Selling Reduction versus Niggli Reduction for Crystallographic Lattices

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(Received 0 XXXXXXX 0000; accepted 0 XXXXXXX 0000)

Unit cell reduction; **Delaunay**; **Delone**; **Niggli**; **Selling**

Abstract

The unit cell reduction described by Selling and used by Delone is explained in a simple form. The transformations needed to implement the reduction are listed. The simplicity of this reduction contrasts with the complexity of Niggli reduction.

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

1. Introduction

The origin of crystallography was the study of minerals (Haüy, 1784). That led to the study of lattices, since it was clear that repetition underlaid the structure of crystals.

In order to systematize the enumeration of lattices (unit cells), the mathematical procedures of reduction were developed to produce compact descriptions, thus providing a method to compare pairs of lattices. Fundamentally, reduction is used to place the lattice in an asymmetric unit of the space of unit cells. For some applications (*e.g.* cell clustering by pairwise comparison), the use of lattice reduction can be computationally time consuming for large data sets. Of the known reduction methods, the Selling reduction is the least time-consuming.

Niggli (1928) and Delone (1933) used reduction methods developed in the 19th century by Eisenstein (1851) and Selling (1874), respectively. Their original goal was to systematize the experimental determination of Bravais lattice types. Each provided tables of the characteristics of the reduced cells with their correspondence to each of the Bravais types. The first edition of International Tables for X-Ray Crystallography originally included a section (Henry & Lonsdale, 1952) on the Delone's methods and Selling reduction and their use. Later editions have instead included only Niggli's method.

The initial impetus for the developments by Delone and Niggli was to determine likely Bravais lattice types based on experimental unit cells. (Probably the best display of Niggli's methods is in Roof (1967).) With time and the progress in crystallography, researchers realized that those tables did not always provide a simple answer due to unavoidable experimental errors in cell determination. Later simply measuring the difference between pairs of lattices became important. Methods have been developed to cope with the resulting approximate cells (reviewed in Andrews & Bernstein (2014)).

Bravais lattice determination has been automated by several methods (see a review in Andrews & Bernstein (2014)). However, accumulation of databases of unit cell parameters, often of closely similar materials, increased the need for perturbation stability. At the present time, the need is for methods that can be used for accessing large databases of unit cell parameters and for cluster analysis of substantial numbers of images from serial crystallography. Bravais lattice determination is no longer the only or even the most important use of lattice reduction methods. Now the most pressing need is for high performance methods for lattice matching.

Andrews & Bernstein (2014) and Andrews & Bernstein (1988) discussed Niggli reduction. In this paper we provide a complete description of the reduction of Selling that can be applied in crystallography as a time-cost-effective alternative to more complex reduction methods. Especially in procedures for handling large numbers of experimental data, reduction can be a significant portion of the processing time. Loading large databases (there are now approximately one million unit cells available) and clustering many images from serial crystallography can be a lengthy process.

One strong advantage of the use of Selling scalars is that they are homogeneous. They are all dot products and of comparable dimensions. There is another lattice representation which is also homogeneous, as seven squared lengths forming a space called $\mathbf{D^7}$. For completeness we present that representation in Appendix A and in supplementary material, inasmuch as literature on $\mathbf{D^7}$ is not easily available elsewhere. The Selling representation as six scalars is computationally more efficient for database work and for clustering than the representation as seven squared lengths. Indeed it appears to be the most efficient available choice when quantifying differences among any large number of crystallographic lattices.

2. The Selling Scalars

As applied to crystallography, the scalars to be reduced by Selling's method are the dot products of the unit cell axes, in addition to the negative of their sum (a body diagonal). Labeling these $\mathbf{a}, \mathbf{b}, \mathbf{c}$, and $\mathbf{d}$ ($\mathbf{d} = -\mathbf{a} - \mathbf{b} - \mathbf{c}$), the scalars are

$$(\mathbf{b}\cdot\mathbf{c},\ \mathbf{a}\cdot\mathbf{c},\ \mathbf{a}\cdot\mathbf{b},\ \mathbf{a}\cdot\mathbf{d},\ \mathbf{b}\cdot\mathbf{d},\ \mathbf{c}\cdot\mathbf{d})$$

(where, *e.g.*, $\mathbf{b} \cdot \mathbf{c}$ represents the dot product of the **b** and **c** axes). For the purpose of organizing these six quantities in this paper, we describe them as a vector, **s**, with components, $s_1, s_2, s_3, ..., s_6$. For the purpose of Selling reduction, zero is considered to be a negative value.

3. The Tetrahedron

An alternate description of the scalars, due to Bravais (1850), is to consider the scalars as the labels of the edges of a tetrahedron spanned by the ends of **a**, **b**, **c**, and **d** (where **d** is the negative sum of **a**, **b**, and **c**). There is no preferred ordering of the four vectors, and each possible right-handed ordering generates the same lattice. Here, $\mathbf{a} \cdot \mathbf{b}$ is the label of the edge between the ends of vectors **a** and **b**, *etc.* In the quote below, opposite refers to a pair of edges of the tetrahedron across the tetrahedron from each other. This is only a formal labeling; associated with each pair of vertices, the edge between is labeled with the dot product of the two vectors ending at those vertices.

4. The Reduction

Delone *et al.* (1975) states *"Select any positive parameter of the tetrahedron and subtract it from the parameter standing on the opposite edge of the tetrahedron (the tetrahedron is at all times thought of as spatial), add it to the parameters standing on the remaining four edges, interchange the places of the obtained parameters on two of these four edges, converging to one of the ends of the original edge (it makes no difference to which), and, finally, change the sign of the positive parameter itself being considered."*

The goal of Selling reduction is to produce a set, S, of scalars where all elements of S are negative or zero. By "opposite", here, is meant pairs of scalars that do not have a common element (and are on opposite edges of the Bravais tetrahedron):

$\mathbf{b}\cdot\mathbf{c}$ and $\mathbf{a}\cdot\mathbf{d}$ (s_1 and s_4)

$\mathbf{a}\cdot\mathbf{c}$ and $\mathbf{b}\cdot\mathbf{d}$ (s_2 and s_5)

$\mathbf{a}\cdot\mathbf{b}$ and $\mathbf{c}\cdot\mathbf{d}$ (s_3 and s_6)

For example, assuming that s_1 is positive, the reduction step for s_1 produces:

$(-s_1,\ s_2+s_1,\ s_5+s_1,\ s_4-s_1,\ s_3+s_1,\ s_6+s_1\ )$ or

$(-s_1,\ s_6+s_1,\ s_3+s_1,\ s_4-s_1,\ s_5+s_1,\ s_2+s_1\ )$

This is continued until all six scalars are negative, known to be a "unique" solution (Bravais, 1850). The reason that the choice doesn't matter is that the two choices are related by one of the reflections.

In the previous paragraph, "unique" means that the list of the six scalars is unique. Their arrangement is not unique. In terms of the tetrahedron, there are 24 allowed relabelings (reflections) of the vertices. That means that for any reduced cell, there are 24 reflections (permutations of the scalars correspond to permutations of $(\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d})$ that are all "reduced".

Finally as a check on the process and on the correctness of the lattice, the negative sum of the six scalars must decrease in each reduction step.

If we define the six-dimensional space of scalars as $\mathbf{S^6}$, the full set of $\mathbf{S^6}$ reduction operations as matrices on $\mathbf{S^6}$, two alternative matrices per scalar being reduced is:

for $\mathbf{b}\cdot\mathbf{c}=\mathbf{0}$ boundary

$[\bar{1}00000/110000/100010/\bar{1}00100/101000/100001]$

or $[\bar{1}00000/100001/101000/\bar{1}00100/100010/110000]$

for $\mathbf{a}\cdot\mathbf{c}=\mathbf{0}$ boundary

$[110000/0\bar{1}0000/010100/011000/0\bar{1}0010/010001]$

or $[010001/0\bar{1}0000/011000/010100/0\bar{1}0010/110000]$

for $\mathbf{a} \cdot \mathbf{b} = \mathbf{0}$ boundary

$$[101000/001100/00\bar{1}000/011000/001010/00\bar{1}001]$$

$$\text{or } [001010/011000/00\bar{1}000/001100/101000/00\bar{1}001]$$

for $\mathbf{a} \cdot \mathbf{d} = \mathbf{0}$ boundary

$$[100\bar{1}00/001100/010100/000\bar{1}00/000110/000101]$$

$$\text{or } [100\bar{1}00/010100/001100/000\bar{1}00/000101/000110]$$

for $\mathbf{b} \cdot \mathbf{d} = \mathbf{0}$ boundary

$$[001010/0100\bar{1}0/100010/000110/0000\bar{1}0/000011]$$

$$\text{or } [100010/0100\bar{1}0/001010/000011/0000\bar{1}0/000110]$$

for $\mathbf{c} \cdot \mathbf{d} = \mathbf{0}$ boundary

$$[010001/100001/00100\bar{1}/000101/000011/00000\bar{1}]$$

$$\text{or } [100001/010001/00100\bar{1}/000011/000101/00000\bar{1}]$$

Note that the second of each pair is just a permutation of the first, so we only need the first of each pair for reduction.

We include a pseudocode implementation of the reduction. Here, "ReduceTheLargestScalar" applies the corresponding operation from the list of matrices above.

```
bool Reduce( in, out ) {
   out = in
   while ( HasPositiveScalar(out) )
      FindIndexOfLargestScalar(out)
      out = ReduceTheLargestScalar(out)
      if(CountOfReductionCycle>1000 OR
          NegativeSumOfTheSixScalars(out) < 0.0)
          return false
   }
   return true
}
```

Experience has shown that Selling reduction is faster to execute than Niggli reduction (see Figure 1). In many applications it is important to reduce all cells before processing. A large fraction of the cells to be considered have already been reduced before the application is run, but reduction is so important that the reduction methods are applied to all cells to at least verify that they have been reduced. Even for cells that were already reduced, the difference in timing between “Niggli” and “Selling” is due to the difference in complexity for checking whether reduction is complete. The simple pseudocode above can be contrasted with the more complex algorithm for Niggli reduction (see Gruber (1973) and Andrews & Bernstein (1988)). In addition, when working in Selling space, this same difference in complexity for reduction is reflected in a difference in the number of boundary polytopes for the fundamental region, which means that applications such as clustering and cell database searching will be faster when working with Selling-reduced cells. For example, when the cell database program SAUC (McGill *et al.*, 2014) is modified to use Selling reduction, a search of half a million PDB and COD cells for the nearest 500 cells to (P 100 100 100 90 90 90) runs in 137 seconds cpu time and 8 seconds real time on a 12-core AMD Threadripper for Niggli reduction, but the same search runs in 52 seconds cpu time and 4 seconds real time for Selling reduction.

