments of the reported cells.

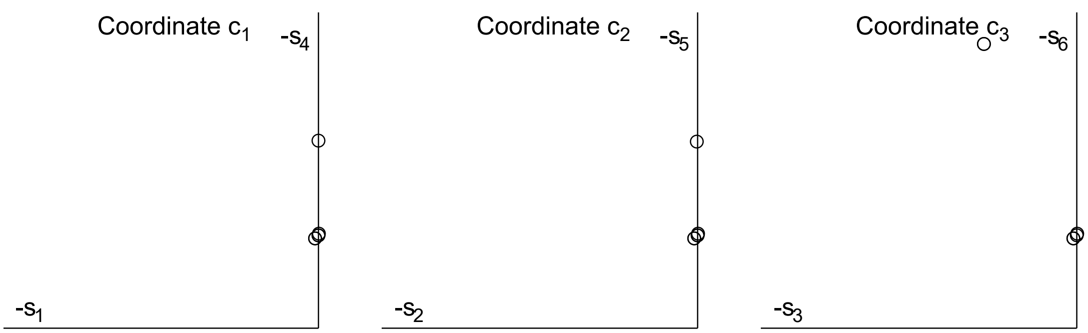

Fig. 1. Phospholipase A2 unit cells as reported.

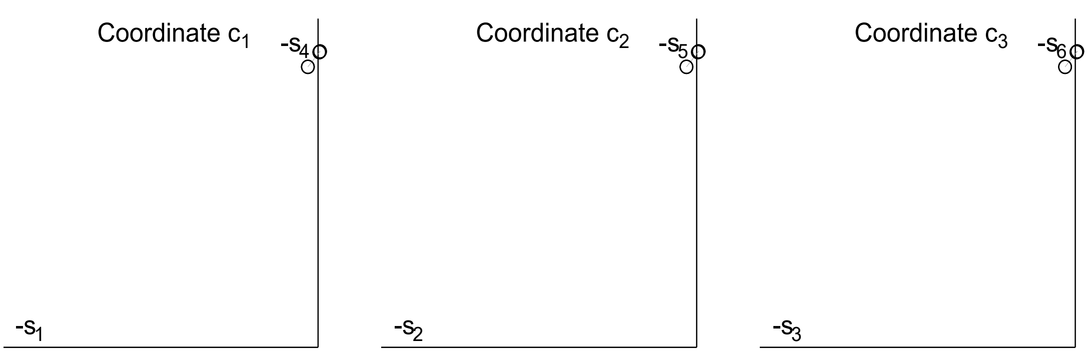

Fig. 2. The PLA2 unit cells Niggli-reduced. The similarity of the 3 projections is indicative of the exact or nearly exact rhombohedral symmetry.

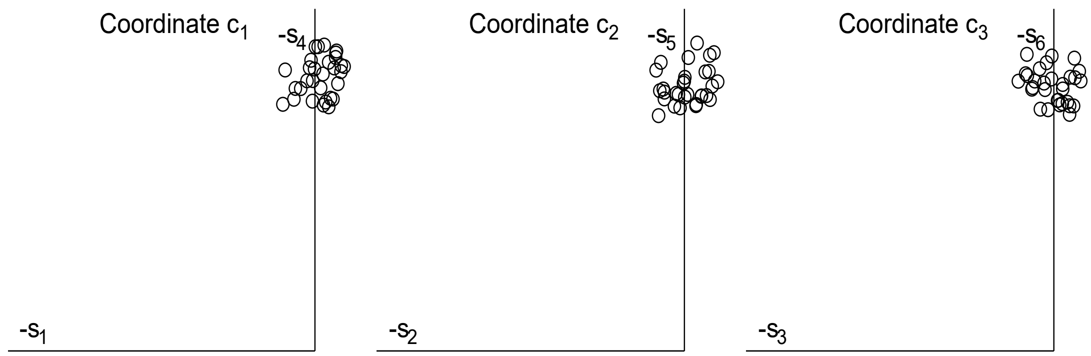

Fig. 3. The PLA2 unit cells, Niggli-reduced, and five copies were perturbed 10% orthogonally to $\mathbf{S^6}$ vector.

