

An Invertible Seven-Dimensional Dirichlet Cell Characterization of Lattices

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Dirichlet Cell; Voronoi Cell; Wigner-Seitz Cell; Niggli Reduction

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 vectors) or by Delaunay-reduced cells (based on four non-coplanar 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 as they are to any other lattice point.

For the case of Niggli reduction, we call the three non-coplanar lattice vectors \mathbf{x}_{xx} chosen, the Niggli-reduced cell edges. 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 lengths are sufficient: three edge lengths, the three shorter of each pair of face-diagonal lengths, and the shortest body-diagonal length. These seven are sufficient to recover the Niggli-reduced cell.

1. Introduction

Algorithms for quantifying the differences among lattices are used for Bravais lattice determination, for database lookup of unit cells to select candidates for molecular replacement, and for clustering to group together images from serial crystallography. In order to create a distance measure, it is necessary to define metric representation of lattices. The current paper describes a new representation with sufficient detail for creating a complete distance measure.

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. While suitable for database searches, \mathbf{V}^7 was found to have difficulties in some other uses. For lattice type determination, issues arose when working near right angles.
- Andrews & Bernstein (1988) then 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 rep-

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 three linearly independent vectors \mathbf{a} , \mathbf{b} , \mathbf{c} spanning the lattice, and defining \mathbf{d} ($\mathbf{d} = -\mathbf{a} - \mathbf{b} - \mathbf{c}$), the Selling 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} vectors). 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, $s_1, s_2, s_3, \dots, s_6$. 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 Buerger-reduced cell that quickly reduces to a Niggli-reduced cell??. Note that the negatives of the Selling scalars of a Selling-reduced cell are non-negative so that the six square roots provide a convenient six-parameter characterization of a lattice (Kurlin, 2022).

2. A new representation

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-reduced cell edges, the six Niggli-reduced cell face-diagonals, and the four body-diagonals, but seven of the Niggli-reduced cell lattice vector lengths are sufficient: three Niggli-reduced cell-edge lengths, the three shorter of each pair of face-diagonal lengths, and the shortest body-

diagonal length. The Niggli-reduced cell may be recovered easily from these seven quantities.

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.

When one is creating a metric to compute distances between lattices they are likely to be based directly or indirectly either on the components of the Niggli-reduced cell or on the components of the Selling-reduced cell. One disadvantage in use of the former is that the space of Niggli-reduced cells admits both all-acute and all-obtuse presentations, dividing the space into two distinct components with a disruptive boundary between them. Use of Selling-reduction avoids this problem by restricting our attention to the all-obtuse case, making it easier to find smooth metrics. The Wigner-Seitz cell is often presented entirely in the context of Selling-reduction, but in this paper we are using the approach of (Hart *et al.*, 2019) and working in terms of Niggli-reduction in order to understand the primary static characteristics of the space, especially the invertibility of this presentation. The question of improving stability – especially when computing distances between lattices in the $---$ and $+++$ components is left for a future investigation.

3. 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 (minerals in this case) (Steno, 1669). See Fig. 2 for a timeline of lattice characterization from Steno onward. 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. See (Andrews & Bernstein, 2023) for additional background information on the problem.

3.1. *Reduced Cells*

Niggli (1928) and Delaunay (1933) (aka Delone) 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. Roof (1967) provided an updated and authoritative reference to the lattice characters of Niggli-reduced cells.

Finally, in the 1970s, the National Institute of Health (NIH) and the Environmental Protection Agency (EPA) joined to create the online searchable Chemical Information System (CIS) (Heller *et al.*, 1976) (Bernstein & Andrews, 1979). Along with physical measurements such as nuclear magnetic resonance and infrared, 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”. An exact

match is not sufficient.

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 face-centered cell $[10\sqrt{2}, 10\sqrt{2}, 10\sqrt{2}, 90, 90, 90]$ has primitive unit cells $[10, 10, 10, 60, 60, 60]$ and $[10, 10, 10, 120, 120, 90]$ (among many other choices) are two different choices from a single crystal lattice. Only the first of these is Niggli reduced, but lattice variation or experimental error may make the second the reduced one.

4. The Unsorted DC⁷ 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:

$$\begin{aligned}
 &(1, 0, 0), (0, 1, 0), (0, 0, 1), (-1, 0, 0), (0, -1, 0), (0, 0, -1), \\
 &(0, 1, 1), (1, 0, 1), (1, 1, 0), (0, 1, -1), (-1, 0, 1), (1, -1, 0), \\
 &(0, -1, -1), (-1, 0, -1), (-1, -1, 0), (0, -1, 1), (1, 0, -1), (-1, 1, 0), \\
 &(1, 1, 1), (1, -1, -1), (-1, 1, -1), (-1, -1, 1), \\
 &(-1, -1, -1), (-1, 1, 1), (1, -1, 1), (1, 1, -1)
 \end{aligned}$$

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

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

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

$$(1, 1, 1), (1, -1, -1), (-1, 1, -1), (-1, -1, 1),$$

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

Let \mathbf{R} be the space of reals, \mathbf{Z} be the space of integers. 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 $h\mathbf{a} + k\mathbf{b} + l\mathbf{c}, h \in \mathbf{Z}, k \in \mathbf{Z}, l \in \mathbf{Z}$ spans L and $\|\mathbf{a}\|, \|\mathbf{b}\|, \|\mathbf{c}\|$ are minimal. We define the Wigner-Seitz cell of L as

