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

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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.

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## 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  $\alpha, \beta$ , and  $\gamma$ , 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  $(\alpha, a), (\beta, b)$ , and  $(\gamma, c)$ . 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
$\mathfrak{M}_r$	$\mathfrak{M}_r(c_j)$	$(-x_j, -x_j + y_j)$	Minus real
$\mathfrak{M}_i$	$\mathfrak{M}_i(c_j)$	$(x_j - y_j, -y_j)$	Minus imag
$\mathfrak{P}_r$	$\mathfrak{P}_r(c_j)$	$(x_j, x_j)$	Plus real
$\mathfrak{P}_i$	$\mathfrak{P}_i(c_j)$	$(y_j, y_j)$	Plus imag
$\mathfrak{R}$	$\mathfrak{R}(c_j)$	$x_j$	Real
$\mathfrak{I}$	$\mathfrak{I}(c_j)$	$y_j$	Imaginary

## 3. Matrices of boundary transformations

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

$$\begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathfrak{I}\mathfrak{R} & \mathfrak{R} \\ \mathfrak{P}_r & \mathfrak{I}\mathfrak{I} & \mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathfrak{I}\mathfrak{I} & \mathfrak{I} \\ \mathfrak{P}_r & \mathfrak{I}\mathfrak{R} & \mathfrak{R} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathfrak{R} & \mathfrak{I}\mathfrak{R} \\ \mathfrak{P}_r & \mathfrak{I} & \mathfrak{I}\mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathfrak{I} & \mathfrak{I}\mathfrak{I} \\ \mathfrak{P}_r & \mathfrak{R} & \mathfrak{I}\mathfrak{R} \end{bmatrix}$$

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

$$\begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathfrak{I}\mathfrak{R} & \mathfrak{R} \\ \mathfrak{P}_i & \mathfrak{I}\mathfrak{I} & \mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathfrak{I}\mathfrak{I} & \mathfrak{I} \\ \mathfrak{P}_i & \mathfrak{I}\mathfrak{R} & \mathfrak{R} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathfrak{R} & \mathfrak{I}\mathfrak{R} \\ \mathfrak{P}_i & \mathfrak{I} & \mathfrak{I}\mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathfrak{I} & \mathfrak{I}\mathfrak{I} \\ \mathfrak{P}_i & \mathfrak{R} & \mathfrak{I}\mathfrak{R} \end{bmatrix}$$

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

$$\begin{bmatrix} \mathfrak{I}\mathfrak{R} & \mathfrak{P}_r & \mathfrak{R} \\ 0 & \mathfrak{M}_r & 0 \\ \mathfrak{I}\mathfrak{I} & \mathfrak{P}_r & \mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{I}\mathfrak{I} & \mathfrak{P}_r & \mathfrak{I} \\ 0 & \mathfrak{M}_r & 0 \\ \mathfrak{I}\mathfrak{R} & \mathfrak{P}_r & \mathfrak{R} \end{bmatrix} \begin{bmatrix} \mathfrak{R} & \mathfrak{P}_r & \mathfrak{I}\mathfrak{R} \\ 0 & \mathfrak{M}_r & 0 \\ \mathfrak{I} & \mathfrak{P}_r & \mathfrak{I}\mathfrak{I} \end{bmatrix} \begin{bmatrix} \mathfrak{I} & \mathfrak{P}_r & \mathfrak{I}\mathfrak{I} \\ 0 & \mathfrak{M}_r & 0 \\ \mathfrak{R} & \mathfrak{P}_r & \mathfrak{I}\mathfrak{R} \end{bmatrix}$$

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

$$\begin{bmatrix} i\Re & \Re_i & \Re \\ 0 & \Re_i & 0 \\ i\Im & \Re_i & \Im \end{bmatrix} \begin{bmatrix} i\Im & \Re_i & \Im \\ 0 & \Re_i & 0 \\ i\Re & \Re_i & \Re \end{bmatrix} \begin{bmatrix} \Re & \Re_i & i\Re \\ 0 & \Re_i & 0 \\ \Im & \Re_i & i\Im \end{bmatrix} \begin{bmatrix} \Im & \Re_i & i\Im \\ 0 & \Re_i & 0 \\ \Re & \Re_i & i\Re \end{bmatrix}$$

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

$$\begin{bmatrix} i\Re & \Re & \Re_r \\ i\Im & \Im & \Re_r \\ 0 & 0 & \Re_r \end{bmatrix} \begin{bmatrix} i\Im & \Im & \Re_r \\ i\Re & \Re & \Re_r \\ 0 & 0 & \Re_r \end{bmatrix} \begin{bmatrix} \Re & i\Re & \Re_r \\ \Im & i\Im & \Re_r \\ 0 & 0 & \Re_r \end{bmatrix} \begin{bmatrix} \Im & i\Im & \Re_r \\ \Re & i\Re & \Re_r \\ 0 & 0 & \Re_r \end{bmatrix}$$

