An Invertible Seven-Dimensional Dirichlet Cell Characterization of Lattices

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Abstract

Characterization of crystallographic lattices is an important tool in structure solution, crystallographic database searches and clustering of diffraction images in serial crystallography. Characterization of lattices by Niggli-reduced cells (based on the three shortest non-coplanar lattice edge vectors) or by Delaunay-reduced cells (based on four edge vectors summing to zero and all meeting at obtuse or right angles) are commonly used. The Niggli cell derives from Minkowski reduction. The Delaunay cell derives from Selling reduction. All are related to the Wigner-Seitz (or Dirichlet, or Voronoi) cell of the lattice, which consists of the points at least as close to a chosen lattice point than they are to any other lattice point. Starting from a Niggli-reduced cell, the Dirichlet cell is characterized by the planes determined by thirteen lattice half-edges: the midpoints of the three Niggli cell edges, the six Niggli cell face diagonals and the four body-diagonals, but seven of the edge lengths are sufficient: three

edge lengths, the three shorter of each pair of face-diagonal lengths and the shortest body-diagonal length, from which the Niggli-reduced cell may be recovered.

1. Introduction

Algorithms for quantifying the differences among lattices are used for Bravais lattice determination, database lookup for unit cells to select candidates for molecular replacement, and for clustering to group together images from serial crystallography. For crystallography, there are many alternative representations to choose from as a basis for distance calculations. Andrews *et al.* (1980) defined $\mathbf{V}^7$, a perturbation-stable space in which, using real and reciprocal space Niggli reduction, a lattice is represented by three cell edge lengths, three reciprocal cell edge lengths and the cell volume, which was proposed for cell database searches, but which has difficulties when used for lattice determination. Andrews & Bernstein (1988) defined $\mathbf{G}^6$ that uses a modified metric tensor and an iterative search through 25 alternative reduction boundary transforms (Gruber, 1973) to work in a satisfactory manner both for database searches and lattice identification in the presence of experimental error. Andrews & Bernstein (2014) discussed sewing together regions of the fundamental region of $\mathbf{G}^6$ under Niggli reduction at fifteen boundaries. Andrews *et al.* (2019) presented the simplest and fastest currently known representation of lattices as the six Selling scalars obtained from 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 $\mathbf{b}$ and $\mathbf{c}$ axes). For the purpose of organizing these six quantities as a vector space in which one can compute simple Euclidean distances, we describe the set of scalars as a vector, $\mathbf{s}$, with components,

$s_1, s_2, s_3, ..., s_6$. The cell is Selling-reduced if all six components are negative or zero (Delone, 1933). Reversing Allman's observation that a Buerger-reduced cell is a good stepping stone to a Selling-reduced cell (Allmann, 1968), a Selling-reduced cell can be an efficient stepping stone to a Niggli-reduced cell.

In this paper we consider lattice representation based on the Wigner-Seitz (Wigner & Seitz, 1933) (or Dirichlet, or Voronoi) cell of the lattice, which consists of the points at least as close to a chosen lattice point as they are to any other lattice point. Starting from a Niggli-reduced cell, the Dirichlet cell is characterized by the planes determined by thirteen lattice half-edges: the midpoints of the three Niggli cell edges, the six Niggli cell face-diagonals and the four body-diagonals, but seven of the edge lengths are sufficient: three edge lengths, the three shorter of each pair of face-diagonal lengths and the shortest body-diagonal length, from which the Niggli-reduced cell may be recovered.

A Wigner-Seitz cell is a polyhedron of six, eight, ten, twelve or fourteen faces. The general fourteen face case is a truncated octahedron. See Fig. 1.

2. Background

That crystals are built from some regular assembly of basic parts was clear already in ancient times. In 1611 Kepler described this relationship (Kepler, 1611) translated in (Kepler *et al.*, 1966). Steno was asked to prepare a catalog of a "cabinet of curiosities"; this is considered the first database of crystals (mineral in this case) (Steno, 1669). See Fig. 2 for a timeline of lattice characterization from Steno onwards. In the 19th century indices were published with interaxial angles of crystals, specifically for the identification of minerals. Following the discovery of x-rays, catalogs of unit cell parameters started to be published (Wyckoff, 1931).