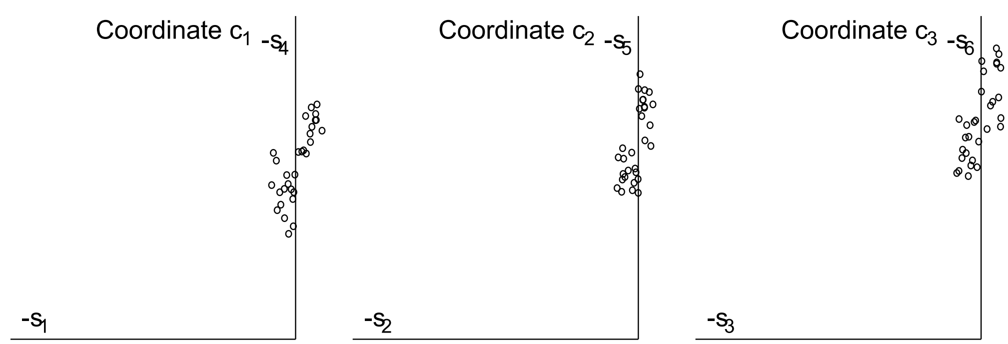

Fig. 4. The PLA2 unit cells, Niggli-reduced, and five copies were perturbed 10% orthogonally to $\mathbf{S^6}$ vector, followed by Niggli reduction.

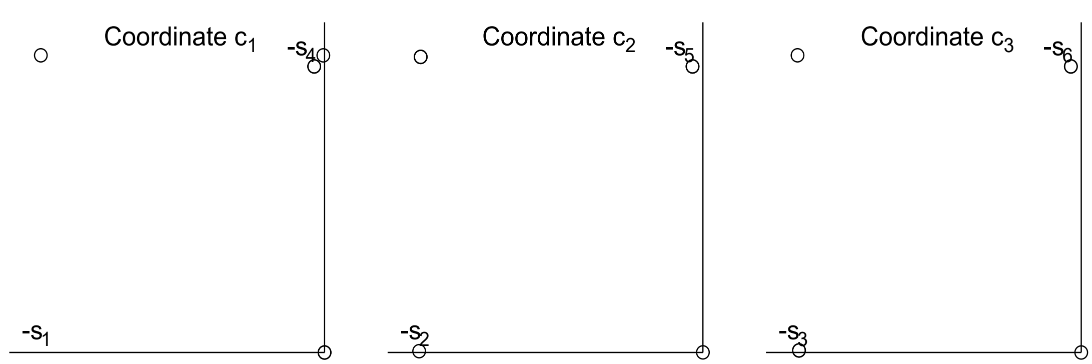

Fig. 5. The PLA2 unit cells Delone-reduced.

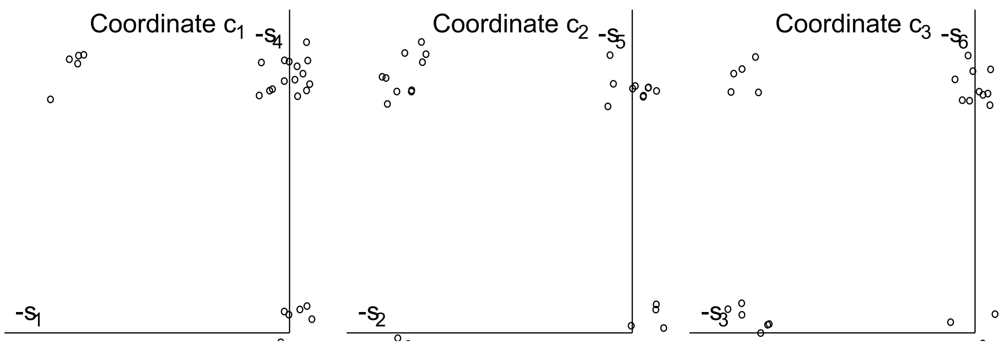

Fig. 6. The PLA2 cells Delone reduced and 5 copies perturbed by 10%.