5. Difficulties in Applying Selling Reduction to the Methods of Delone, 1933

Of the available cell reduction methods, Selling reduction has the fastest performance. As x-ray detectors become faster and data collection moves to higher and higher speeds, the performance of data analysis pipelines also needs to be improved. In any system, the total system performance will not improve until the last bottleneck is removed, and in serial crystallography there are many bottlenecks to be addressed.

The choice of reduction method is an important parameter to consider in this regard. As we have shown, Selling reduction as considered by Delone has much to recommend it, yet the coders of many current applications, especially for Bravais lattice identification, have favored Niggli reduction over Delone's methods because of the issues to be discussed in the paragraphs below. Clearly, Delone's methods are not completely forgotten as Oishi-Tomiyasu (2012) used both Niggli and Delone methods. The solution of these problems is best dealt with algebraically by considering a lattice to be represented by a point in a vector space. This topic will be addressed in a forthcoming paper.

First, the identification of lattice types is usually described in terms of matching a reduced set of scalars to one of the pictures of the 24 different Bravais tetrahedra (Delone, 1933) corresponding to the various lattice types (such as body-centered cubic, etc.). This is a complex step: the user must relabel the axes of his/her own lattice picture to agree with each of the types (equivalent to choosing one or more of the 24 reflections of his/her picture to match the orientation of those of the 24 types that seem possible).

Second, the user must make decisions about how close to zero each scalar is. Each zero or near zero generates additional decisions that must be made. Further, the user may need to make a choice as to whether a near-zero value (negative after reduction) is so close to zero that another reduction should be done with that value considered positive.

Third, several of the reflections might give similar matches to a picture, and there may always be multiple matches (for instances, all cubic cells will match some orthorhombic cells).

None of these issues can outweigh the performance gains of Selling reduction over Niggli reduction in clustering and cell-database use, but, as noted above, they need to be addressed for other applications such as lattice identification, so we will not have to deal with two very different views of the same lattice in pipelines of applications. Especially when visualization rather than just computation is involved in lattice identification, the conversion from Niggli reduction back to Selling reduction to gain performance can be a complex undertaking. This will have to be addressed one application at a time in the future.

Appendix A
A Seven-Space Representation of Lattices Based on Sorted Delone Reduction

We review the relationship between Niggli reduction and Delone reduction and revive a representation due to Delaunay (as Delone) of cells in a seven dimensional space within which the fundamental unit including sorting is convex and equivalent to the conventional representations.

A.1. Notation

- {...} an unordered ensemble
- [...] an ordered list
- $||\vec{x}||$ the norm of vector $\vec{x}$
- $\vec{a},\ \vec{b},\ \vec{c}$ three cell edge vectors giving a unit cell of a lattice
- $\vec{d} = -\vec{a} - \vec{b} - \vec{c}$ the negative of the main cell body diagonal, the fourth vector for Delone reduction
- $[g_1,\ g_2,\ g_3,\ g_4,\ g_5,\ g_6] =$

$$[||\vec{a}||^2,\ ||\vec{b}||^2,\ ||\vec{c}||^2,\ 2\vec{b}\cdot\vec{c},\ 2\vec{a}\cdot\vec{c},\ 2\vec{a}\cdot\vec{b}]$$

the $\mathbf{G^6}$ vector of $[\vec{a},\ \vec{b},\ \vec{c}]$

- $[P,\ Q,\ R,\ S,\ T,\ U] =$

$$[s_{23}, s_{13}, s_{12}, s_{14}, s_{24}, s_{34}] =$$

$$[\vec{b}\cdot\vec{c},\ \vec{a}\cdot\vec{c},\ \vec{a}\cdot\vec{b},\ \vec{a}\cdot\vec{d},\ \vec{b}\cdot\vec{d},\ \vec{c}\cdot\vec{d}]$$

the Selling (Delaunay, Delone) scalars of $[\vec{a},\ \vec{b},\ \vec{c},\ \vec{d}]$

- $[d_1,\ d_2,\ d_3,\ d_4,\ d_5,\ d_6,\ d_7] =$

$$[||\vec{a}||^2,\ ||\vec{b}||^2,\ ||\vec{c}||^2,\ ||\vec{d}||^2,\ ||\vec{b}+\vec{c}||^2,\ ||\vec{a}+\vec{c}||^2,\ ||\vec{a}+\vec{b}||^2] =$$

$$[||\vec{a}||^2,\ ||\vec{b}||^2,\ ||\vec{c}||^2,\ ||\vec{d}||^2,\ ||\vec{d}+\vec{a}||^2,\ ||\vec{d}+\vec{b}||^2,\ ||\vec{d}+\vec{c}||^2]$$

the $\mathbf{D^7}$ vector of $[\vec{a},\ \vec{b},\ \vec{c},\ \vec{d}]$

A.2. Delone Reduction

Given three cell edge vectors $\vec{a},\ \vec{b},\ \vec{c}$, that cell is called Delone-reduced if the four vectors (the Bravais tetrahedron (Delone, 1933)) $\vec{a},\ \vec{b},\ \vec{c},\ \vec{d} = -\vec{a}-\vec{b}-\vec{c}$, numbered 1 through 4, all form right angles or obtuse angles relative to one another. In terms of $\mathbf{G^6}$, (Andrews & Bernstein, 1988) given a cell described by $[g_1, g_2, g_3, g_4, g_5, g_6]$, converting from the Selling (Selling, 1874) scalar $\mathbf{S^6}$ $[P, Q, R, S, T, U]$ notation for the inner products of (Henry & Lonsdale, 1952), based on (Ito, 1950) and (Delone, 1933), the six doubled inner products among the Bravais tetrahedron vectors are:

$$2P = 2\vec{b}.\vec{c} = 2s_{23} = g_4 \tag{A.1}$$

$$2Q = 2\vec{a}.\vec{c} = 2s_{13} = g_5 \tag{A.2}$$

$$2R = 2\vec{a}.\vec{b} = 2s_{12} = g_6 \tag{A.3}$$

$$2S = 2\vec{a}.(-\vec{a}-\vec{b}-\vec{c}) = -2\vec{a}.\vec{a} - 2\vec{a}.\vec{b} - 2\vec{a}.\vec{c} = 2s_{14} = -2g_1 - g_6 - g_5 \tag{A.4}$$

$$2T = 2\vec{b}.(-\vec{a} - \vec{b} - \vec{c}) = -2\vec{b}.\vec{a} - 2\vec{b}.\vec{b} - 2\vec{b}.\vec{c} = 2s_{24} = -g_6 - 2g_2 - g_4 \quad \text{(A.5)}$$

$$2U = 2\vec{c}.(-\vec{a} - \vec{b} - \vec{c}) = -2\vec{c}.\vec{a} - 2\vec{c}.\vec{b} - 2\vec{c}.\vec{c} = 2s_{34} = -g_5 - g_4 - 2g_3 \quad \text{(A.6)}$$

equivalently

$$g_1 = -Q - R - S$$

$$g_2 = -P - R - T$$

$$g_3 = -P - Q - U$$

$$g_4 = 2P$$

$$g_5 = 2Q$$

$$g_6 = 2R$$

For a Delone-reduced cell all of expressions A.1 through A.6 must be zero or negative. This is equivalent to saying that all the cell angles must be obtuse or right angles. No acute angles are permitted.

Patterson & Love (1957) used a slightly different notation and presented a very efficient algorithm for Delone-reduction.

To a minimal extent, in the past one level of ambiguity in presentation was removed by imposing various symmetry dependent orderings. We go further in this appendix by imposing a strict ordering on the lengths of the tetrahedron vectors $||\vec{a}|| \leq ||\vec{b}|| \leq ||\vec{c}|| \leq ||\vec{d}||$ This ordering, while not essential to doing the reduction, clarifies the presentation of each cell.

A.3. Converting from the $\mathbf{G^6}$ or $\mathbf{E^3}$ representation of a Niggli-reduced cell to Delone-reduced

It is possible to achieve Delone reduction by first doing Niggli reduction. See B.1 in the supplementary material for a summary of the Niggli conditions.

(Allmann, 1968) presented the transformation from a Burger-reduced cell to a Delone-reduced cell. We restate that algorithm in full detail and specialize it to deal with the Niggli-reduction conditions.

Most of the Niggli conditions are not relevant to conversion from Niggli reduction to Delone reduction. The relevant Niggli conditions can be stated as:

$$g_1 \leq g_2 \leq g_3$$

$$|g_4| \leq g_2 \leq g_3$$

$$|g_5| \leq g_1 \leq g_2 \leq g_3$$

$$|g_6| \leq g_1 \leq g_2 \leq g_3$$

and $g_{\{4,5,6\}}$ are all strictly positive or all less than or equal to zero.

A.3.1. The Niggli-reduced $---$ case If we have $g_{\{4,5,6\}}$ all less than or equal to zero, examine each element of expressions A.1 through A.6:

$$g_6 \leq 0$$

$$g_5 \leq 0$$

$$-2g_1 - g_5 - g_6 = (-g_5 - g_1) + (-g_6 - g_1) \leq 0$$

$$g_4, \leq 0$$

$$-g_6 - 2g_2 - g_4 = (-g_4 - g_2) + (-g_6 - g_2) \leq 0$$

$$-g_5 - g_4 - 2g_3 = (-g_4 - g_3) + (-g_5 - g_3) \leq 0$$

so the Niggli reduction case of $g_{\{4,5,6\}}$ all less than or equal to zero is already Delone reduced. Recall, that for these $---$ Niggli-reduced cells,

$$0 \leq g_1 \leq g_2 \leq g_3 \leq g_1 + g_2 + g_3 + g_4 + g_5 + g_6$$

$$-g_2 \leq g_4 \leq 0$$

$$-g_1 \leq g_5 \leq 0$$

$$-g_1 \leq g_6 \leq 0$$

A.3.2. The Niggli-reduced $+++$ cases Now consider the remaining case of $g_{\{4,5,6\}}$ all greater than zero. For these $+++$ Niggli-reduced cells,

$$0 \leq g_1 \leq g_2 \leq g_3 \leq g_1 + g_2 + g_3 + g_4 + g_5 + g_6$$

$$0 \leq g_4 \leq g_2$$

$$0 \leq g_5 \leq g_1$$

$$0 \leq g_6 \leq g_1$$

At least one of $g_{\{4,5,6\}}$ is minimal. It is possible for more than one to be minimal.