Often, these were arranged by crystal system and then sorted by some of the cell

parameters. However, related minerals with distortions or deformed into another crystal system or incorrectly attributed to another could be difficult to find. Clearly a metric for relating unit cells was required.

2.1. Reduced Cells

Niggli (Niggli, 1928) and Delone (Delone, 1933) devised "reduced cells', which allowed for a more standard presentation of some of the crystal data. The Buerger-reduced cell is simpler than the Niggli-reduced cell, having fewer constraints (Buerger, 1957) (Azaroff & Buerger, 1958) (Buerger, 1960). All Niggli-reduced cells are Buerger-reduced, but not all Buerger-reduced cells are Niggli-reduced.

Finally, in the 1970s, NIH and EPA joined to create the online searchable Chemical Information System (CIS) (Heller *et al.*, 1976) (Bernstein & Andrews, 1979). Along with physical measurements such as NMR and IR, NIH/EPA wanted to include unit cell searching. At the time, there was no commonly accepted method to compute the "distance" between two unit cells (equivalently, lattices).

There were two problems.

The first problem was that measured unit cell parameters (conventionally, [a, b, c, alpha, beta, gamma] for the cell lengths and angles) always have experimental error in their determinations. Further, closely related compounds of interest might have slightly different cell edge parameters. That means that the problem to be solved is "the nearest neighbor problem" also known as "the post office problem". Exact match is not good enough.

The second issue is related to the problem of experimental error, but it manifests in a different way. It is well-known that for any given lattice, there is an infinity of unit cells that can be chosen. The problem is that two unit cells from the same lattice may not look the same. The cells: [10, 10, 10, 90, 90, 90] and [10, 10, 10, 120, 120, 90]

are two different choices from a single crystal lattice. Only the first of these is Niggli reduced, but lattice variation may make the second the reduced one.

3. The Unsorted DC^7 Cell, dc7unsrt

We define the Wigner-Seitz cell as consisting of the points which are no farther from a given lattice point than they are from any other lattice point. As Hart *et al.* (2019) has shown the Wigner-Seitz cell centered on a given lattice point is contained entirely within the convex envelope of the immediate neighbors of a given lattice point, *i.e.* in terms of twenty-six Miller indices:

$(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(\overline{1},0,0)$, $(0,\overline{1},0)$, $(0,0,\overline{1})$,

$(0,1,1)$, $(1,0,1)$, $(1,1,0)$, $(0,1,\overline{1})$, $(\overline{1},0,1)$, $(1,\overline{1},0)$,

$(0,\overline{1},\overline{1})$, $(\overline{1},0,\overline{1})$, $(\overline{1},\overline{1},0)$, $(0,\overline{1},1)$, $(1,0,\overline{1})$, $(\overline{1},1,0)$,

$(1,1,1)$, $(1,\overline{1},\overline{1})$, $(\overline{1},1,\overline{1})$, $(\overline{1},\overline{1},1)$,

$(\overline{1},\overline{1},\overline{1})$, $(\overline{1},1,1)$, $(1,\overline{1},1,)$, $(1,1,\overline{1})$

We organize the lattice in terms of a basis of the three shortest distances. The Wigner-Seitz cell is symmetric around the lattice point, so the thirteen Miller indices are sufficient:

$(1,0,0)$, $(0,1,0)$, $(0,0,1)$,

$(0,1,1)$, $(1,0,1)$, $(1,1,0)$, $(0,1,\overline{1})$, $(\overline{1},0,1)$, $(1,\overline{1},0)$,

$(1,1,1)$, $(1,\overline{1},\overline{1})$, $(\overline{1},1,\overline{1})$, $(\overline{1},\overline{1},1)$,

Formally, the definition of the Wigner-Seitz cell is:

Let L be an $\mathbf{R}^3$ lattice with Minkowski basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ $\in \mathbf{R}^3$, i.e. such that $h\mathbf{a} + k\mathbf{b} + l\mathbf{c}, h \in Z, k \in Z, l \in Z$ spans L and $||\mathbf{a}||, ||\mathbf{b}||, ||\mathbf{c}||$ are minimal. We define the Wigner-Seitz cell of L as

$$WS(L) = \{w \in \mathbf{R}^3 \ni \forall x \in L, x \neq 0, ||w|| \leq ||x - w||\}$$

If we translate this cell to each element of L, we tile the space and have a Voronoi decomposition.