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

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

$$\begin{aligned} & \{r, s, t, u, v, w\} \\ &= \{\mathbf{a} \cdot \mathbf{a}, \mathbf{b} \cdot \mathbf{b}, \mathbf{c} \cdot \mathbf{c}, 2\mathbf{b} \cdot \mathbf{c}, 2\mathbf{a} \cdot \mathbf{c}, 2\mathbf{a} \cdot \mathbf{b}\} \end{aligned}$$

As a Niggli-reduced cell, we either have all of $u, v, w \leq 0$, which we annotate as the $---$ case, or all of $u, v, w > 0$, which we annotate as the $+++$ case, and in both cases $|u| \leq s, |v| \leq r, |w| \leq r$.

The full set of conditions for a Niggli-reduced cell are given in conditions 1 – 16:

$$\text{require } 0 < r \leq s \leq t \tag{1}$$

$$\text{if } r = s; \text{ then require } |u| \leq |v| \tag{2}$$

$$\text{if } s = t; \text{ then require } |v| \leq |w| \tag{3}$$

$$\text{require } u > 0 \text{ and } v > 0 \text{ and } w > 0 \text{ or} \tag{4}$$

$$\text{require } u \leq 0 \text{ and } v \leq 0 \text{ and } w \leq 0 \quad (5)$$

$$\text{require } |u| \leq s \quad (6)$$

$$\text{require } |v| \leq r \quad (7)$$

$$\text{require } |w| \leq r \quad (8)$$

$$\text{require } t \leq r + s + t + u + v + w \quad (9)$$

$$\text{if } u = s \text{ then require } w \leq 2v \quad (10)$$

$$\text{if } v = r \text{ then require } w \leq 2u \quad (11)$$

$$\text{if } w = r \text{ then require } v \leq 2u \quad (12)$$

$$\text{if } u = -s \text{ then require } w = 0 \quad (13)$$

$$\text{if } v = -r \text{ then require } w = 0 \quad (14)$$

$$\text{if } w = -r \text{ then require } v = 0 \quad (15)$$

$$\text{if } t = r + s + t + u + v + w \text{ then require } 2r + 2v + w \leq 0 \quad (16)$$

Using the \mathbf{G}^6 vector component definitions, 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.*:

$$\begin{aligned} dc_{13,raw}(r, s, t, u, v, w) = \\ [r, s, t, \\ s + t - u, s + t + u, r + t - v, r + t + v, r + s - w, r + s + w, \\ r + s + t + u + v + w, r + s + t + u - v - w, \\ r + s + t - u + v - w, r + s + t - u - v + w] \end{aligned}$$

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 $r+s+t+u+v+w \leq \{ r+s+t+u-v-w, r+s+t-u+v-w, r+s+t-u-v+w \}$. In this — — — case, the 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 squares of the lengths of longer face diagonals formed by the Niggli-reduced cell-edge vector sums are strictly greater than the corresponding shorter face diagonals formed by the Niggli-reduced cell-edge vector differences. Turning to the body diagonals, the square of the length of the main body diagonal is $r+s+t+u+v+w$.

The squares of the lengths of the other three body diagonals are $\{r + s + t + u - v - w, r + s + t - u + v - w, r + s + t - u - v + w\}$. Thus the square of the length of 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 explained in the following theorem and proof.

4.1. Theorem

Let $g = r, s, t, u, v, w$ be a \mathbf{G}^6 Niggli-reduced cell satisfying the Niggli-reduction conditions 1 – 16. Let

$$\begin{aligned}
 dc7_{unsrt} &= [dc7_{unsrt,1}, dc7_{unsrt,2}, dc7_{unsrt,3}, \\
 &dc7_{unsrt,4}, dc7_{unsrt,5}, dc7_{unsrt,6}, dc7_{unsrt,7}] \\
 &= [r, s, t, s + t - |u|, r + t - |v|, r + s - |w|, \\
 &min(r + s + t + u + v + w, r + s + t + u - v - w, \\
 &r + s + t - u + v - w, r + s + t - u - v + w)] \\
 &= [r, s, t, s + t - |u|, r + t - |v|, r + s - |w|, \\
 &r + s + t - |u| - |v| - |w| + 2min(max(0, u), max(0, v), max(0, w))]
 \end{aligned}$$

be the unsorted \mathbf{DC}^7 presentation of g . Then the values of the components of $dc7_{unsrt}$ unambiguously determine the values of the components of g .

4.1.1. Proof of Theorem 4.1

In the Niggli-reduced $---$ case we have

$$dc7_{unsrt} = [r, s, t, s + t + u, r + t + v, r + s + w, r + s + t + u + v + w] \quad (17)$$

and in the Niggli-reduced $+++$ case we have

$$dc7_{unsrt} = [r, s, t, s + t - u, r + t - v, r + s - w, r + s + t - u - v - w + 2 \min(u, v, w)] \quad (18)$$

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, τ , 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 $dc7_{unsrt}$. Q.E.D.