A.3.3. The Niggli-reduced $+++$, g_6 minimal case Suppose $g_6 \leq g_4$, $g_6 \leq g_5$. In this case consider the Bravais tetrahedron

$$\vec{a},\ -\vec{b},\ -\vec{c}+\vec{b},\ \vec{c}-\vec{a} \tag{A.7}$$

The first two components are of lengths $||\,\vec{a}\,||$ and $||\,\vec{b}\,||$ from the Niggli cell. Both lengths $||-\vec{c}+\vec{b}\,||$ and $||\,\vec{c}-\vec{a}\,||$ are greater than or equal to $||\,\vec{c}\,||$. If either were smaller, $\vec{a}, \vec{b}, \vec{c}$ would not be Niggli-reduced. There are two $\mathbf{G^6}$ vectors to consider, using the shorter of the last two vectors in place of $\vec{c}$. The remaining vector becomes the fourth tetrahedron edge.

$$[g_1,\ g_2,\ g_2 + g_3 - g_4,\ g_4 - 2g_2,\ -g_5 + g_6,\ -g_6]$$

$$[g_1,\ g_2,\ g_1 + g_3 - g_5,\ g_6 - g_4,\ g_5 - 2g_1,\ -g_6]$$

which are $---$ vectors in this case, and the elements of expressions A.1 through A.6 are

$$-g_6,\ \ g_6-g_5,\ \ g_5-2g_1,\ \ g_4-2g_2,\ \ g_6-g_4,\ \ g_5-2g_3+g_4-g_6$$

$$-g_6,\ \ g_5-2g_1,\ \ g_6-g_5,\ \ g_6-g_4,\ \ g_4-2g_2,\ \ g_5-2g_3+g_4-g_6$$

respectively, all of which are less than or equal to zero.

A.3.4. The Niggli-reduced $+++$, g_5 minimal case Suppose $g_5 \leq g_4$, $g_5 \leq g_6$. In this case consider the Bravais tetrahedron

$$\vec{a},\ \ \vec{b}-\vec{a},\ \ -\vec{c},\ \ \vec{c}-\vec{b} \tag{A.8}$$

The first and third components are of lengths $||\,\vec{a}\,||$ and $||\,\vec{c}\,||$, respectively, from the Niggli cell. $||\,\vec{b}-\vec{a}\,||^2 = g_1 - g_6 + g_2 \geqslant g_2$ and $||\,\vec{b}-\vec{c}||^2 = g_2 - g_4 + g_3 \geqslant g_3$. It is possible that $||\,\vec{b}-\vec{a}\,||^2 \geqslant g_3$ in which case $\vec{c}$ will replace $\vec{b}$ and the smaller of $\vec{b}-\vec{a}$ and $\vec{c}-\vec{b}$ will replace $\vec{c}$. Otherwise the smaller of $\vec{b}-\vec{a}$ and $\vec{c}-\vec{b}$ will replace $\vec{c}$. In any of these cases, there are two $\mathbf{G^6}$ vectors to consider, using either the second or fourth component in addition to $\vec{a}$ and $\vec{c}$

$$[g_1,\ \ -g_6+g_2+g_1,\ \ g_3,\ \ g_5-g_4,\ \ -g_5,\ \ g_6-2g_1]$$

$$[g_1,\ \ -g_4+g_3+g_2,\ \ g_3,\ \ g_4-2g_3,\ \ -g_5,\ \ g_5-g_6]$$

which are $---$ vectors in this case, and the elements of expressions A.1 through A.6 are

$$g_6-2g_1,\ \ -g_5,\ \ g_5-g_6,\ \ g_5-g_4,\ \ g_4-2g_2-g_5+g_6,\ \ g_4-2g_3$$

$$g_5-g_6,\ \ -g_5,\ \ g_6-2g_1,\ \ g_4-2g_3,\ \ g_4-g_5+g_6-2g_2,\ \ g_5-g_4$$

respectively, all of which are less than or equal to zero.

A.3.5. The Niggli-reduced $+++$, g_4 minimal case Suppose $g_4 \leq g_5$, $g_4 \leq g_6$. In this case consider the Bravais tetrahedron

$$\vec{b} - \vec{a},\ \ -\vec{b},\ \ \vec{c},\ \ \vec{a} - \vec{c} \tag{A.9}$$

The second and third components are of lengths $||\vec{b}||$ and $||\vec{c}||$, respectively, from the Niggli cell. The length of $\vec{b} - \vec{a}$ is greater than or equal to the length of $\vec{b}$. The length of $\vec{a} - \vec{c}$ is greater than of equal to the length of $\vec{c}$. Therefore the three shortest edges of the Bravais tetrahedron will be some combination of $-\vec{b}$, $||\vec{c}||$ and the shorter of $\vec{b} - \vec{a}$ and $\vec{a} - \vec{c}$, so there are two $\mathbf{G^6}$ vectors to consider

$$[-g_6 + g_2 + g_1,\ \ g_2,\ \ g_3,\ \ -g_4,\ \ g_4 - g_5,\ \ g_6 - 2g_2]$$

$$[-g_5 + g_3 + g_1,\ \ g_2,\ \ g_3,\ \ -g_4,\ \ g_5 - 2g_3,\ \ g_4 - g_6]$$

which are $---$ vectors in this case, and the elements of expressions A.1 through A.6 are

$$g_6 - 2g_2,\ \ g_4 - g_5,\ \ -g_4 + g_5 + g_6 - 2g_1,\ \ -g_4,\ \ g_4 - g_6,\ \ g_5 - 2g_3$$

$$g_4 - g_6,\ \ g_5 - 2g_3,\ \ -g_4 + g_5 + g_6 - 2g_1,\ \ -g_4,\ \ g_6 - 2g_2,\ \ g_4 - g_5$$

respectively, all of which are less than or equal to zero.

Note that in all cases for a Bravais tetrahedron, the three shortest edge vectors are either from a $---$ Niggli cell, or, in the case of a Bravais tetrahedron derived from a $+++$ Niggli cell, two of the three shortest edges are from that Niggli cell with the direction of one edge reversed and the third of the shortest edges is a face diagonal from a face involving the third Niggli cell edge.

A.4. The effects of perturbations

Perturbations of a cell can cause exchanges of edges with face diagonals or body diagonals. Because a Delone cell only has obtuse (or right) angles the diagonals produced by sums are closer in length to the original edges than those involving differences. Therefore, in many cases, Delone reduction of a cell close to

$$\vec{a},\ \vec{b},\ \vec{c},\ -\vec{a}-\vec{b}-\vec{c}$$

will use the additive face and body diagonals

$$\vec{a}+\vec{b},\ \vec{a}+\vec{c},\ \vec{a}-\vec{a}-\vec{b}-\vec{c},\ \vec{b}+\vec{c},$$

$$\vec{b}-\vec{a}-\vec{b}-\vec{c},\ \vec{c}-\vec{a}-\vec{b}-\vec{c},\ \vec{a}+\vec{b}+\vec{c},\ \vec{a}+\vec{b}-\vec{a}-\vec{b}-\vec{c},$$

$$\vec{a}+\vec{c}-\vec{a}-\vec{b}-\vec{c},\ \vec{b}+\vec{c}-\vec{a}-\vec{b}-\vec{c}$$

$$=\vec{a}+\vec{b},\ \vec{a}+\vec{c},\ -\vec{b}-\vec{c},\ \vec{b}+\vec{c},$$

$$-\vec{a}-\vec{c},\ -\vec{a}-\vec{b},\ \vec{a}+\vec{b}+\vec{c},\ -\vec{c},\ -\vec{b},\ -\vec{a}$$

A.5. The 7-Dimensional Delone Space $\mathbf{D^7}$

Consider the Bravais tetrahedron $\vec{a}$, $\vec{b}$, $\vec{c}$, $\vec{d}=-\vec{a}-\vec{b}-\vec{c}$

If we consider only lengths, then the total ensemble of seven unique lengths resulting from the Bravais tetrahedron and the additive face and body diagonals is

$$\{||\vec{a}||,\ ||\vec{b}||,\ ||\vec{c}||,\ ||\vec{d}||,\ ||\vec{b}+\vec{c}||,\ ||\vec{a}+\vec{c}||,\ ||\vec{a}+\vec{b}||\}$$

Taking squares of these lengths gives a seven-vector defined by (Delone *et al.*, 1975) in a space we call $\mathbf{D^7}$ for Delone 7-space.

In Appendix B (supplementary Material), the necessary and sufficient conditions for a well-defined cell to be Delone reduced are given and the fundamental region of points in seven-space satisfying those conditions are shown to be convex with seven 5-dimensional boundaries.

Appendix B
A Seven-Space Representation of Lattices Based on Sorted Delone Reduction – Supplementary Material

For notation and background, see the main paper sections A.1 and 1.

We review the relationship between Niggli reduction and Delone reduction and present a representation of Delone-reduced cells in a seven-dimensional space of squared lengths, $\mathbf{D^7}$, as an alternative to the six-dimensional $\mathbf{S^6}$ space Selling inner products, within which the fundamental unit including sorting is convex and equivalent to the conventional representations.

See A.2 for Delone (Delaunay) reduction. Compare this to the more complex Niggli conditions B.1. Next we turn to the structure of $\mathbf{D^7}$.

B.1. The Niggli Conditions

The Niggli-reduced cell of a lattice is a unique choice from among the infinite number of alternate cells that generate the same lattice (Niggli, 1928). A Buerger-reduced cell, which is equivalent to a Minkowski-reduced cell (Minkowski, 1905)) for a given lattice is any cell that generates that lattice, chosen such that no other cell has shorter cell edges (Buerger, 1960). Even after allowing for the equivalence of cells in which the directions of axes are reversed or axes of the same length are exchanged, there can be up to five alternate Buerger-reduced cells for the same lattice (Gruber, 1973). The Niggli conditions allow the selection of a unique reduced cell for a given lattice from among the alternate Buerger-reduced cells for that lattice.

Niggli reduction consists of converting the original cell to a primitive one and then alternately applying two operations: conversion to standard presentation and reduction (Andrews & Bernstein, 1988). The convention for meeting the combined Buerger and Niggli conditions is based on increasingly restrictive layers of constraints:

If $g_1 < g_2 < g_3$, $|g_4| < g_2$, $|g_5| < g_1$, $|g_6| < g_1$ and either $g_{\{4,5,6\}} > 0$ or $g_{\{4,5,6\}} \leq 0$ then we have a Niggli-reduced cell, and we are done.

The remaining conditions are imposed when any of the above inequalities becomes an equality or the elements of $g_{\{4,5,6\}}$ are not consistently all strictly positive or are not consistently all less than or equal to zero.