Niggli-reduction provides an unambiguous Minkowski reduction. Assume the cell formed by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is Niggli reduced, with $||\mathbf{a}|| \leq ||\mathbf{b}|| \leq ||\mathbf{c}||$. Define the $\mathbf{G}^6$ vector of the cell as

$$\{r,\, s,\, t,\, u,\, v,\, w\}$$

$$= \{\mathbf{a}\cdot\mathbf{a},\, \mathbf{b}\cdot\mathbf{b},\, \mathbf{c}\cdot\mathbf{c},\, 2\mathbf{b}\cdot\mathbf{c},\, 2\mathbf{a}\cdot\mathbf{c},\, 2\mathbf{a}\cdot\mathbf{b}\}$$

As a Niggli-reduced cell, we either have all of $u, v, w \leq 0$ or all of $u, v, w > 0$.

We define a $\mathbf{DC}^{13}$ cell as the squares of the three edge lengths, the six face diagonal lengths and the four body diagonal lengths, *i.e.*:

$$dc_{13,raw}(r, s, t, u, v, w) =$$

$$[r,\, s,\, t,$$

$$s+t-u,\, s+t+u,\, r+t-v,\, r+t+v,\, r+s-w,\, r+s+w,$$

$$r+s+t+u+v+w,\, r+s+t+u-v-w,$$

$$r+s+t-u+v-w,\, r+s+t-u-v+w]$$

If we sort the elements of $\mathbf{DC}^{13}$ and only present the first seven elements, we have $\mathbf{DC}^7$ as discussed in (Bernstein & Andrews, 2021), which is a smooth but ambiguous characterization of lattices. $\mathbf{DC}^7$ is not invertible in some cases unless the symmetry is known *a priori*, or some elements after the seventh are retained. Bright (Bright, 2021) has demonstrated the $\mathbf{DC}^7$ ambiguity with the cells i: [2.8284, 3.162277, 3.4641, 117.157, 107.8295, 116.5651] and ii: [2.8284, 3.162277, 3.4641, 123.211, 107.8295, 109.59748] as $[a, b, c, \alpha, \beta, \gamma]$, or i: [8, 10, 12, −10, −6, −4] and ii: [8, 10, 12, −12, −6, −3] as the $\mathbf{G}^6$ vectors $[r,\, s,\, t,\, u,\, v,\, w]$ for which the sorted $\mathbf{DC}^{13}$ elements after Niggli reduction

are

i: 2.44949, 2.82843, 3.16228,

3.16228, 3.4641, 3.4641, 3.74166, **4**,

4.24264, 4.47214, 5.09902, 5.09902, 6.16441,

and

ii: 2.44949, 2.82843, 3.16228,

3.16228, 3.4641, 3.4641, 3.74166, **4.24264**,

4.24264, 4.89898, 4.89898, 5.2915, 5.65685,

respectively, which do not differ until the eighth element.

If all of u, v, $w \leq 0$, then $s+t+u \leq s+t-u$, $r+t+v \leq r+t-v$, $r+s+w \leq r+s-w$, *i.e.* the three summed squares of the face diagonals are no larger than the corresponding differences, and $r+s+t+u+v+w \leq \{\ r+s+t+u-v-w,\ r+s+t-u+v-w,\ r+s+t-u-v+w\ \}$, *i.e.* the summed squared main body diagonal is no larger than the three remaining body diagonals.

On the other hand, if all of $u, v, w > 0$, then $s+t+u > s+t-u$, $r+t+v > r+t-v$, $r+s+w > r+s-w$, *i.e.* the three summed squares of the face diagonals are strictly greater than the corresponding differences, and $r+s+t+u+v+w\ >$ each of $\{r+s+t+u-v-w,\ r+s+t-u+v-w,\ r+s+t-u-v+w\}$, *i.e.* the smallest squared body diagonal is strictly less than $r+s+t+u+v+w$, and strictly greater than $r+s+t-|u|-|v|-|w|$

Thus we can recover r, s, t, u, v, w from the three cell edge lengths, the three shorter of each pair of face diagonal lengths, and the shortest squared body diagonal length as follows.