4.2. Recovering the components of the Bright example

For example, the Niggli-reduced \mathbf{G}^6 versions of the cells in the Bright example above 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 3 shows the unsorted \mathbf{DC}^7 vectors and the process of recovery of the \mathbf{G}^6 vectors.

4.3. Examples using Phospholipase A2

As noted in (McGill *et al.*, 2014), the structures in the PDB for Phospholipase A2 include slightly different experimental determinations of presented as different lattices, *e.g.* 1U4J in space group H 3 as [80.36, 80.36, 99.44, 90, 90, 120], 1G2X in space group C 1 2 1 as

[80.949, 80.572, 57.098, 90, 90.35, 90] , and 1FE5 in space group R32 as

[57.98, 57.98, 57.98, 92.02, 92.02, 92.02]. The primitive Niggli-reduced \mathbf{G}^6 $[r, s, t, u, v, w]$ vectors are:

$$1U4J: [3251.278, 3251.278, 3251.27, 44.826, 44.826, 44.826]$$

$$1G2X: [3260.182, 3261.147, 3261.147, 30.447, 28.234, 28.234]$$

$$1FE5: [3361.68, 3361.68, 3361.68, -236.987, -236.987, -236.987]$$

from which we compute the three \mathbf{DC}^7 vectors as

$$[r, s, t, s + t - |u|, r + t - |v|, r + s - |w|, r + s + t - |u| - |v| - |w| + 2\min(|u|, |v|, |w|)]$$

in the first two $+++$ cases and as

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

in the final $---$ case:

$$1\text{U4J: } [3251.278, 3251.278, 3251.278, 6457.73, 6457.73, 6457.73, 9709.008]$$

$$1\text{G2X: } [3260.182, 3261.147, 3261.147, 6491.847, 6493.095, 6493.095, 9752.029]$$

$$1\text{FE5: } [3361.68, 3361.68, 3361.68, 6486.373, 6486.373, 6486.373, 9374.079]$$

In each case the original primitive Niggli-reduced $\mathbf{G}^6 [r, s, t, u, v, w]$ vectors can be recovered by simply copying the first three elements of the unsorted \mathbf{DC}^7 vector, r, s, t then computing the three absolute values of u, v, w as the differences $s + t$ minus the fourth element of the unsorted \mathbf{DC}^7 vector, $r + t$ minus the fifth element of the unsorted \mathbf{DC}^7 vector, and $r + s$ minus the sixth element. What remains is to compute $\tau = r + s + t - |u| - |v| - |w|$ and compare it to the seventh element. If they are the same to within rounding error, as they are, indeed, for the 1FE5 case, then this is a $---$ case and the absolute values of u, v, w we have computed are the negatives of the actual values. Otherwise this is a $+++$ case. Completion of this example is left as an exercise to the reader, but to help in checking your work, the three values of τ are 9619.356, 9695.561, and 9374.079.

4.4. Example of the effect of Small Perturbations an F-centered Cell

A well-know example occurs for face-centered cubic lattices. Choosing an initial face-centered unit cell of $(10\sqrt{2}, 10\sqrt{2}, 10\sqrt{2}, 90, 90, 90)$, the primitive Niggli-reduced cell is $(10, 10, 10, 60, 60, 60)$. However, small changes in the original F-centered cell can change the primitive Niggli-reduced cell to $(10...., 10...., 10...., 90, 120, 120)$. The cells in Table 1 are all derived from F-centered $(14.14, 14.14, 14.14, 90, 120, 120)$

perturbing by 0.01% normal to the vector. The resulting unsorted \mathbf{DC}^7 vectors are given in Table 2.

While these look very different, when the differences are smoothed by permutations and gluing at boundaries, the distances among these cells are all small.

5. 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) and then applying equations (17) and (18) to the \mathbf{G}^6 descriptions of the boundaries. The manifold of Wigner-Seitz-reduced cells in unsorted \mathbf{DC}^7 is divided similarly to the way in which the manifold of Niggli-reduced cells is divided on the basis of whether $\tau < dc7_{usrt,7}$ for $+++$ or $\tau = dc7_{usrt,7}$ for $---$. The fifteen boundary polytopes are sufficient to then describe the primitive lattice characters, but, as with \mathbf{G}^6 , seven additional special-position subspaces are needed to fully describe some of the centered cases. See Andrews & Bernstein (2014) for a discussion of the special-position subspaces.

For consistency, we break from past tradition and use u, v, w for both the all-positive and all-negative cases rather than using $-u, -v, -w$ for the $---$ case.

Recall that in linear algebra an orthogonal projector P into a subspace S_{sub} of a space S is a symmetric matrix that maps any element $s \in S$ into an element $s_{sub} \in S_{sub}$ and satisfies $P^2 = P$. Orthogonal projectors are commonly just called "projectors". Note that $(I - Ps)$ is perpendicular to Ps for any projector Ps . Projec-

tors are often computed by *ad hoc* singular value decomposition (SVD). In this case they were computed by the column-space operations of the symbolic algebra package maxima, the open source version of DOE macsyms (Bogen, 1974)

5.1. Equal-cell-edge case

Recall that $r \leq s \leq t$ for Niggli-reduced cells. The first two boundaries are the equal-edge boundary cases. For both of these cases, the boundaries subdivide into one $---$ subcase and three $+++$ subcases, one for each of u , v , or w being minimal. Then at least one of $r + s + t + u - v - w$, $r + s + t - u + v - w$, or $r + s + t - u - v + w$ respectively is the minimal body diagonal.