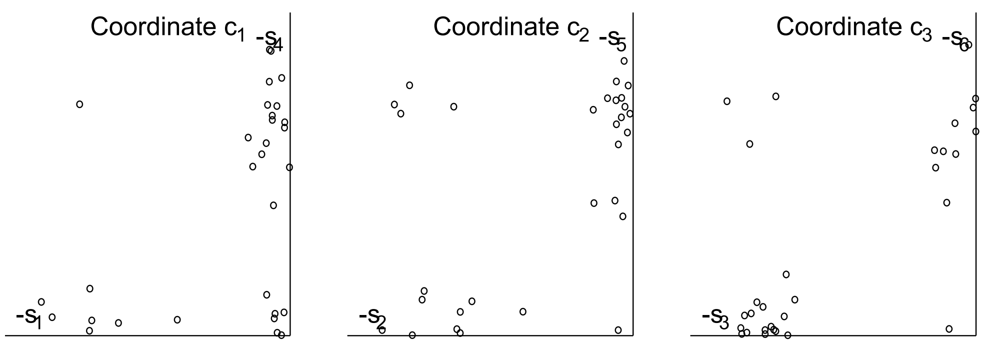

Fig. 7. The same cells as plotted in Figure 6 and Delone reduced.

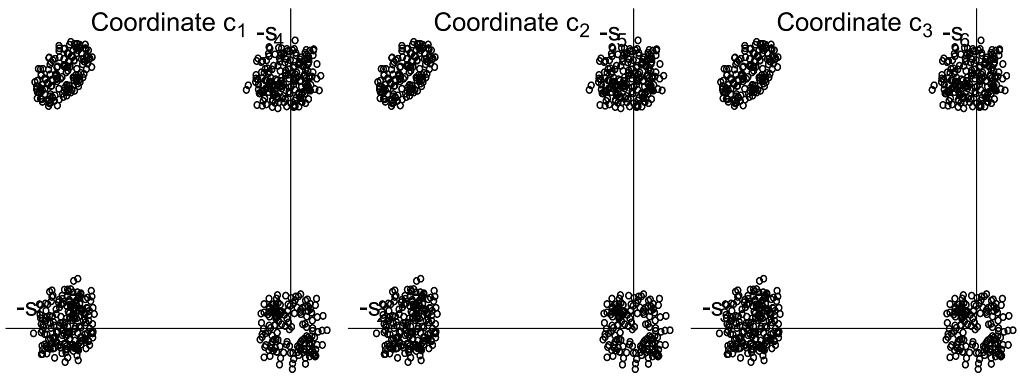

Fig. 8. The same cells as plotted in Figure 6 and Delone reduced, and then each multiplied by the 24 $\mathbf{S^6}$ reflections.

6. Summary

The transformation matrices shown above demonstrate the considerable regularity of Selling reduction, as used by Delaunay (1932). The reduction operations of Niggli reduction (Niggli, 1928) are more complex. While all the boundaries of the non-positive orthant of $\mathbf{S^6}$ are essentially the same (and related by reflections), the boundaries formed in Niggli reduction are of multiple types, and the fundamental unit of the space representing Niggli-reduced cells ($\mathbf{G^6}$, see Andrews & Bernstein (2014)) is non-convex.

Several aspects of $\mathbf{C^3}$ are evident from inspecting the matrices. First, each boundary has four possible transformations that can be applied. Since each of the transformations at boundaries are self-inverse, they are the same transformations that would be used in the process of cell (lattice) reduction. Delaunay (1932) and Delone *et al.* (1975) give only two choices, presumably for simplicity, omitting transformations that use the "exchange" operator (see Andrews *et al.* (2019b)).

7. Availability of code

The C^{++} code for $\mathbf{C^3}$ and related software tools is available in github.com, in `https://github.com/duck10/LatticeRepLib.git`. The program CmdToC3 uses the required files.

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Synopsis

The space $\mathbf{C^3}$ is explained in more detail than in the original description. Boundary transformations of the fundamental unit are described in detail. A graphical presentation of the basic coordinates is described and illustrated.