$dc7_{unsrt} = [dc7_{unsrt,1}, dc7_{unsrt,2}, dc7_{unsrt,3},$

$dc7_{unsrt,4}, dc7_{unsrt,5}, dc7_{unsrt,6}, dc7_{unsrt,7}]$

$= [r, s, t, s + t - |u|, r + t - |v|, r + s - |w|,$

$min(r + s + t + u + v + w, r + s + t + u - v - w,$

$r + s + t - u + v - w, r + s + t - u - v + w)]$

If we subtract the face diagonal from the matching pairs of edges, we get the absolute values of u, v, w

$dc7_{unsrt,2} + dc7_{unsrt,3} - dc7_{unsrt,4}$

$= s + t - (s + t - |u|) = |u|$

$dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5}$

$= r + t - (r + t - |v|) = |v|$

$dc7_{unsrt,1} + dc7_{unsrt,2} - dc7_{unsrt,6}$

$= r + s - (r + s - |w|) = |w|$

from which we can compute an estimate of the shortest body diagonal that is exact for $---$ and a strict underestimate for $+++$:

$\tau = r + s + t - |u| - |v| - |w|$

$= dc7_{unsrt,1} + dc7_{unsrt,2} + dc7_{unsrt,3}$

$-(dc7_{unsrt,2}, + dc7_{unsrt,3}, - dc7_{unsrt,4})$

$-(dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5})$

$-(dc7_{unsrt,1} +, dc7_{unsrt,2} - dc7_{unsrt,6})$

$= -dc7_{unsrt,1} - dc7_{unsrt,2} - dc7_{unsrt,3}$

$+ dc7_{unsrt,4} + dc7_{unsrt,5} + dc7_{unsrt,6}$

If $\tau = dc7_{unsrt,7}$, we can be certain that all of u, v, $w \leq 0$. If $\tau \neq dc7_{unsrt,7}$ and the difference is larger than the possible experimental or rounding errors, we can be certain that all of $u, v, w > 0$. Thus the Niggli cell can be recovered from $dc7_{unsrt}$.

For example, the Niggli-reduced $\mathbf{G}^6$ versions of the cells in the Bright example are i: [6, 8, 10, 8, 4, 2] and ii: [6, 8, 10, −6, −2, −4] Note that the former has all of u, v, w positive and the latter negative. Table 1 shows the unsorted $\mathbf{DC}^7$ vectors and the process of recovery of the $\mathbf{G}^6$ vectors.

4. The Boundaries of Unsorted $\mathbf{DC}^7$

Whether we are working in seven dimensions with $\mathbf{DC}^7$ or in six dimensions with $\mathbf{G}^6$, the reduced cells form a manifold for which it is useful to understand the boundaries. Inasmuch as seven-dimensional unsorted $\mathbf{DC}^7$ cells are invertibly derived from six-dimensional $\mathbf{G}^6$ cells, the six-dimensional boundary polytopes of the manifold of valid Wigner-Seitz-reduced cells in $\mathbf{DC}^7$ can be derived directly from the fifteen five-dimensional boundary polytopes of the manifold of valid Niggli-reduced cells in $\mathbf{G}^6$ as described in (Andrews & Bernstein, 2014). Recall that the manifold of Niggli-reduced cells in $\mathbf{G}^6$ is divided into two components for which in one component all of the cell angles are acute, which we mark "+ + +" and in the other component all of the cell angles are obtuse (less than or equal to zero), which we mark "− − −". The manifold of Wigner-Seitz-reduced cells in unsorted $\mathbf{DC}^7$ is similarly divided on the basis of whether $\tau \neq dc7_{usrt,7}$ for + + + or $\tau = dc7_{usrt,7}$ for − − −.

4.1. Equal-cell-edge case

Recall that $r \leq s \leq t$. The first two boundaries are the equal-edge boundary cases.

- Case 1. $r = s$: The cells in this case may be either + + + or − − −.

  $dc7_{unsrt,1} = dc7_{unsrt,2}$.