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

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

$$dc7_{unsrt} \text{ subspace } 1 = [r, r, t, r + t - |u|, r + t - |v|, 2r - |w|,$$

$$2r + t - |u| - |v| - |w| + \min(\max(0, u), \max(0, v), \max(0, w))]$$

$$dc7_{unsrt} \text{ boundary } 1 \text{ --- projector } =$$

$$\begin{pmatrix} \frac{5}{14} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{5}{14} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 1 \text{ +++ minimal } u \text{ projector } =$$

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{4}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{-1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{5} & \frac{4}{5} & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} \\ 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{4}{5} & \frac{-1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{4}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{4}{5} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 1 + + + minimal v projector =

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{4}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{-1}{5} & \frac{4}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{4}{5} & \frac{1}{5} & \frac{-1}{5} \\ 0 & 0 & \frac{-1}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{4}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{4}{5} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 1 + + + minimal w projector =

$$\begin{pmatrix} \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} \\ \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 1 transforms =

$$- - - : [s, r, t, v + t + r, u + t + s, w + s + r, w + v + u + t + s + r]$$

$$+ + + : [s, r, t, -v + t + r, -u + t + s, -w + s + r, -w - v + 2\min(u, v, w) - u + t + s + r]$$

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

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

$$dc7_{unsrt} \text{ subspace } 2 = [r, s, s, 2s - |u|, r + s - |v|, r + s - |w|,$$

$$r + 2s - |u| - |v| - |w| + \min(\max(0, u), \max(0, v), \max(0, w))]$$

$$dc7_{unsrt} \text{ boundary } 2 \text{ --- projector } =$$

$$\begin{pmatrix} \frac{6}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 2 \text{ +++ minimal } u \text{ projector } =$$

$$\begin{pmatrix} \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 2 \text{ +++ minimal } v \text{ projector } =$$

$$\begin{pmatrix} \frac{4}{5} & 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{-1}{5} & 0 & 0 & \frac{4}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{1}{5} \\ \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{4}{5} & \frac{1}{5} & \frac{-1}{5} \\ \frac{-1}{5} & 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{4}{5} & \frac{1}{5} \\ \frac{1}{5} & 0 & 0 & \frac{-1}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{4}{5} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 2 \text{ } + + + \text{ minimal } w \text{ projector } =$$

$$\begin{pmatrix} \frac{4}{5} & 0 & 0 & \frac{-1}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{-1}{5} & 0 & 0 & \frac{4}{5} & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{-1}{5} & 0 & 0 & \frac{-1}{5} & \frac{4}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{4}{5} & \frac{-1}{5} \\ \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} & \frac{4}{5} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 2 \text{ transforms } =$$

$$- - - : [r, t, s, u + t + s, w + s + r, v + t + r, w + v + u + t + s + r]$$

$$+ + + : [r, t, s, -u + t + s, -w + s + r, -v + t + r, -w - v + 2\min(u, v, w) - u + t + s + r]$$

The special-position subspaces $\hat{1}$ and $\hat{2}$ are obtained by adding the constraints $1'$: $\{u = v\}$ and $2'$: $\{v = w\}$, respectively.

5.2. 90° case

The 90° case marks a possible transition between $- - -$ and $+ + +$. All the cells with a 90° angle are in $- - -$.

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

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

$$dc7_{unsrt} \text{ subspace } 3 = [r, s, t, s + t, r + t + v, r + s + w, r + s + t + v + w]$$

$$dc7_{unsrt} \text{ boundary } 3 \text{ projector } =$$

$$\begin{pmatrix} \frac{3}{4} & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{-1}{4} \\ 0 & \frac{2}{3} & \frac{-1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{-1}{3} & \frac{2}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{1}{4} & 0 & 0 & 0 & \frac{3}{4} & \frac{-1}{4} & \frac{1}{4} \\ \frac{1}{4} & 0 & 0 & 0 & \frac{-1}{4} & \frac{3}{4} & \frac{1}{4} \\ \frac{-1}{4} & 0 & 0 & 0 & \frac{1}{4} & \frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 3 transform =

$$[r, s, t, -u + t + s, v + t + r, w + s + r, w + v + 2\min(u, -v, -w) - u + t + s + r]$$

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

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

$$dc7_{unsrt} \text{ subspace 4} = [r, s, t, s + t + u, r + t, r + s + w, r + s + t + u + w]$$

$dc7_{unsrt}$ boundary 4 projector =

$$\begin{pmatrix} \frac{2}{3} & 0 & \frac{-1}{3} & 0 & \frac{1}{3} & 0 & 0 \\ 0 & \frac{3}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & \frac{-1}{4} \\ \frac{-1}{3} & 0 & \frac{2}{3} & 0 & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{4} & 0 & \frac{3}{4} & 0 & \frac{-1}{4} & \frac{1}{4} \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{2}{3} & 0 & 0 \\ 0 & \frac{1}{4} & 0 & \frac{-1}{4} & 0 & \frac{3}{4} & \frac{1}{4} \\ 0 & \frac{-1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & \frac{3}{4} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 4 transform =

$$[r, s, t, u + t + s, -v + t + r, w + s + r, w - v + u + 2\min(-u, v, -w) + t + s + r]$$