The full set of combined Niggli conditions, in addition to those for the cell edge lengths being minimal, is:

require $0 \leq g_1 \leq g_2 \leq g_3$

if $g_1 = g_2,$ then require $|g_4| \leq |g_5|$

if $g_2 = g_3,$ then require $|g_5| \leq |g_6|$

require $\{g_4 > 0$ and $g5 > 0$ and $g6 > 0\}$

or require $\{g_4 \leq 0$ and $g_5 \leq 0$ and $g6 \leq 0\}$

require $|g_4| \leq g_2$

require $|g_5| \leq g_1$

require $|g_6| \leq g_1$

require $g_3 \leq g_1 + g_2 + g_3 + g_4 + g_5 + g_6$

if $g_4 = g_2,$ then require $g_6 \leq 2g_5$

if $g_5 = g_1,$ then require $g_6 \leq 2g_4$

if $g_6 = g_1,$ then require $g_5 \leq 2g_4$

if $g_4 = -g_2,$ then require $g_6 = 0$

if $g_5 = -g_1,$ then require $g_6 = 0$

if $g_6 = -g_1$, then require $g_5 = 0$

if $g_3 = g_1 + g_2 + g_3 + g_4 + g_5 + g_6$, then require $2g_1 + 2g_5 + g_6 \leq 0$

The $\mathbf{G^6}$ transformations associated with each of these steps are enumerated in (Andrews & Bernstein, 1988). Application of these transformations must be repeated until all conditions are satisfied.

B.2. The 7-Dimensional Delone Space $\mathbf{D^7}$

Consider the Bravais tetrahedron $\vec{a}$, $\vec{b}$, $\vec{c}$, $\vec{d} = -\vec{a} - \vec{b} - \vec{c}$

If we consider only lengths, then the total ensemble of seven unique lengths resulting from the Bravais tetrahedron and the additive face and body diagonals is

$$\{||\,\vec{a}\,||,\ \ ||\,\vec{b}\,||,\ \ ||\,\vec{c}\,||,\ \ ||\,\vec{d}\,||,\ \ ||\,\vec{b}+\vec{c}\,||,\ \ ||\,\vec{a}+\vec{c}\,||,\ \ ||\,\vec{a}+\vec{b}\,||\,\}$$

Taking squares of these lengths gives a seven-vector defined by (Delone *et al.*, 1975) in a space we call $\mathbf{D^7}$ for Delone 7-space:

$$[d_1 = ||\,\vec{a}\,||^2,\ \ d_2 = ||\,\vec{b}\,||^2,\ \ d_3 = ||\,\vec{c}\,||^2,\ \ d_4 = ||\,\vec{d}\,||^2,$$

$$d_5 = ||\,\vec{b}+\vec{c}\,||^2,\ \ d_6 = ||\,\vec{a}+\vec{c}\,||^2,\ \ d_7 = ||\,\vec{a}+\vec{b}\,||^2]$$

$$= [d_1 = ||\,\vec{a}\,||^2,\ \ d_2 = ||\,\vec{b}\,||^2,\ \ d_3 = ||\,\vec{c}\,||^2,\ \ d_4 = ||\,\vec{d}\,||^2,$$

$$d_5 = ||\,\vec{a}+\vec{d}\,||^2,\ \ d_6 = ||\,\vec{b}+\vec{d}\,||^2,\ \ d_7 = ||\,\vec{c}+\vec{d}\,||^2]$$

$$= [g_1,\ \ g_2,\ \ g_3,\ \ g_1 + g_2 + g_3 + g_4 + g_5 + g_6,$$

$$g_2 + g_3 + g_4,\ \ g_1 + g_3 + g_5,\ \ g_1 + g_2 + g_6]$$

$$= [-Q - R - S,\ \ -P - R - T,\ \ -P - Q - U,\ \ -S - T - U, -Q - R - T - U,$$

$$-P - R - S - U,\ \ -P - Q - S - T]$$

and

$$P = -d_2/2 - d_3/2 + d_5/2$$

$Q = d_2/2 + d_4/2 - d_5/2 - d_7/2$

$R = -d_1/2 - d_2/2 + d_7/2$

$S = -d_1/2 - d_4/2 + d_5/2$

$T = d_1/2 + d_3/2 - d_5/2 - d_7/2$

$U = -d_3/2 - d_4/2 + d_7/2$

In $\mathbf{D^7}$ the Delone reduced cells are defined by:

$$d_1,\ d_2,\ d_3,\ d_4,\ d_5,\ d_6,\ d_7 > 0 \tag{B.1}$$

$$d_1 + d_2 + d_3 + d_4 - d_5 - d_6 - d_7 = 0 \tag{B.2}$$

$$d_1 \le d_2 \le d_3 \le d_4 \tag{B.3}$$

$$d_5 \le d_2 + d_3 \tag{B.4}$$

$$d_5 \le d_1 + d_4 \tag{B.5}$$

$$d_6 \le d_1 + d_3 \tag{B.6}$$

$$d_6 \le d_2 + d_4 \tag{B.7}$$

$$d_7 \le d_1 + d_2 \tag{B.8}$$

$$d_7 \le d_3 + d_4 \tag{B.9}$$

$$d_5 \ge d_2 - d_3 \tag{B.10}$$

$$d_5 \ge d_1 - d_4 \tag{B.11}$$

$$d_6 \ge d_1 - d_3 \tag{B.12}$$

$$d_6 \geq d_2 - d_4 \tag{B.13}$$

$$d_7 \geq d_1 - d_2 \tag{B.14}$$

$$d_7 \geq d_3 - d_4 \tag{B.15}$$

Boundaries may be defined by equalities in the above relationships.

As we will show, the conditions B.1 through B.15 are necessary and sufficient for a well-defined cell to be Delone reduced, and for the fundamental region of points in seven-space satisfying those conditions to be convex, with seven 5-dimensional boundaries.

B.3. Comments on projectors and boundaries

All the currently accepted reduction processes depend on obeying constraining linear inequalities. Such inequalities determine boundaries of the space of reduced cells. Because they are linear, the results are linear polytopes defining boundaries of the fundamental region of reduced cells. The highest dimension polytopes completely determine the shape of the fundamental region. For example. the highest order boundaries in G6 (which is a 6-dimensional space) are 5-dimensional polytopes. The lower dimensional boundary polytopes are all the result of the intersections of the higher dimensional polytopes.

Given a unit cell, the distance from that cell to another cell depends on whether we draw a line directly between the two cells or look at lines that are interrupted by boundaries. Metrics in spaces of reduced cells depend on an understanding of where each cell stands in relation to each boundary. For that we need projection matrices that project from a cell to the nearest cell in a boundary. The boundaries can be determined entirely algebraically; however it is more efficient to start with computational experiments that probe all boundaries and reveal which ones are more populated and likely to be higher dimensional and therefore more fundamental to this necessary understanding.

The boundaries presented here were discovered first by Monte Carlo experiments and then by confirming algebraic analysis using the reduction inequalities that fundamentally determine the boundaries.

The process of finding projectors began by randomly generating a large number of vectors satisfying the boundary conditions. For one of the boundaries, a group of vectors that is sufficient to span the boundary polytope is generated. Treating the vectors as an m by n matrix (n vectors of m dimension), singular value decomposition gives one the eigenvectors that span the boundary polytope and those eigenvectors serve as the projector. A simpler confirming method is to take powers of the product of the m by n matrix and its transpose.

For distance calculations, the "perp", the unit matrix minus the projector, is also needed. This is represented in the equations by the $^{\perp}$ symbol.

B.4. Necessity of conditions B.1 through B.15

The necessity of B.1 follows from the definition of each of d_1 through d_7 as a length, which, as norms, must be non-negative. The zero cases can only arise from a tetrahedron with a zero edge in the first four cases, or a 180 degree angle in the last three cases.

We show the necessity of B.2 from the representations in terms of $\mathbf{G^6}$ components.

$$d_1 + d_2 + d_3 + d_4 - d_5 - d_6 - d_7$$

$$= g_1 + g_2 + g_3 + g_1 + g_2 + g_3 + g_4 + g_5 + g_6$$

$$-g_2 - g_3 - g_4 - g_1 - g_3 - g_5 - g_1 - g_2 - g_6$$

$$= (1 + 1 - 1 - 1) * g_1 + (1 + 1 - 1 - 1) * g_2 + (1 + 1 - 1 - 1) * g_3$$

$$+(1-1)*g4+(1-1)*g5+(1-1)*g6=0$$

Conditions B.4 through B.9 are just a restatement of the Delone reduction condition of obtuse or right angles among the four cell edges, and thus are necessary.

Finally, the remaining conditions follow from the Cauchy-Schwarz inequality and from the tetrahedron cell edge length ordering we have chosen. For example

$$|\vec{b}.\vec{c}| \le ||\vec{b}||||\vec{c}|| \le ||\vec{c}||^2$$

$$\implies -g_4 \le 2g_3 \implies -g_3 \le g_3+g_4 \implies g_2-g_3 \le g_2+g_3+g_4$$

which is equivalent to B.10

The necessity of all B.10 through B.15 follows similarly.

B.5. Sufficiency of conditions B.1 through B.15

In order to show that conditions B.1 through B.15 are sufficient to define Delone reduction, we need to map from $\mathbf{D^7}$ to $\mathbf{G^6}$ and verify that the left-hand sides in A.1 through A.6 are all less than or equal to zero when B.1 through B.15 are satisfied.

Given a cell $v=(v_1,v_2,v_3,v_4,v_5,v_6,v_7) \in \mathbf{D^7}$, we define the mapping from $\mathbf{D^7}$ to $\mathbf{G^6}$ by:

$$\mathbf{D^7\_to\_G^6}(v_1,v_2,v_3,v_4,v_5,v_6,v_7)$$

$$=(v_1,v_2,v_3,v_5-v_2-v_3,v_6-v_1-v_3,v_7-v_1-v_2)$$

The requirement that A.1 through A.3 be less than or equal to zero is satisfied by applying B.4, B.6, and B.8. The requirement that A.4 through A.6 be less than or equal to zero can be seen to be satisfied by combining condition B.2 with one of conditions B.5, B.7 or B.9. For example, A.4 is equivalent to

$$0 \ge -2v_1-(v_7-v_1-v_2)-(v_6-v_1-v_3)$$

$$=-v_7+v_2-v_6+v_3$$

applying B.2 by subtracting it

$$= -v_7 + v_2 - v_6 + v_3 - (v_1 + v_2 + v_3 + v_4 - v_5 - v_6 - v_7)$$

$$= -v_1 - v_4 + v_5$$

which is equivalent to condition B.5. The other conditions are similarly satisfied. Note that we have not used all of B.1 through B.15. The system has strong redundancies. This is inherent because we are using a seven-dimensional representation of a six-dimensional space. We do this because it changes complex mappings involving the body diagonals into simple permutations.