- Case 2. $s = t$: The cells in this case may be either $+++$ or $---$.

  $dc7_{unsrt,2} = dc7_{unsrt,3}$.

4.2. 90° *case*

The 90° case marks a possible transition between $---$ and $+++$.

- Case 3. $u = 0$: The cells in this case must be $---$.

  $dc7_{unsrt,2} + dc7_{unsrt,3} - dc7_{unsrt,4} = 0$

- Case 4. $v = 0$: The cells in this case must be $---$.

  $dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5} = 0$

- Case 5. $w = 0$: The cells in this case must be $---$.

  $dc7_{unsrt,1} + dc7_{unsrt,2} - dc7_{unsrt,6} = 0$

4.3. Face-diagonal case

Recall that $|u| \leq s$, $|v| \leq r$, and $|w| \leq r$. Equality marks the transition from edges being smaller than face diagonals to face diagonals possibly being smaller.

- Case 6. $s = u, v \geq w$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,2} = dc7_{unsrt,2} + dc7_{unsrt,3} - dc7_{unsrt,4}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,4}$

  $dc7_{unsrt,3} - dc7_{unsrt,5} \geq dc7_{unsrt,2} - dc7_{unsrt,6}$

- Case 7. $s = u, v < w$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,2} = dc7_{unsrt,2} + dc7_{unsrt,3} - dc7_{unsrt,4}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,4}$

  $dc7_{unsrt,3} - dc7_{unsrt,5} < dc7_{unsrt,2} - dc7_{unsrt,6}$

- Case 8. $s = -u$: The cells in this case must be $---$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) = dc7_{unsrt,7}$

  $dc7_{unsrt,2} = dc7_{unsrt,2} + dc7_{unsrt,3} - dc7_{unsrt,4}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,4}$

- Case 9. $r = v, u \geq w$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,5}$

  $dc7_{unsrt,3} - dc7_{unsrt,4} \geq dc7_{unsrt,1} - dc7_{unsrt,6}$

- Case A. $r = v, u < w$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,5}$

  $dc7_{unsrt,3} - dc7_{unsrt,4} < dc7_{unsrt,1} - dc7_{unsrt,6}$

- Case B. $r = -v$: The cells in this case must be $---$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) = dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,3} - dc7_{unsrt,5}$

  equivalent to $dc7_{unsrt,3} = dc7_{unsrt,5}$

- Case C. $r = w, u \geq v$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,2} - dc7_{unsrt,6}$

  equivalent to $dc7_{unsrt,2} = dc7_{unsrt,6}$

  $dc7_{unsrt,2} - dc7_{unsrt,4)\geq dc7_{unsrt,1} - dc7_{unsrt,5}}$

- Case D. $r = w, u < v$: The cells in this case must be $+++$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) < dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,2} - dc7_{unsrt,6}$

equivalent to $dc7_{unsrt,2} = dc7_{unsrt,6}$

$dc7_{unsrt,2} - dc7_{unsrt,4)<dc7_{unsrt,1}-dc7_{unsrt,5}}$

- Case E. $r = -w$: The cells in this case must be $---$.

  $\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i}) = dc7_{unsrt,7}$

  $dc7_{unsrt,1} = dc7_{unsrt,1} + dc7_{unsrt,2} - dc7_{unsrt,6}$

  equivalent to $dc7_{unsrt,2} = dc7_{unsrt,6}$

4.4. Body-diagonal case

Recall that $t <= r + s + t + u + v + w$ for a Niggli-reduced cell, otherwise the main body diagonal would be shorter than c. Equality can occur in $---$ and marks the transition from edges being smaller than the main body diagonal to the main body diagonal possibly being smaller.