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

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

$$dc7_{unsrt} \text{ subspace 5} = [r, s, t, s + t + u, r + t + v, r + s, r + s + t + u + v]$$

$dc7_{unsrt}$ boundary 5 projector =

$$\begin{pmatrix} \frac{2}{3} & \frac{-1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 \\ \frac{-1}{3} & \frac{2}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{3}{4} & \frac{1}{4} & \frac{1}{4} & 0 & \frac{-1}{4} \\ 0 & 0 & \frac{1}{4} & \frac{3}{4} & \frac{-1}{4} & 0 & \frac{1}{4} \\ 0 & 0 & \frac{1}{4} & \frac{-1}{4} & \frac{3}{4} & 0 & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & \frac{-1}{4} & \frac{1}{4} & \frac{1}{4} & 0 & \frac{3}{4} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 5 transform =

$$[r, s, t, u+t+s, v+t+r, -w+s+r, -w+v+u+2\min(-u, -v, w)+t+s+r]$$

In each ninety-degree case, the special-position subspace consists of $\hat{3}, \hat{4}, \hat{5} : \{u = v = w = 0\}$, *i.e.* the primitive orthorhombic case, and we take $3' : \{v = w = 0\}$, $4' : \{u = w = 0\}$, and $5' : \{u = v = 0\}$.

5.3. 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 than the Niggli-reduced cell edges.

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace 6} = [r, s, t, t, r+t-v, r+s-w, r+t-v+w], v \geq w > 0$$

$dc7_{unsrt}$ boundary 6 projector =

$$\begin{pmatrix} \frac{4}{5} & \frac{-1}{5} & 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{-1}{5} & \frac{4}{5} & 0 & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{-1}{5} & \frac{-1}{5} & 0 & 0 & \frac{4}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{4}{5} & \frac{-1}{5} \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{-1}{5} & \frac{4}{5} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 6 transform =

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

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace } 7 = [r, s, t, t, r + t - v, r + s - w, r + t + v - w], w > v > 0$$

$dc7_{unsrt}$ boundary 7 projector =

$$\begin{pmatrix} \frac{6}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{5}{14} & \frac{5}{14} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 7 transform =

$$[r, s, -u+t+s, t, -w+v-u+t+s+r, -w+s+r, -2*w+v+2*min(2*s-u, w, w-v)+t+r]$$

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

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

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

$$\text{equivalent to } dc7_{unsrt,3} = dc7_{unsrt,4}.$$

$$dc7_{unsrt} \text{ subspace } 8 = [r, s, t, t, r+t+v, r+s+w, r+t+v+w], v, w \leq 0$$

$$dc7_{unsrt} \text{ boundary } 8 \text{ projector } =$$

$$\begin{pmatrix} \frac{4}{5} & \frac{-1}{5} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} \\ \frac{-1}{5} & \frac{4}{5} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & \frac{4}{5} & \frac{-1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & 0 & 0 & \frac{-1}{5} & \frac{4}{5} & \frac{1}{5} \\ \frac{-1}{5} & \frac{-1}{5} & 0 & 0 & \frac{1}{5} & \frac{1}{5} & \frac{4}{5} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary } 8 \text{ transform } =$$

$$[r, s, u+t+s, t, w+v+u+t+s+r, w+s+r, 2w+v+2*min(u+2*s, -w-v, -w)+t+r]$$

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace } 9 = [r, s, t, s+t-u, t, r+s-w, s+t-u+w], 0 < w \leq u$$

$$dc7_{unsrt} \text{ boundary } 9 \text{ projector } =$$

$$\begin{pmatrix} \frac{4}{5} & \frac{-1}{5} & 0 & \frac{-1}{5} & 0 & \frac{1}{5} & \frac{1}{5} \\ \frac{-1}{5} & \frac{4}{5} & 0 & \frac{-1}{5} & 0 & \frac{1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{-1}{5} & \frac{-1}{5} & 0 & \frac{4}{5} & 0 & \frac{1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & \frac{1}{5} & 0 & \frac{4}{5} & \frac{-1}{5} \\ \frac{1}{5} & \frac{1}{5} & 0 & \frac{1}{5} & 0 & \frac{-1}{5} & \frac{4}{5} \end{pmatrix}$$

$dc7_{unsrt}$ boundary 9 transform =

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

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace A} = [r, s, t, s + t - u, t, r + s - w, s + t + u - w], 0 < u < w$$