B.6. The Seven 5-D Boundaries Polytopes of $\mathbf{D^7}$

The full 7-dimensional space is projected to a 6-dimensional space by the linear constraint B.2. We start the exploration of this space by identifying the 5-dimensional boundary polytopes that result from considering one equality in the above relationships at a time.

B.7. Cases 1, 2 and 3: Equal Bravais tetrahedron Edge Lengths

These cases arise when two Bravais tetrahedron edges have equal lengths, the equality cases in expression B.3. Consider for example $d_1 = d_2$. The boundary transformation would be based on exchanging $\vec{a}$ and $\vec{b}$, but that simple exchange would reverse the handedness of the cell, so we also negate all resulting edges to restore the handedness.

B.7.1. Case 1 $d_1 = d_2$, $Q + S = P + T$, $||\,\vec{a}\,||^2 = ||\,\vec{b}\,||^2$, $\vec{a} \to -\vec{b}$, $\vec{b} \to -\vec{a}$, $\vec{c} \to -\vec{c}$, $\vec{d} \to \vec{a} + \vec{b} + \vec{b} = -\vec{d}$

$$MD_1 =$$

$$(\mathbf{01}00000/\mathbf{10}00000/0010000/0001000/0000\mathbf{01}0/0000\mathbf{10}0/0000001)$$

$PD_1 =$

$$\left(\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\right)$$

$PD_1^{\perp} =$

$$\left(\frac{9}{14}\frac{\bar{5}}{14}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{5}}{14}\frac{9}{14}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\right)$$

$\mathbf{D^7}$ subspace: $(r, r, s, t, u, v, 2r + s + t - u - v)$

B.7.2. *Case 2* $d_2 = d_3$, $R + T = Q + U$, $||\vec{b}||^2 = ||\vec{c}||^2$, $\vec{a} \to -\vec{a}$, $\vec{b} \to -\vec{c}$, $\vec{c} \to -\vec{b}$, $\vec{d} \to \vec{a} + \vec{b} + \vec{b} = -\vec{d}$

$MD_2 = (1000000/0\mathbf{01}0000/0\mathbf{10}0000/0001000/0000100/00000\mathbf{01}/00000\mathbf{10})$

$PD_2 =$

$$\left(\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\right)$$

$PD_2^{\perp} =$

$$\left(\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{9}{14}\frac{\bar{5}}{14}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{\bar{5}}{14}\frac{9}{14}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\right)$$

$\mathbf{D^7}$ subspace: $(r, s, s, t, u, v, r + 2s + t - u - v)$

B.7.3. *Case 3* $d_3 = d_4$, $P + Q = S + T$, $||\vec{c}||^2 = ||\vec{d}||^2 = ||\vec{a} + \vec{b} + \vec{c}||^2$, $\vec{a} \to -\vec{a}$, $\vec{b} \to -\vec{b}$, $\vec{c} \to \vec{a} + \vec{b} + \vec{c}$, $\vec{d} \to -\vec{c}$

$MD_3 = (1000000/0100000/00\mathbf{01}000/00\mathbf{10}000/0000\mathbf{01}0/0000\mathbf{10}0/0000001)$

$PD_3 =$

$$\left(\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{5}{14}\frac{5}{14}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{5}{14}\frac{5}{14}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\right)$$

$PD_3^{\perp} =$

$$\left(\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{9}{14}\frac{\bar{5}}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{\bar{5}}{14}\frac{9}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\right)$$

$\mathbf{D^7}$ subspace: $(r, s, t, t, u, v, r + s + 2t - u - v)$

B.7.4. Other equality cases Consider the other possible edge length equality cases. The other potential boundary polytopes to consider are:

$$d_1 = d_3 \tag{B.16}$$

$$d_1 = d_4 \tag{B.17}$$

$$d_1 = d_5 \tag{B.18}$$

$$d_1 = d_6 \tag{B.19}$$

$$d_1 = d_7 \tag{B.20}$$

$$d_2 = d_4 \tag{B.21}$$

$$d_2 = d_5 \tag{B.22}$$

$$d_2 = d_6 \tag{B.23}$$

$$d_2 = d_7 \tag{B.24}$$

$$d_3 = d_5 \tag{B.25}$$

$$d_3 = d_6 \tag{B.26}$$

$$d_3 = d_7 \tag{B.27}$$

$$d_4 = d_5 \tag{B.28}$$

$$d_4 = d_6 \tag{B.29}$$

$$d_4 = d_7 \tag{B.30}$$

$$d_5 = d_6 \tag{B.31}$$

$$d_5 = d_7 \tag{B.32}$$

$$d_6 = d_7 \tag{B.33}$$

The boundary polytopes B.16, B.17, and B.21 are of dimensions 4, 3 and 4, respectively, because they imply additional equalities from the ordering in B.3. Many of the others arise in mapping Niggli characters into Delone conditions.

B.8. Cases 4, 5, 6, 7, 8, 9: Right angle cases

There are six cases, cases 4, 5, 6, 7, 8, 9 given by expressions B.4 through B.9 with inequality replaced by equality, in which edges of the Bravais tetrahedron meet at right angles. Cases 4, 5, 6, and 8 are 5-dimensional and cases 7 and 9 are of lower dimension. Consider for example

$$d_5 = d_2 + d_3$$

$$g_2 + g_3 + g_4 = g_2 + g_3$$

$$g_4 = 2\vec{b}.\vec{c} = 0$$

The full set of resulting equations in the same ordering as expressions B.4 through B.9 are

$$2\vec{b}.\vec{c} = g_4 = 0; P = 0 \tag{B.34}$$

$$2\vec{a}.\vec{d} = 2\vec{a}.(-\vec{a} - \vec{b} - \vec{c}) = -2g_1 - g_6 - g_5 = 0; S = 0 \tag{B.35}$$

$$2\vec{a}.\vec{c} = g_5 = 0; Q = 0 \tag{B.36}$$

$$2\vec{b}.\vec{d} = 2\vec{b}.(-\vec{a} - \vec{b} - \vec{c}) = -g_6 - 2g_2 - g_4 = 0; T = 0; \tag{B.37}$$

$$2\vec{a}.\vec{b} = g_6 = 0; R = 0 \tag{B.38}$$

$$2\vec{c}.\vec{d} = 2\vec{c}.(-\vec{a} - \vec{b} - \vec{c}) = -g_5 - g_4 - 2g_3 = 0; U = 0; \tag{B.39}$$

The right angle cases are Delone reduced. However a slight perturbation will introduce an acute angle, necessitating a transformation to return to $\mathbf{D^7}$. In order to understand the necessary transformation, consider a Delone-reduced cell with tetrahedron

$$\vec{a}_{orig}, \vec{b}_{orig}, \vec{c}_{orig}, -\vec{a}_{orig} - \vec{b}_{orig} - \vec{c}_{orig}$$

for which $2\vec{b}_{orig}.\vec{c}_{orig} = 0$. Impose a slight perturbation on $\vec{b}_{orig}$ to form $\vec{b}_{ptrb}$ such that $\vec{b}_{ptrb}.\vec{c}_{orig} = \epsilon > 0$, and such that all other inner products remain non-positive. We convert from the $+--$ presentation to $+++$ by changing +the sign of $\vec{a}$. If we define $\vec{a}_{ptrb} = -\vec{a}_{orig}$ with a small additional perturbation to guarantee that

$$2\vec{a}_{ptrb}.\vec{c}_{orig} > 0$$

$$2\vec{a}_{ptrb}.\vec{b}_{ptrb} > 0$$

then we are starting from a $+++$ case with a small g_4 and can apply the transformation in expression A.9 to return to the $---$ case using the tetrahedron

$$\vec{b}_{ptrb} - \vec{a}_{ptrb}, -\vec{b}_{ptrb}, \vec{c}_{orig}, \vec{a}_{ptrb} - \vec{c}_{orig}$$

which says, up to reordering, if the $+++$ case we generated is Niggli-reduced, the boundary transform takes the tetrahedron to

$$\vec{b} + \vec{a}, -\vec{b}, \vec{c}, -\vec{a} - \vec{c}$$

There is only one mapping back into $\mathbf{D^7}$ for each right angle case, but in each of these cases several permuted versions of the boundary transform may be needed to ensure that the results are ordered $d_1 \leq d_2 \leq d_3 \leq d_4$. While there are, in general, 24 permutations of 4 objects, the ordering constraint reduces the number of acceptable permutations to eight, six, or zero cases that represent 5-dimensional boundaries. The remaining permutations imply additional constraints that lower the dimensionality of the resulting boundary polytope.

The general pattern is that the new Bravais tetrahedron resulting from a right-angle boundary mapping will change the sign of one of the two edges involved in the right angle and leave the other edge that is involved unchanged.

B.8.1. Case 4: $d_5 = d_2 + d_3$ (see equation B.4). This is equivalent to $g_4 = 0$. The Bravais tetrahedron edges to be ordered are

$$\vec{a} + \vec{b}, -\vec{b}, \vec{c}, -\vec{a} - \vec{c}$$

In this case, the only acceptable permutations are ones that preserve the relative ordering of $||\,\vec{a}\,||^2 \leq ||\,\vec{b}\,||^2 \leq ||\,\vec{c}\,||^2 \leq ||\,\vec{d}\,||^2$ with obtuse angles. If $||\,\vec{b}\,||^2$ is presented first, all six permutations of the remaining three edges are feasible. It is not possible to present $||\,\vec{c}\,||^2$ first, because that would leave no room to present $||\,\vec{b}\,||^2$, except in the lower-dimensional polytope resulting from the intersection of Case 4 with Case 2.