- case F. $t = r + s + t + u + v + w$. The cells in this case must be $---$.

$$\tau = -\sum_{i=1}^{3}(-dc7_{unsrt,i}) + \sum_{i=4}^{6}(dc7_{unsrt,i})$$

$$= dc7_{unsrt,7} = dc7_{unsrt,3}$$

5. Smoothing by permutations

Because the same boundaries are available in unsorted $\mathbf{DC}^7$ as in $\mathbf{G}^6$, the equivalent algorithmic techniques can be used in improving the distance calculations to improve smoothness. The obvious first step is to deal with boundary cases 1 and 2 by simple permutation of the $dc7_{unsrt}$ vectors, so that

$dc7unsrt\_dist(dc7_1, dc7_2) = min($

$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,3}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$

$-[dc7_{2,1}, dc7_{2,2}, dc7_{2,3}, dc7_{2,4}, dc7_{2,5}, dc7_{2,6}, dc7_{2,7}]||,$

$$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$$

$$-[dc7_{2,1}, dc7_{2,3}, dc7_{2,2}, dc7_{2,4}, dc7_{2,6}, dc7_{2,5}, dc7_{2,7}]||,$$

$$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$$

$$-[dc7_{2,2}, dc7_{2,1}, dc7_{2,3}, dc7_{2,5}, dc7_{2,4}, dc7_{2,6}, dc7_{2,7}]||,$$

$$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$$

$$-[dc7_{2,2}, dc7_{2,3}, dc7_{2,1}, dc7_{2,5}, dc7_{2,6}, dc7_{2,4}, dc7_{2,7}]||,$$

$$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$$

$$-[dc7_{2,3}, dc7_{2,1}, dc7_{2,2}, dc7_{2,6}, dc7_{2,4}, dc7_{2,5}, dc7_{2,7}]||,$$

$$||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]$$

$$-[dc7_{2,3}, dc7_{2,2}, dc7_{2,1}, dc7_{2,6}, dc7_{2,5}, dc7_{2,4}, dc7_{2,7}]||,$$

These cases are simple because cases 1 and 2 do not impact the seventh element. In the general case a fresh Niggli reduction may be needed to regenerate the seventh element for minimal distance calculations.

6. Testing against the Gruber example

Gruber (1973) presented a Niggli-reduced cell with a five-fold Buerger-reduced cell ambiguity. The Niggli-reduced cell is $[a, b, c, \alpha, \beta, \gamma]$ = [2, 4, 4, 60, 79.19, 75.52] which is equivalent to the $\mathbf{G}^6$ cell $[r, s, t, u, v, w]$ = [4, 16, 16, 16, 3, 4] and the unsorted $\mathbf{DC}^7$ cell [4, 16, 16, 17, 19, 16, 16]. The five examples of the alternative Buerger reduced cells are shown in Table 2 as edges and angles, in Table 3 as $\mathbf{G}^6$ $[r, s, t, u, v, w]$, and in Table 4 as unsorted $\mathbf{DC}^7$. Cell i is Niggli reduced. All of the cells are on the 2 boundary with $s = t$ and can equally be presented with s and t interchanged and v and w interchanged. Cells i and ii are both $+++$ and on the 7 and C face-diagonal

boundaries as well as being on the 2 boundary. Cells iii, iv and v are all $---$ and on the F body-diagonal boundary as well as being on 2 boundary and one other face-diagonal boundary. Cell iii is on the 8 face-diagonal boundary and cells iv and v are on the E face-diagonal boundary. Niggli reduction will transform all of these back to cell i and Niggli reduction is the first step in computing unsorted $\mathbf{DC}^7$. Therefore in order to compute the cells in Table 4 the components at the face-diagonal boundaries were reduced in magnitude by 0.01 to prevent the Niggli reduction. The differences among the unsorted $\mathbf{DC}^7$ cells are consistent with the perturbation.

7. Summary and Conclusions

Starting from a Niggli-reduced cell, a crystallographic lattice may be characterized by seven parameters describing the Dirichlet cell: three edge lengths, the three shorter face diagonals and the shortest body diagonal, from which the Niggli-reduced cell may be recovered. This unsorted $\mathbf{DC}^7$ lattice characterization avoids the low-symmetry ambiguities of sorted $\mathbf{DC}^7$ and is worth further investigation as a possible alternative to $\mathbf{S}^6$ for crystallographic databases and clustering.