$dc7_{unsrt}$ boundary A projector =

$$\begin{pmatrix} \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$dc7_{unsrt}$ boundary A transform =

$$[r, s, -v+t+r, -w-v+u+t+s+r, t, -w+s+r, -2w+2\min(2r-v, w, w-u)+u+t+s]$$

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

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

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

$$\text{equivalent to } dc7_{unsrt,3} = dc7_{unsrt,5}.$$

$$dc7_{unsrt} \text{ subspace B} = [r, s, t, s+t+u, t, r+s+w, s+t+u+w], u, w \leq 0$$

$$dc7_{unsrt} \text{ boundary B projector} =$$

$$\begin{pmatrix} \frac{4}{5} & \frac{-1}{5} & 0 & \frac{1}{5} & 0 & \frac{1}{5} & \frac{-1}{5} \\ \frac{-1}{5} & \frac{4}{5} & 0 & \frac{1}{5} & 0 & \frac{1}{5} & \frac{-1}{5} \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & \frac{4}{5} & 0 & \frac{-1}{5} & \frac{1}{5} \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{5} & \frac{1}{5} & 0 & \frac{-1}{5} & 0 & \frac{4}{5} & \frac{1}{5} \\ \frac{-1}{5} & \frac{-1}{5} & 0 & \frac{1}{5} & 0 & \frac{1}{5} & \frac{4}{5} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary B transform} =$$

$$[r, s, v+t+r, w+v+u+t+s+r, t, w+s+r, 2w+2\min(v+2*r, -w-u, -w)+u+t+s]$$

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace C} = [r, s, t, s+t-u, r+t-v, s, s+t-u+v], 0 < v \leq u$$

$$dc7_{unsrt} \text{ boundary C projector} =$$

$$\begin{pmatrix} \frac{4}{5} & 0 & \frac{-1}{5} & \frac{-1}{5} & \frac{1}{5} & 0 & \frac{1}{5} \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ \frac{-1}{5} & 0 & \frac{4}{5} & \frac{-1}{5} & \frac{1}{5} & 0 & \frac{1}{5} \\ \frac{-1}{5} & 0 & \frac{-1}{5} & \frac{4}{5} & \frac{1}{5} & 0 & \frac{1}{5} \\ \frac{1}{5} & 0 & \frac{1}{5} & \frac{1}{5} & \frac{4}{5} & 0 & \frac{-1}{5} \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ \frac{1}{5} & 0 & \frac{1}{5} & \frac{1}{5} & \frac{-1}{5} & 0 & \frac{4}{5} \end{pmatrix}$$

$dc7_{unsrt}$ boundary C transform =

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

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

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

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

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

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

$$dc7_{unsrt} \text{ subspace D} = [r, s, t, s + t - u, r + t - v, s, s + t + u - v], 0 < u < v$$

$dc7_{unsrt}$ boundary D projector =

$$\begin{pmatrix} \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{5}{14} & \frac{-1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} \\ \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} \end{pmatrix}$$

$dc7_{unsrt}$ boundary D transform =

$$[r, -w + s + r, t, -w - v + u + t + s + r, -v + t + r, s, 2\min(v, v - u, 2r - w) - 2v + u + t + s]$$

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

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

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

$$\text{equivalent to } dc7_{unsrt,2} = dc7_{unsrt,6}.$$

$$dc7_{unsrt} \text{ subspace E} = [r, s, t, s+t+u, r+t+v, s, s+t+u+v], u, v \leq 0$$

$$dc7_{unsrt} \text{ boundary E projector} =$$

$$\begin{pmatrix} \frac{4}{5} & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} & 0 & \frac{-1}{5} \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ \frac{-1}{5} & 0 & \frac{4}{5} & \frac{1}{5} & \frac{1}{5} & 0 & \frac{-1}{5} \\ \frac{1}{5} & 0 & \frac{1}{5} & \frac{4}{5} & \frac{-1}{5} & 0 & \frac{1}{5} \\ \frac{1}{5} & 0 & \frac{1}{5} & \frac{-1}{5} & \frac{4}{5} & 0 & \frac{1}{5} \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ \frac{-1}{5} & 0 & \frac{-1}{5} & \frac{1}{5} & \frac{1}{5} & 0 & \frac{4}{5} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary E transform} =$$

$$[r, w+s+r, t, w+v+u+t+s+r, v+t+r, s, 2v+2\min((-v)-u, -v, w+2*r)+u+t+s]$$

The special-position subspaces of the face-diagonal boundary polytopes 6, 8, 9, B, C and E are empty because such a special position would require a common point in the all acute $+++$ and all obtuse $---$ cases, but they only meet at the axial planes of the u, v, w subspace, which are excluded from the all acute $+++$ cases. For cases 7, A and D there are non-trivial special-position subspaces. An invariant point in case 7 would have to satisfy $v = w - v$ or $v = w/2$. Thus we define $7' : \{v = w/2\}$ and similarly define $A' : \{u = w/2\}$ and $D' : \{u = v/2\}$.

5.4. Body-diagonal case

Recall that $t \leq r + s + t + u + v + w$ 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 $- - -$.