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

$$\begin{bmatrix} i\Re & \Re & \Re_i \\ i\Im & \Im & \Re_i \\ 0 & 0 & \Re_i \end{bmatrix} \begin{bmatrix} i\Im & \Im & \Re_i \\ i\Re & \Re & \Re_i \\ 0 & 0 & \Re_i \end{bmatrix} \begin{bmatrix} \Re & i\Re & \Re_i \\ \Im & i\Im & \Re_i \\ 0 & 0 & \Re_i \end{bmatrix} \begin{bmatrix} \Im & i\Im & \Re_i \\ \Re & i\Re & \Re_i \\ 0 & 0 & \Re_i \end{bmatrix}$$

#### 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  $\mathbf{C}^3$  can also be written:

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \Re + i\Im & 0 \\ 0 & 0 & \Re + i\Im \end{bmatrix} \mathbf{c}.$$

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  $c_2$ :

$$\begin{bmatrix} \Re_r & 0 & 0 \\ \Re_r & \Re & i\Re \\ \Re_r & \Im & i\Im \end{bmatrix}$$

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.

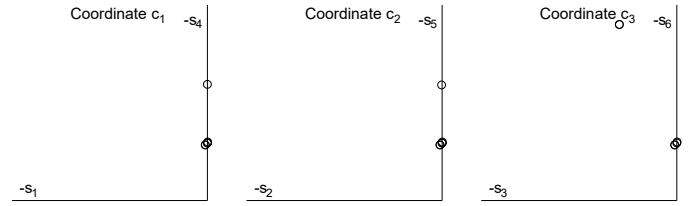
As an example, we use Phospholipase A2 (**PLA2**) (retrieved from the Protein Data Bank (Bernstein *et al.*, 1977)), which has had several similar or identical structures determined (Le Trong & Stenkamp, 2007). Andrews *et al.* (2019b) found additional cases (see Table 2)

PDB id	Centering	a	b	c	$\alpha$	$\beta$	$\gamma$
1DPY	R	57.98	57.98	57.98	92.02	92.02	92.02
1FE5	R	57.98	57.98	57.98	92.02	92.02	92.02
1G0Z	H	80.36	80.36	99.44	90	90	120
1G2X	C	80.95	80.57	57.1	90	90.35	90
1U4J	H	80.36	80.36	99.44	90	90	120
2OSN	R	57.10	57.10	57.10	89.75	89.75	89.75

**Table 2**

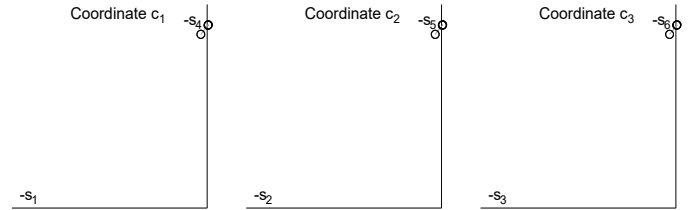
Phospholipase A2 unit cells

Below, Figure 1 shows the unit cells as reported (the centering of lattices has not been removed). The following figures (Figures 2 to 5) show various transformations and embellishments of the reported cells.



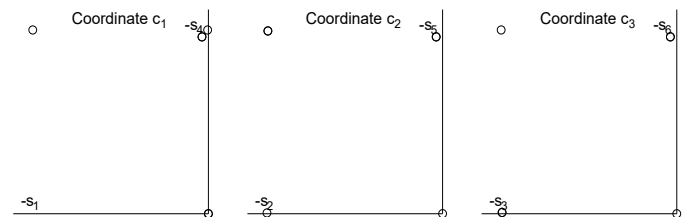
**Figure 1**

Phospholipase A2 unit cells as reported.



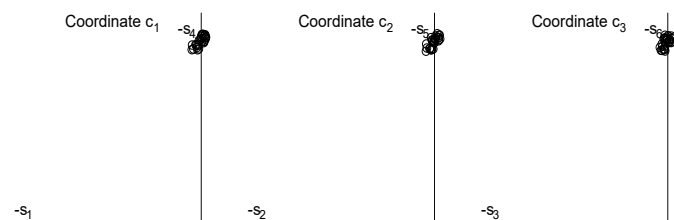
**Figure 2**

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



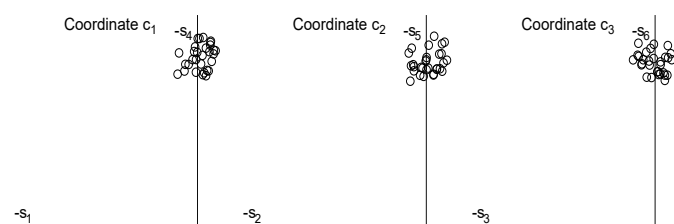
**Figure 3**

The PLA2 unit cells Delone-reduced.



**Figure 4**

The PLA2 unit cells, Niggli-reduced, and five copies were perturbed 2% orthogonally to  $S^6$  vector.



**Figure 5**

The PLA2 unit cells, Niggli-reduced, and five copies were perturbed 10% orthogonally to  $S^6$  vector.

## 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  $S^6$  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 ( $G^6$ , see Andrews & Bernstein (2014)) is non-convex.

Several aspects of  $C^3$  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  $C^3$  and related software tools is available in [github.com](https://github.com/duck10/LatticeRepLib.git), in <https://github.com/duck10/LatticeRepLib.git>. The program CmdToC3 uses the required files.

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