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Table 1. *Bright's* $\mathbf{DC}^7$ *ambiguous example, redone in unsorted* $\mathbf{DC}^7$. *The Niggli-reduced* $\mathbf{G}^6$ *vectors are* [6, 8, 10, 8, 4, 2] *and* [6, 8, 10, −6, −2, −4]. *The former is* + + + *and becomes* [6, 8, 10, 10, 12, 12, 14] *as unsorted* $\mathbf{DC}^7$. *The latter is* − − − *and becomes* [6, 8, 10, 12, 14, 10, 12] *as unsorted* $\mathbf{DC}^7$. *When each is processed to recover* $\mathbf{G}^6$ *the magnitude of* $\mathbf{r}+\mathbf{s}+\mathbf{t}-|\mathbf{u}|-|\mathbf{v}|-|\mathbf{w}|$ *disagrees with the minimum body diagonal for the former and agrees for the latter, giving the correct signs for full recovery of* $\mathbf{G}^6$.

$\mathbf{G}^6$:	**r**	**s**	**t**	**u**	**v**	**v**
i	6	8	10	8	4	2
ii	6	8	10	-6	-2	-4

$\mathbf{DC}^7$ unsrt:	**r**	**s**	**t**	$\mathbf{s}+\mathbf{t}$ $-\lvert\mathbf{u}\rvert$	$\mathbf{r}+\mathbf{t}$ $-\lvert\mathbf{v}\rvert$	$\mathbf{r}+\mathbf{s}$ $-\lvert\mathbf{w}\rvert$	min body diag (MBD)
i	6	8	10	10	12	12	14
ii	6	8	10	12	14	10	12

recover $\mathbf{G}^6$:	**r**	**s**	**t**	$\lvert\mathbf{u}\rvert$	$\lvert\mathbf{v}\rvert$	$\lvert\mathbf{w}\rvert$	$\tau=\mathbf{r}+\mathbf{s}+\mathbf{t}$ $-\lvert\mathbf{u}\rvert-\lvert\mathbf{v}\rvert-\lvert\mathbf{w}\rvert$
i	6	8	10	8	4	2	$\tau\,10 \neq$ MBD 14 (disagree + + +)
ii	8	8	10	6	2	4	$\tau\,12 =$ MBD 12 (agree − − −)

Table 2. *Gruber's example of five-fold alternative Buerger-reduced cells for a lattice as* $[a, b, c, \alpha, \beta, \gamma]$

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cell	a	b	c	α	β	γ
i	2	4	4	60.00	79.1	75.52
ii	2	4	4	60.00	86.42	75.52
iii	2	4	4	120.00	93.58	100.80
iv	2	4	4	117.95	93.58	104.48
v	2	4	4	113.97	100.80	104.48

Table 3. *Gruber's example of five-fold alternative Buerger-reduced cells for a lattice as* $\mathbf{G}^6$ *[**r**,**s**,**t**,**u**,**v**,**w**]*

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cell	**r**	**s**	**t**	**u**	**v**	**w**	**bdry**
i	4	16	16	16	3	4	27C
ii	4	16	16	16	1	4	27C
iii	4	16	16	-16	-1	-3	2F8
iv	4	16	16	-15	-1	-4	2FE
v	4	16	16	-13	-3	-4	2FE

Table 4. *Gruber's example of five-fold alternative Buerger-reduced cells for a lattice as unsorted* **DC**[7]. *In order to get past the fact that all the cell reduces to the same Niggli cell, a small perturbation of .01 was applied to u or w in ii – v to get away from the relevant boundaries.*

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cell	1	2	3	4	5	6	7
i	4	16	16	17	19	16	16
ii	4	16	16	17.01	19	16	16.01
iii	4	16	16	16.01	19	17	16.01
iv	4	16	16	17	19	16.01	16.01
v	4	16	16	19	17	16.01	16.01