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

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

$$dc7_{unsrt} \text{ subspace F} = [r, s, t, s + t + u, r + t + v, -u - v, t], u, v \leq 0$$

$$dc7_{unsrt} \text{ boundary F projector} =$$

$$\begin{pmatrix} \frac{6}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{5}{14} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{-1}{7} & \frac{1}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{-1}{7} & \frac{-1}{7} & \frac{6}{7} & \frac{1}{7} \\ \frac{-1}{7} & \frac{-1}{7} & \frac{5}{14} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{5}{14} \end{pmatrix}$$

$$dc7_{unsrt} \text{ boundary F transform} =$$

$$[r, s, w + v + u + t + s + r, v + t + r, u + t + s, w + s + r, t]$$

In order to have a special-position subspace in case F, in addition to $r + s + t + u + v + w = t$, we need $u = -2s - u - w$ and $v = -2r - v - w$. From this we have $2s + 2u = -w = 2r + 2v$. Then it follows that $F': \{r - s - u + v = 0\}$. This is equivalent to $\|\vec{a} + \vec{c}\| = \|\vec{b} + \vec{c}\|$, *i.e.* the shorter b-face-diagonal is the same length as the shorter a-face-diagonal.

The unsorted \mathbf{DC}^7 subspace descriptions of the non-anorthic lattice characters derived from the \mathbf{G}^6 subspace descriptions given in Table 4 in Andrews & Bernstein (2014) are given in Tables 7 and 8 by applying equations (17) and (18). Except for

three of the monoclinic cases, 55A, 55B and 57C, the boundary polytopes from \mathbf{G}^6 fully describe those for unsorted \mathbf{DC}^7 . In those three cases, the boundary is divided between $0 < u \leq r$ and $r < u \leq s$ with two different forms each for $dc7_{unsrt,7}$, the minimum body diagonal. Such divided boundaries due to overlapping inequalities are encountered in Niggli reduction even when working just in \mathbf{G}^6 , and just as in those cases, this adds combinatorial complexity that needs to be allowed for in distance calculations.

6. 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

$$\begin{aligned}
 dc7_{unsrt_dist}(dc7_1, dc7_2) = \min(\\
 & ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,3}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}] \\
 & - [dc7_{2,1}, dc7_{2,2}, dc7_{2,3}, dc7_{2,4}, dc7_{2,5}, dc7_{2,6}, dc7_{2,7}]||, \\
 & ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}] \\
 & - [dc7_{2,1}, dc7_{2,3}, dc7_{2,2}, dc7_{2,4}, dc7_{2,6}, dc7_{2,5}, dc7_{2,7}]||, \\
 & ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}] \\
 & - [dc7_{2,2}, dc7_{2,1}, dc7_{2,3}, dc7_{2,5}, dc7_{2,4}, dc7_{2,6}, dc7_{2,7}]||, \\
 & ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}] \\
 & - [dc7_{2,2}, dc7_{2,3}, dc7_{2,1}, dc7_{2,5}, dc7_{2,6}, dc7_{2,4}, dc7_{2,7}]||, \\
 & ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}]
 \end{aligned}$$

$$\begin{aligned}
& -[dc7_{2,3}, dc7_{2,1}, dc7_{2,2}, dc7_{2,6}, dc7_{2,4}, dc7_{2,5}, dc7_{2,7}||], \\
& ||[dc7_{1,1}, dc7_{1,2}, dc7_{1,2}, dc7_{1,4}, dc7_{1,5}, dc7_{1,6}, dc7_{1,7}] \\
& -[dc7_{2,3}, dc7_{2,2}, dc7_{2,1}, dc7_{2,6}, dc7_{2,5}, dc7_{2,4}, dc7_{2,7}||].
\end{aligned}$$

These cases are simple because cases 1 and 2 do not impact the seventh element. In the general case, *e.g.* a boundary transform, rather than a simple Niggli-reduced cell-edge permutation, a fresh Niggli reduction may be needed to regenerate the seventh element for minimal distance calculations.

7. 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 4 as edges and angles, in Table 5 as $\mathbf{G}^6 [r, s, t, u, v, w]$, and in Table 6 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 the 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 . In order to compute the cells in Table 6 the components at the face-diagonal boundaries were reduced in magnitude by 0.01 to prevent the Niggli reduction from changing all the examples to be identical. The differences among the unsorted \mathbf{DC}^7 cells are consistent with the perturbation.

8. 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 .

Acknowledgements

Our thanks to Frances C. Bernstein for careful copy-editing and helpful suggestions. Our thanks to Elizabeth Kincaid for the timeline figure.

Work supported in part by US Dept. of Energy, Office of Science, DOE Office of Biological and Environmental Research, grant KP1607011 and DOE Office of Basic Energy Sciences Program, contract DE-SC0012704, US NIH National Institute of General Medical Sciences P30GM133893, U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI).

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Table 1. *Cells derived from F-centered [14.14, 14.14, 14.14, 90, 90, 90] perturbing by 0.01% normal to the respective Selling vector and scaling a to 10. These are the primitive*

Niggli-reduced cells. They are sorted with alpha increasing.