If $||\,\vec{a} + \vec{b}\,||^2$ is presented first, then we must have $||\,\vec{a} + \vec{b}\,||^2 \leq ||-\vec{b}\,||^2$ which is equivalent to

$$||\,\vec{a}\,||^2 + 2\vec{a}.\vec{b} \leq 0 \tag{B.40}$$

From the ordering constraint $||\,\vec{c}\,||^2 \leq ||\,\vec{d}\,||^2$ and equation B.40 it follows that

$$0 \leq ||\,\vec{a}\,||^2 + ||\,\vec{b}\,||^2 + 2\vec{b}.\vec{c} + 2\vec{a}.\vec{c} + 2\vec{a}.\vec{b} \leq ||\,\vec{b}\,||^2 + 2\vec{b}.\vec{c} + 2\vec{a}.\vec{c} = || - \vec{a} - \vec{c}|| - ||\,\vec{c}\,||^2 + 2\vec{b}.\vec{c}$$

but from the obtuseness of the angles in a Bravais tetrahedron, we have

$$|| - \vec{a} - \vec{c}|| - ||\,\vec{c}\,||^2 \geq 0$$

i.e.

$$|| -\vec{a}-\vec{c}|| \geq ||\,\vec{c}\,||^2$$

which allows only one ordering in this case. Similarly there is only one ordering when $||\,\vec{a}+\vec{c}\,||^2$ is presented first. Thus there is a total of eight 5-dimensional cases:

$$MD_{4.1} = (0100000/0010000/0000010/0000001/1000000/0001000/0220\bar{1}00)$$

$$MD_{4.2} = (0100000/0010000/0000001/0000010/0001000/1000000/0220\bar{1}00)$$

$$MD_{4.3} = (0100000/0000010/0010000/0000001/1000000/0220\bar{1}00/0001000)$$

$$MD_{4.4} = (0100000/0000010/0000001/0010000/0220\bar{1}00/1000000/0001000)$$

$$MD_{4.5} = (0100000/0000001/0010000/0000010/0001000/0220\bar{1}00/1000000)$$

$$MD_{4.6} = (0100000/0000001/0000010/0010000/0220\bar{1}00/0001000/1000000)$$

$$MD_{4.7} = (0000010/0100000/0010000/0000001/0220\bar{1}00/1000000/0001000)$$

$$MD_{4.8} = (0000001/0100000/0010000/0000010/0220\bar{1}00/0001000/1000000)$$

$PD_4 =$

$$\left(\frac{3}{4}00\frac{\bar{1}}{4}0\frac{1}{4}\frac{1}{4}/0\frac{2}{3}\frac{\bar{1}}{3}0\frac{1}{3}00/0\frac{\bar{1}}{3}\frac{2}{3}0\frac{1}{3}00/\frac{\bar{1}}{4}00\frac{3}{4}0\frac{1}{4}\frac{1}{4}/0\frac{1}{3}\frac{1}{3}0\frac{2}{3}00/\frac{1}{4}00\frac{1}{4}0\frac{3}{4}\frac{\bar{1}}{4}/\frac{1}{4}00\frac{1}{4}0\frac{\bar{1}}{4}\frac{3}{4}\right)$$

$PD_4^{\perp} =$

$$\left(\frac{1}{4}00\frac{1}{4}0\frac{\bar{1}}{4}\frac{\bar{1}}{4}/0\frac{1}{3}\frac{1}{3}0\frac{\bar{1}}{3}00/0\frac{1}{3}\frac{1}{3}0\frac{\bar{1}}{3}00/\frac{1}{4}00\frac{1}{4}0\frac{\bar{1}}{4}\frac{\bar{1}}{4}/0\frac{\bar{1}}{3}\frac{\bar{1}}{3}0\frac{1}{3}00/\frac{\bar{1}}{4}00\frac{\bar{1}}{4}0\frac{1}{4}\frac{1}{4}/\frac{\bar{1}}{4}00\frac{\bar{1}}{4}0\frac{1}{4}\frac{1}{4}\right)$$

This implies $\mathbf{D^7}$ cells of the form $[r, s, t, u, s{+}t, v, r{+}u{-}v]$, $0 \le r \le s \le t \le u \le r{+}v$ $v \le s + u$. As $\mathbf{G^6}$ cells, these cells are of the form $[r, s, t, 0, v - t - r, u - v - s]$.

B.8.2. Case 4 Internal Boundaries The eight permutations that constitute the case 4 five-dimensional case in terms of $\mathbf{D^7}$ components are

d_2, d_3, d_6, d_7

d_2, d_3, d_7, d_6

d_2, d_6, d_3, d_7

d_2, d_6, d_7, d_3

d_2, d_7, d_3, d_6

d_2, d_7, d_6, d_3

d_6, d_2, d_3, d_7

d_7, d_2, d_3, d_6

so the internal boundaries are:

$\{4.1, 4.2\} : d_6 = d_7$

$\{4.1, 4.3\} : d_3 = d_6$

$\{4.3, 4.4\} : d_3 = d_7$

$\{4.2, 4.5\} : d_3 = d_7$

$\{4.4, 4.6\} : d_6 = d_7$

$\{4.3, 4.7\} : d_2 = d_6$

$\{4.5, 4.8\} : d_2 = d_7$

leaving the conditions $d_6 = d_7$, $d_3 = d_6$, $d_3 = d_7$, $d_2 = d_6$, and $d_2 = d_7$, all subject to the case 4 conditions $d_5 = d_2 + d_3$, $g_4 = 0$ and the general Bravais tetrahedron condition $d_1 + d_2 + d_3 + d_4 - d_5 - d_6 - d_7$ to analyze.

The projectors onto the 4-dimensional internal boundaries are:

$$PD_{4\_67} =$$

$$\left(\frac{3}{4}00\frac{\bar{1}}{4}0\frac{1}{4}\frac{1}{4}/0\frac{2}{3}\frac{\bar{1}}{3}0\frac{1}{3}00/0\frac{\bar{1}}{3}\frac{2}{3}0\frac{1}{3}00/\frac{\bar{1}}{4}00\frac{3}{4}0\frac{1}{4}\frac{1}{4}/0\frac{1}{3}\frac{1}{3}0\frac{2}{3}00/\frac{1}{4}00\frac{1}{4}0\frac{1}{4}\frac{1}{4}/\frac{1}{4}00\frac{1}{4}0\frac{1}{4}\frac{1}{4}\right)$$

$$PD_{4\_36} =$$

$$(\frac{12}{17}\frac{\bar{1}}{17}\frac{2}{17}\frac{\bar{5}}{17}\frac{1}{17}\frac{2}{17}\frac{5}{17}/\frac{\bar{1}}{17}\frac{10}{17}\frac{\bar{3}}{17}\frac{\bar{1}}{17}\frac{7}{17}\frac{\bar{3}}{17}\frac{1}{17}/\frac{2}{17}\frac{\bar{3}}{17}\frac{6}{17}\frac{2}{17}\frac{3}{17}\frac{6}{17}\frac{\bar{2}}{17}/\frac{\bar{5}}{17}\frac{\bar{1}}{17}\frac{2}{17}\frac{12}{17}\frac{1}{17}\frac{2}{17}\frac{5}{17}$$
$$\frac{1}{17}\frac{7}{17}\frac{3}{17}\frac{1}{17}\frac{10}{17}\frac{3}{17}\frac{\bar{1}}{17}/\frac{2}{17}\frac{\bar{3}}{17}\frac{6}{17}\frac{2}{17},\frac{3}{17}\frac{6}{17}\frac{\bar{2}}{17}/\frac{5}{17}\frac{1}{17}\frac{\bar{2}}{17}\frac{5}{17}\frac{\bar{1}}{17}\frac{\bar{2}}{17}\frac{12}{17})$$

$$PD_{4\_37} =$$

$$(\frac{12}{17}\frac{\bar{1}}{17}\frac{2}{17}\frac{\bar{5}}{17}\frac{1}{17}\frac{5}{17}\frac{2}{17}/\frac{\bar{1}}{17}\frac{10}{17}\frac{\bar{3}}{17}\frac{\bar{1}}{17}\frac{7}{17}\frac{1}{17}\frac{\bar{3}}{17}/\frac{2}{17}\frac{\bar{3}}{17}\frac{6}{17}\frac{2}{17}\frac{3}{17}\frac{\bar{2}}{17}\frac{6}{17}/\frac{\bar{5}}{17}\frac{\bar{1}}{17}\frac{2}{17}\frac{12}{17}\frac{1}{17}\frac{5}{17}\frac{2}{17}$$
$$\frac{1}{17}\frac{7}{17}\frac{3}{17}\frac{1}{17}\frac{10}{17}\frac{\bar{1}}{17}\frac{3}{17}/\frac{5}{17}\frac{1}{17}\frac{\bar{2}}{17}\frac{5}{17}\frac{\bar{1}}{17}\frac{12}{17}\frac{\bar{2}}{17}/\frac{2}{17}\frac{\bar{3}}{17}\frac{6}{17}\frac{2}{17}\frac{3}{17}\frac{\bar{2}}{17}\frac{6}{17})$$

$$PD_{4\_26} =$$

$$(\frac{12}{17}\frac{2}{17}\frac{\bar{1}}{17}\frac{\bar{5}}{17}\frac{1}{17}\frac{2}{17}\frac{5}{17}/\frac{2}{17}\frac{6}{17}\frac{\bar{3}}{17}\frac{2}{17}\frac{3}{17}\frac{6}{17}\frac{\bar{2}}{17}/\frac{\bar{1}}{17}\frac{\bar{3}}{17}\frac{10}{17}\frac{\bar{1}}{17}\frac{7}{17}\frac{\bar{3}}{17}\frac{1}{17}/\frac{\bar{5}}{17}\frac{2}{17}\frac{\bar{1}}{17}\frac{12}{17}\frac{1}{17}\frac{2}{17}\frac{5}{17}$$
$$\frac{1}{17}\frac{3}{17}\frac{7}{17}\frac{1}{17}\frac{10}{17}\frac{3}{17}\frac{\bar{1}}{17}/\frac{2}{17}\frac{6}{17}\frac{\bar{3}}{17}\frac{2}{17}\frac{3}{17}\frac{6}{17}\frac{\bar{2}}{17}/\frac{5}{17}\frac{\bar{2}}{17}\frac{1}{17}\frac{5}{17}\frac{\bar{1}}{17}\frac{\bar{2}}{17}\frac{12}{17})$$

$$PD_{4\_27} =$$

$$(\frac{12}{17}\frac{2}{17}\frac{\bar{1}}{17}\frac{\bar{5}}{17}\frac{1}{17}\frac{5}{17}\frac{2}{17}/\frac{2}{17}\frac{6}{17}\frac{\bar{3}}{17}\frac{2}{17}\frac{3}{17}\frac{\bar{2}}{17}\frac{6}{17}/\frac{\bar{1}}{17}\frac{\bar{3}}{17}\frac{10}{17}\frac{\bar{1}}{17}\frac{7}{17}\frac{1}{17}\frac{\bar{3}}{17}/\frac{\bar{5}}{17}\frac{2}{17}\frac{\bar{1}}{17}\frac{12}{17}\frac{1}{17}\frac{5}{17}\frac{2}{17}$$
$$\frac{1}{17}\frac{3}{17}\frac{7}{17}\frac{1}{17}\frac{10}{17}\frac{\bar{1}}{17}\frac{3}{17}/\frac{5}{17}\frac{\bar{2}}{17}\frac{1}{17}\frac{5}{17}\frac{\bar{1}}{17}\frac{12}{17}\frac{\bar{2}}{17}/\frac{2}{17}\frac{6}{17}\frac{\bar{3}}{17}\frac{2}{17}\frac{3}{17}\frac{\bar{2}}{17}\frac{6}{17})$$

B.8.3. Case 5: $d_5 = d_1 + d_4$ (see equation B.5). The Bravais tetrahedron edges to be ordered are

$$-\vec{a}, \vec{a} + \vec{b}, \vec{a} + \vec{c}, \vec{d} = -\vec{a} - \vec{b} - \vec{c}$$

As in case 4, above, the original Bravais tetrahedron edge ordering must be respected in selecting permutations, which limits us to permutations that begin with $||-\vec{a}\,||^2$, $||\,\vec{a}+\vec{b}\,||^2$ or $||\,\vec{a}+\vec{c}\,||^2$. If we were to begin with $||\,\vec{d}\,||^2$ there would be no room for $||-\vec{a}\,||^2$ except in the lower-dimensional case of the intersection of case 5 with cases 1, 2 and 3.