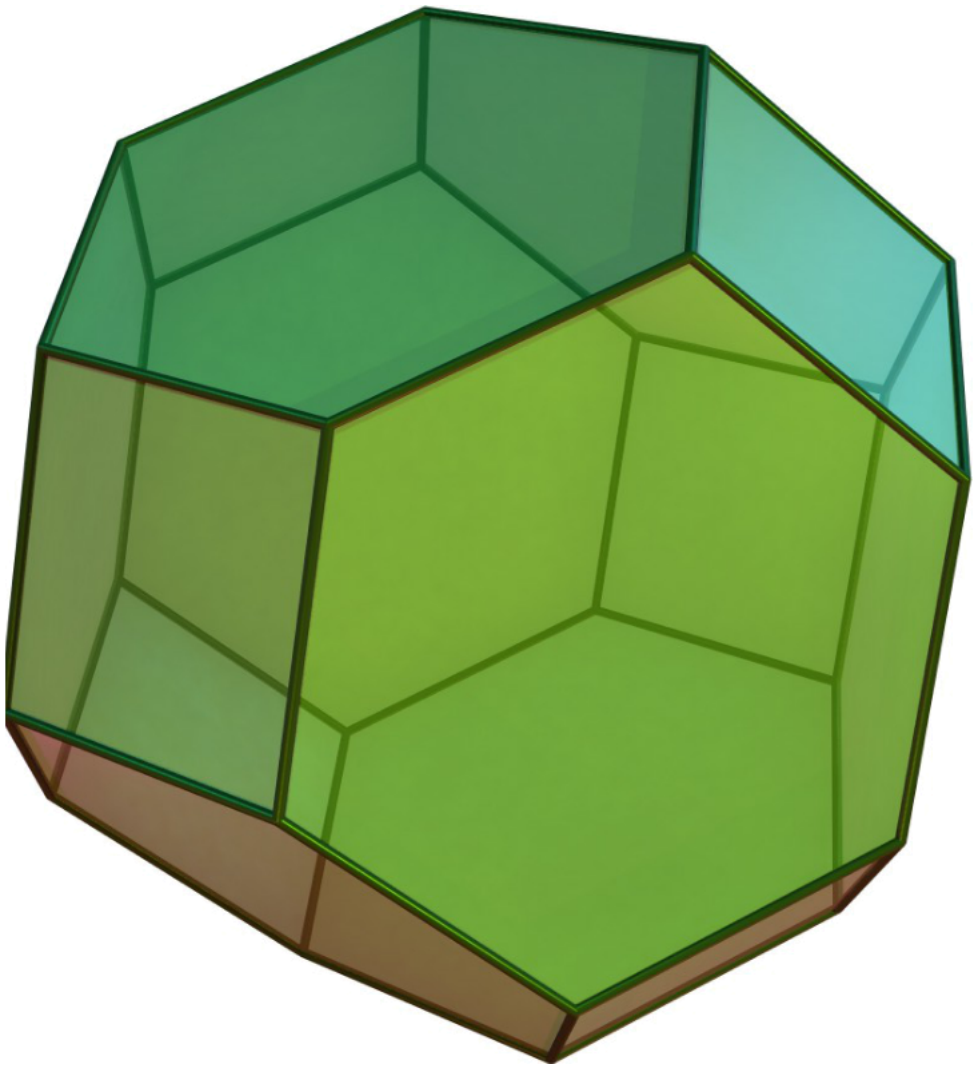

Fig. 1. Truncated octahedron (Wikipedia, 2017). Image licensed under the Creative Commons Attribution-Share Alike 3.0 Unported license. Subject to disclaimers. See web site.

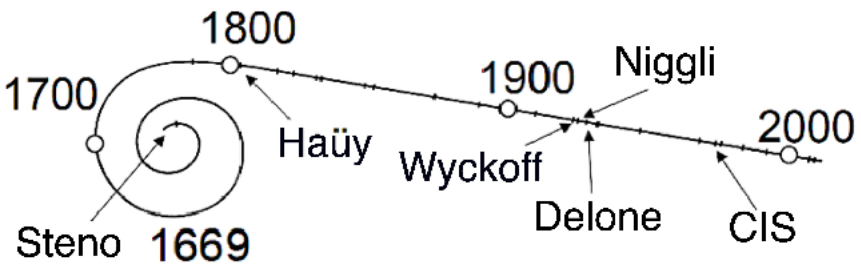

Fig. 2. Historical timeline of studies of crystallographic lattice characterization. Figure drawn by E. Kincaid. Used with permission of the artist.

Synopsis

Starting from a Niggli-reduced cell, a crystallographic lattice may be characterized by seven parameters describing the Dirichlet cell: three edge lengths, the three shorter of each pair of face diagonal lengths and the shortest body diagonal length, from which the Niggli-reduced cell may be recovered.