Consider the permutations that begin with $||-\vec{a}\,||^2$. There are six possible permtations of $||\,\vec{d}\,||^2$, $||\,\vec{a}+\vec{b}\,||^2$, and $||\,\vec{a}+\vec{c}\,||^2$ to consider. If $||-\vec{a}\,||^2$ does not come first, then it must come second and only either $||\,\vec{a}+\vec{b}\,||^2$ or $||\,\vec{a}+\vec{c}\,||^2$ may come before it or we are forced into lower-dimensional cases.

$$MD_{5.1} = (1000000/0001000/0000010/0000001/0100000/0010000/2002\bar{1}00)$$

$$MD_{5.2} = (1000000/0001000/0000001/0000010/0010000/0100000/2002\bar{1}00)$$

$$MD_{5.3} = (1000000/0000010/0001000/0000001/0100000/2002\bar{1}00/0010000)$$

$$MD_{5.4} = (1000000/0000010/0000001/0001000/2002\bar{1}00/0100000/0010000)$$

$$MD_{5.5} = (1000000/0000001/0001000/0000010/0010000/2002\bar{1}00/0100000)$$

$$MD_{5.6} = (1000000/0000001/0000010/0001000/2002\bar{1}00/0010000/0100000)$$

$$MD_{5.7} = (0000010/1000000/0001000/0000001/2002\bar{1}00/0100000/0010000)$$

$$MD_{5.8} = (0000001/1000000/0001000/0000010/2002\bar{1}00/0010000/0100000)$$

$$PD_5 =$$

$$\left(\frac{2}{3}00\frac{\bar{1}}{3}\frac{1}{3}00/0\frac{3}{4}\frac{\bar{1}}{4}00\frac{1}{4}\frac{1}{4}/0\frac{\bar{1}}{4}\frac{3}{4}00\frac{1}{4}\frac{1}{4}/\frac{\bar{1}}{3}00\frac{2}{3}\frac{1}{3}00/\frac{1}{3}00\frac{1}{3}\frac{2}{3}00/0\frac{1}{4}\frac{1}{4}00\frac{3}{4}\frac{\bar{1}}{4}/0\frac{1}{4}\frac{1}{4}00\frac{\bar{1}}{4}\frac{3}{4}\right)$$

$$PD_5^{\perp} =$$

$$\left(\frac{1}{3}00\frac{1}{3}\frac{\bar{1}}{3}00/0\frac{1}{4}\frac{1}{4}00\frac{\bar{1}}{4}\frac{\bar{1}}{4}/0\frac{1}{4}\frac{1}{4}00\frac{\bar{1}}{4}\frac{\bar{1}}{4}/\frac{1}{3}00\frac{1}{3}\frac{\bar{1}}{3}00/\frac{\bar{1}}{3}00\frac{\bar{1}}{3}\frac{1}{3}00/0\frac{\bar{1}}{4}\frac{\bar{1}}{4}00\frac{1}{4}\frac{1}{4}/0\frac{\bar{1}}{4}\frac{\bar{1}}{4}00\frac{1}{4}\frac{1}{4}\right)$$

This implies $\mathbf{D^7}$ cells of the form $[r, s, t, u, r+u, v, s+t-v]$, $0 \le r \le s \le t \le u$, $u+r \le t+s$, $t \le r+v$, $v \le r+t$, which are $\mathbf{G^6}$ cells of the form $[r, s, t, u-t-s+r, v-t-r, t-r-v]$.

B.8.4. Case 6: $d_6 = d_1 + d_3$, (see equation B.6). The Bravais tetrahedron edges to be ordered are

$$\vec{a}, -\vec{a}-\vec{b}, -\vec{c}, \vec{b}+\vec{c}$$

As with case 4, there are 8 permutations that result in 5-dimensional boundary polytopes.

$$MD_{6.1} = (1000000/0010000/0000100/0000001/0100000/0001000/20200\bar{1}0)$$

$$MD_{6.2} = (1000000/0010000/0000001/0000100/0001000/0100000/20200\bar{1}0)$$

$$MD_{6.3} = (1000000/0000100/0010000/0000001/0100000/20200\bar{1}0/0001000)$$

$$MD_{6.4} = (1000000/0000100/0000001/0010000/20200\bar{1}0/0100000/0001000)$$

$$MD_{6.5} = (1000000/0000001/0010000/0000100/0001000/20200\bar{1}0/0100000)$$

$$MD_{6.6} = (1000000/0000001/0000100/0010000/20200\bar{1}0/0001000/0100000)$$

$$MD_{6.7} = (0000100/1000000/0010000/0000001/20200\bar{1}0/0100000/0001000)$$

$$MD_{6.8} = (0000001/1000000/0010000/0000100/20200\bar{1}0/0001000/0100000)$$

$$PD_6 =$$
$$\left(\frac{2}{3}0\frac{\bar{1}}{3}00\frac{1}{3}0/0\frac{3}{4}0\frac{\bar{1}}{4}\frac{1}{4}0\frac{1}{4}/\frac{\bar{1}}{3}0\frac{2}{3}00\frac{1}{3}0/0\frac{\bar{1}}{4}0\frac{3}{4}\frac{1}{4}0\frac{1}{4}/0\frac{1}{4}0\frac{1}{4}\frac{3}{4}0\frac{\bar{1}}{4}/\frac{1}{3}0\frac{1}{3}00\frac{2}{3}0/0\frac{1}{4}0\frac{1}{4}\frac{\bar{1}}{4}0\frac{3}{4}\right)$$

$$PD_6^{\perp} =$$
$$\left(\frac{1}{3}0\frac{1}{3}00\frac{\bar{1}}{3}0/0\frac{1}{4}0\frac{1}{4}\frac{\bar{1}}{4}0\frac{\bar{1}}{4}/\frac{1}{3}0\frac{1}{3}00\frac{\bar{1}}{3}0/0\frac{1}{4}0\frac{1}{4}\frac{\bar{1}}{4}0\frac{\bar{1}}{4}/0\frac{\bar{1}}{4}0\frac{\bar{1}}{4}\frac{1}{4}0\frac{1}{4}/\frac{\bar{1}}{3}0\frac{\bar{1}}{3}00\frac{1}{3}0/0\frac{\bar{1}}{4}0\frac{\bar{1}}{4}\frac{1}{4}0\frac{1}{4}\right)$$

This implies $\mathbf{D^7}$ cells of the form $[r, s, t, u, v, r+t, s+u-v]$, $0 \leq r \leq s \leq t \leq u \leq r+v$, $v \leq s+u$, which are $\mathbf{G^6}$ cells of the form $[r, s, t, v-t-s, 0, u-v-r]$.

B.8.5. Case 7, a subboundary of Case 6: $d_6 = d_2 + d_4$ (see equation B.7). The Bravais tetrahedron edges to be ordered are

$$\vec{a} + \vec{b}, -\vec{b}, \vec{b} + \vec{c}, \vec{d} = -\vec{a} - \vec{b} - \vec{c}$$

This is not a 5-dimensional boundary. If we call the original case 7 boundary Bravais tetrahedron

$$\vec{a_7}, \vec{b_7}, \vec{c_7}.\vec{d_7} = -\vec{a_7} - \vec{b_7} - \vec{c_7}$$

with the ordering

$$|| \vec{a_7} ||^2 \leq || \vec{b_7} ||^2 \leq || \vec{c_7} ||^2 \leq || \vec{d_7} ||^2$$

which, by subtracting $|| \vec{c_7} ||^2$ from the third and fourth terms implies

$$0 \leq || \vec{a_7} ||^2 + || \vec{b_7} ||^2 + 2\vec{b_7}.\vec{c_7} + 2\vec{a_7}.\vec{c_7} + 2\vec{a_7}.\vec{b_7}$$

$$= (|| \vec{a_7} ||^2 - || \vec{b_7} ||^2) + (|| \vec{b_7} ||^2 - || \vec{b_7} ||^2) + (2\vec{a_7}.\vec{c_7}) + (2|| \vec{b_7} ||^2 + 2\vec{a_7}.\vec{b_7} + 2\vec{b_7}.\vec{c_7})$$

in which each of the parenthesized terms is less than or equal to zero, which means each of them is, indeed, equal to zero, so that

$$|| \vec{a_7} ||^2 = || \vec{b_7} ||^2$$

and

$$2\vec{a_7}.\vec{c_7} = 0$$

then this all, combined with $d_6 = d_1 + d_3$, gives three constraints, thereby lowering the dimension of this boundary to three.

The three-dimensional projector, with "C" in place of "12" and "D" in place of "13" is:

$$PD_7 = \frac{(77\overline{3}\overline{3}242/77\overline{3}\overline{3}242/\overline{3}\overline{3}77242/\overline{3}\overline{3}77242/2222C4\overline{8}/4444484/2222\overline{8}4C)}{20}$$

$$PD_7^{\perp} = \frac{(D\overline{7}33\overline{2}\overline{4}\overline{2}/\overline{7}D33\overline{2}\overline{4}\overline{2}/33D\overline{7}\overline{2}\overline{4}\overline{2}/33D\overline{7}\overline{2}\overline{4}\overline{2}/\overline{2}\overline{2}\overline{2}\overline{2}8\overline{4}8/\overline{4}\overline{4}\overline{4}\overline{4}\overline{4}C\overline{4}/\overline{2}\overline{2}\overline{2}\overline{2}8\overline{4}8)}{20}$$

This implies $\mathbf{D^7}$ cells of the form $[r, r, s, s, t, r+s, r+s-t]$, $0 \leq r \leq s$ $0 \leq t \leq r+s$, $s \leq r+t$, which are $\mathbf{G^6}$ cells of the form $[r, r, s, t-s-r, 0, -t+s-r]$. Thus all case 7 cells are also case 6 cells.

B.8.6. Case 8: $d_7 = d_1 + d_2$ (see equation B.8). This is equivalent to $g_6 = 0$. The Bravais tetrahedron edges to be ordered are

$$\vec{a}, -\vec{b}, \vec{b} + \vec{c}, -\vec{a} - \vec{c}$$

As in case 4, above, the original Bravais tetrahedron edge ordering must be respected in selecting permutations, which requires that $||a||^2 \leq ||b||^2$. In addition, neither $||\,\vec{a}\,||^2$ nor $||\,\vec{b}\,||^2$ can be larger than both $||\,\vec{b}+\vec{c}\,||^2$ and $||-\vec{a}-\vec{c}\,||^2$ or we will force $||\,\vec{d}\,||^2$ to be equal to $||\,\vec{a}\,||^2$ or $||\,\vec{b}\,||^2$, respectively, thereby lowering the dimension of the boundary. This leaves the following six feasible 5-dimensional polytopes.

$$MD_{8.1} = (1000000/0100000/0000100/0000010/0010000/0001000/220000\overline{1})$$

$$MD_{8.2} = (1000000/0100000/0000010/0000100/0001000/0010000/220000\overline{1})$$

$$MD_{8.3} = (1000000/0000100/0100000/0000010/0010000/220000\overline{1}/0001000)$$

$$MD_{8.4} = (1000000/0000010/0100000/0000100/0001000/220000\overline{1}/0010000)$$

$$MD_{8.5} = (0000010/1000000/0100000/0000100/220000\overline{1}/0001000/0010000)$$

$$MD_{8.6} = (0000100/1000000/0100000/0000010/220000\overline{1}/0010000/0001000)$$

$$PD_8 =$$

$$\left(\frac{2}{3}\frac{\bar{1}}{3}0000\frac{1}{3}/\frac{\bar{1}}{3}\frac{2}{3}0000\frac{1}{3}/00\frac{3}{4}\frac{\bar{1}}{4}\frac{1}{4}\frac{1}{4}0/00\frac{\bar{1}}{4}\frac{3}{4}\frac{1}{4}\frac{1}{4}0/00\frac{1}{4}\frac{1}{4}\frac{3}{4}\frac{\bar{1}}{4}0/00\frac{1}{4}\frac{1}{4}\frac{\bar{1}}{4}\frac{3}{4}0/\frac{1}{3}\frac{1}{3}0000\frac{2}{3}\right)$$

$$PD_8^{\perp} =$$

$$\left(\frac{1}{3}\frac{1}{3}0000\frac{\bar{1}}{3}/\frac{1}{3}\frac{1}{3}0000\frac{\bar{1}}{3}/00\frac{1}{4}\frac{1}{4}\frac{\bar{1}}{4}\frac{\bar{1}}{4}0/00\frac{1}{4}\frac{1}{4}\frac{\bar{1}}{4}\frac{\bar{1}}{4}0/00\frac{\bar{1}}{4}\frac{\bar{1}}{4}\frac{1}{4}\frac{1}{4}0/00\frac{\bar{1}}{4}\frac{\bar{1}}{4}\frac{1}{4}\frac{1}{4}0/\frac{\bar{1}}{3}\frac{\bar{1}}{3}0000\frac{1}{3}\right)$$

This implies $\mathbf{D^7}$ cells of the form $[r, s, t, u, v, t+u-v, r+s]$, $0 \leq r \leq s \leq t \leq u$, $t \leq u-v$, $v \leq s+u$, which are $\mathbf{G^6}$ cells of the form $[r, s, t, v-t-s, u-v-r, 0]$.

B.8.7. Case 9, as subboundary of Case 8: $d_7 = d_3 + d_4$ (see equation B.9). The Bravais tetrahedron edges to be ordered are

$$-\vec{c}, \vec{a}+\vec{c}, \vec{b}+\vec{c}, \vec{d} = -\vec{a}-\vec{b}-\vec{c}$$

This is not a 5-dimensional boundary. If we call case 9 boundary Bravais tetrahedron

$$\vec{a_9}, \vec{b_9}, \vec{c_9}.\vec{d_9} = -\vec{a_9}-\vec{b_9}-\vec{c_9}$$

with the ordering

$$||\,\vec{a_9}\,||^2 \leq ||\,\vec{b_9}\,||^2 \leq ||\,\vec{c_9}\,||^2 \leq ||\,\vec{d_9}\,||^2$$

which, by subtracting $||\,\vec{c_9}\,||^2$ from the third and fourth terms implies

$$0 \leq ||\,\vec{a_9}\,||^2 + ||\,\vec{b_9}\,||^2 + 2\vec{b_9}.\vec{c_9} + 2\vec{a_9}.\vec{c_9} + 2\vec{a_9}.\vec{b_9}$$

$$= (||\,\vec{a_9}\,||^2 - ||\,\vec{c_9}\,||^2) + (||\,\vec{b_9}\,||^2 - ||\,\vec{c_9}\,||^2) + (2\vec{a_9}.\vec{b_9}) + (2||\,\vec{c_9}\,||^2 + 2\vec{a_9}.\vec{c_9} + 2\vec{b_9}.\vec{c_9}) \leq 0$$

in which each of the parenthesized terms in less than or equal to zero, which means each of them is, indeed, equal to zero, so that

$$||\,\vec{a_9}\,||^2 = ||\,\vec{b_9}\,||^2 = ||\,\vec{c_9}\,||^2$$

and

$$2\vec{a_9}.\vec{b_9} = 0$$

then this all, combined with $d_7 = d_3 + d_4$, gives four constraints, thereby lowering the dimension of this boundary to two.

Monte Carlo experiments have not produced any examples of this boundary thus far. If these cases do exist, they should be permutations of

$$MD_{9.1} = (0010000/0000010/0000100/0001000/\bar{2}\bar{2}00221/0100000/1000000)$$

The 2-dimensional projector for case 9 is

$$PD_9 = \frac{(1111112/1111112/1111112/1111112/11116\bar{4}2/1111\bar{4}62/2222224)}{10}$$

$$PD_9^{\perp} = \frac{(9\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}\bar{2}/\bar{1}9\bar{1}\bar{1}\bar{1}\bar{1}\bar{2}/\bar{1}\bar{1}9\bar{1}\bar{1}\bar{1}\bar{2}/\bar{1}\bar{1}\bar{1}9\bar{1}\bar{1}\bar{2}/\bar{1}\bar{1}\bar{1}\bar{1}44\bar{2}/\bar{1}\bar{1}\bar{1}\bar{1}44\bar{2}/\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}6)}{10}$$

This implies $\mathbf{D^7}$ cells of the form $[r, r, r, r, s, 2r - s, 2r]$, $0 \leq r$, $0 \leq s \leq 2r$, which are $\mathbf{G^6}$ cells of the form $[r, r, r, s - 2r, -s, 0]$. Thus all case 9 cells are also case 8 cells.

Acknowledgements

We thank the referees for careful reading and for useful suggestions for improvement. Careful copy-editing and corrections by Frances C. Bernstein are gratefully acknowledged. Our thanks to Jean Jakoncic and Alexei Soares for helpful conversations and access to data and facilties at Brookhaven National Laboratory.

Funding information

Funding for this research was provided in part by: U.S. Department of Energy Offices of Biological and Environmental Research and of Basic Energy Sciences (grant No. DE-AC02-98CH10886; grant No. E-SC0012704); U.S. National Institutes of Health (grant No. P41RR012408; grant No. P41GM103473; grant No. P41GM111244; grant No. R01GM117126); and Dectris, Ltd.

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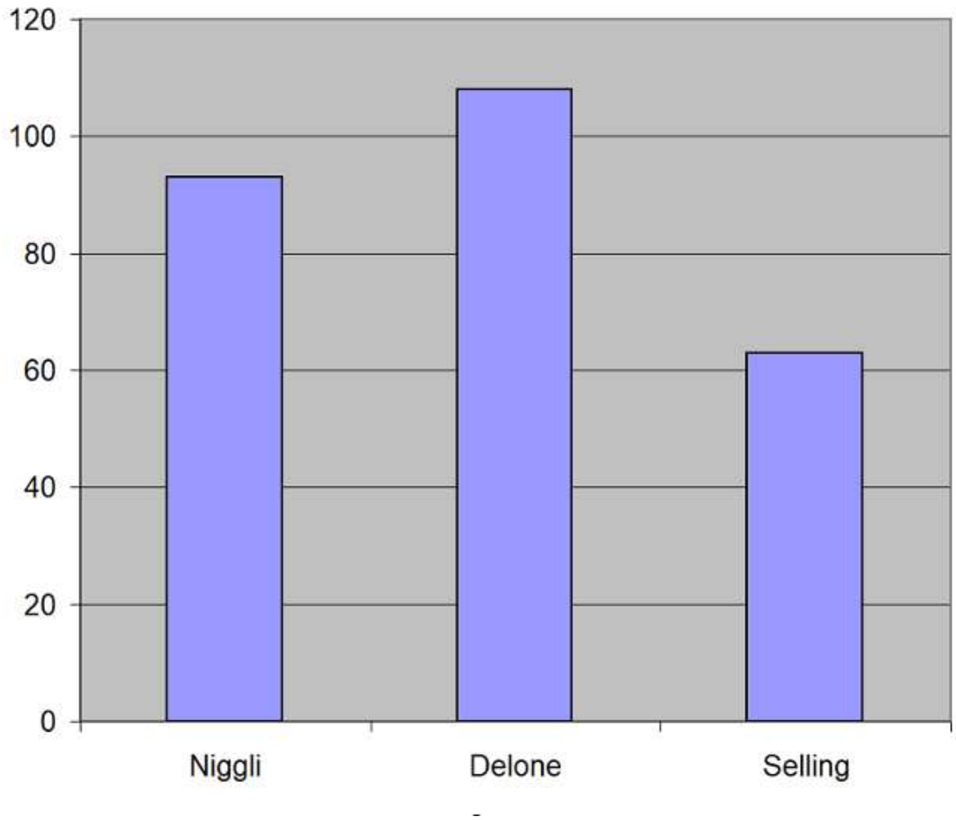
Reduction timing for 89539 unit cells taken from the Protein Data Bank (milliseconds). The times given are for primitive cells.



Synopsis

The unit cell reduction described by Selling and used by Delone (Delaunay) is explained in a simple form.