| | | | | | | |
|---|--------|--------|--------|---------|---------|---------|
| P | 10.000 | 10.000 | 10.003 | 60.010 | 60.038 | 89.977 |
| P | 10.000 | 10.003 | 10.008 | 60.017 | 89.961 | 60.031 |
| P | 10.000 | 10.006 | 10.008 | 60.025 | 60.046 | 60.101 |
| P | 10.000 | 10.002 | 10.009 | 60.039 | 60.057 | 60.082 |
| P | 10.000 | 10.002 | 10.006 | 60.041 | 60.028 | 60.102 |
| P | 10.000 | 10.001 | 10.004 | 60.047 | 60.050 | 60.016 |
| P | 10.000 | 10.003 | 10.006 | 60.049 | 60.036 | 60.025 |
| P | 10.000 | 10.000 | 10.008 | 60.049 | 60.051 | 60.030 |
| P | 10.000 | 10.001 | 10.002 | 60.049 | 60.059 | 60.047 |
| P | 10.000 | 10.005 | 10.008 | 60.052 | 60.048 | 60.076 |
| P | 10.000 | 10.002 | 10.004 | 89.997 | 60.032 | 60.026 |
| P | 10.000 | 10.001 | 10.008 | 90.018 | 119.955 | 119.980 |
| P | 10.000 | 10.001 | 10.004 | 90.019 | 119.984 | 119.941 |
| P | 10.000 | 10.005 | 10.006 | 90.051 | 119.942 | 119.972 |
| P | 10.000 | 10.006 | 10.007 | 90.074 | 119.940 | 119.951 |
| P | 10.000 | 10.001 | 10.003 | 119.938 | 119.984 | 90.024 |
| P | 10.000 | 10.005 | 10.005 | 119.968 | 119.978 | 90.011 |
| P | 10.000 | 10.000 | 10.006 | 119.971 | 90.032 | 119.963 |
| P | 10.000 | 10.009 | 10.012 | 119.981 | 90.022 | 119.949 |
| P | 10.000 | 10.010 | 10.011 | 119.990 | 90.007 | 119.947 |

Table 2. *unsorted \mathbf{DC}^7 vectors from the cells in Table 1.*

| r | s | t | $s + t - u $ | $r + t - v $ | $r + s - w $ | $r + s + t - u - v - w + 2 * \max(0, \min(u, v, w))$ |
|---------|---------|---------|---------------|---------------|---------------|--|
| 100.000 | 100.006 | 100.054 | 100.060 | 100.141 | 199.927 | 100.147 |
| 100.000 | 100.056 | 100.154 | 100.157 | 200.017 | 100.123 | 100.224 |
| 100.000 | 100.119 | 100.164 | 100.216 | 100.221 | 100.367 | 100.273 |
| 100.000 | 100.044 | 100.181 | 100.230 | 100.263 | 100.269 | 100.312 |
| 100.000 | 100.046 | 100.119 | 100.206 | 100.145 | 100.333 | 100.232 |
| 100.000 | 100.016 | 100.078 | 100.189 | 100.190 | 100.057 | 100.230 |
| 100.000 | 100.054 | 100.118 | 100.234 | 100.167 | 100.104 | 100.271 |
| 100.000 | 100.000 | 100.152 | 100.224 | 100.232 | 100.090 | 100.304 |
| 100.000 | 100.020 | 100.036 | 100.178 | 100.197 | 100.152 | 100.309 |
| 100.000 | 100.108 | 100.168 | 100.295 | 100.228 | 100.285 | 100.355 |
| 100.000 | 100.013 | 100.160 | 200.109 | 100.217 | 100.067 | 100.221 |
| 100.000 | 100.031 | 100.072 | 200.092 | 100.133 | 100.094 | 100.228 |
| 100.000 | 100.017 | 100.088 | 200.037 | 100.091 | 100.187 | 100.211 |
| 100.000 | 100.107 | 100.130 | 200.058 | 100.240 | 100.137 | 100.199 |
| 100.000 | 100.118 | 100.143 | 200.004 | 100.252 | 100.209 | 100.203 |
| 100.000 | 100.014 | 100.055 | 100.221 | 100.076 | 199.930 | 100.159 |
| 100.000 | 100.090 | 100.108 | 100.195 | 100.120 | 200.050 | 100.167 |
| 100.000 | 100.000 | 100.125 | 100.150 | 200.014 | 100.112 | 100.152 |
| 100.000 | 100.179 | 100.242 | 100.269 | 200.167 | 100.243 | 100.258 |
| 100.000 | 100.202 | 100.227 | 100.246 | 200.202 | 100.263 | 100.280 |

Table 3. *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 : | \mathbf{r} | \mathbf{s} | \mathbf{t} | \mathbf{u} | \mathbf{v} | \mathbf{w} |
|------------------|--------------|--------------|--------------|--------------|--------------|--------------|
| i | 6 | 8 | 10 | 8 | 4 | 2 |
| ii | 6 | 8 | 10 | -6 | -2 | -4 |

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

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

Table 4. *Gruber (1973) example of five-fold alternative Buerger-reduced cells for a lattice as*
 $[a, b, c, \alpha, \beta, \gamma]$

| cell | <i>a</i> | <i>b</i> | <i>c</i> | α | β | γ |
|------|----------|----------|----------|----------|---------|----------|
| i | 2 | 4 | 4 | 60.00 | 79.19 | 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 5. *Gruber (1973) example of five-fold alternative Buerger-reduced cells for a lattice as*
 $\mathbf{G}^6 [r, s, t, u, v, w]$.

| cell | <i>r</i> | <i>s</i> | <i>t</i> | <i>u</i> | <i>v</i> | <i>w</i> | boundary |
|------|----------|----------|----------|----------|----------|----------|----------|
| 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 6. *Gruber (1973) example of five-fold alternative Buerger-reduced cells for a lattice as unsorted \mathbf{DC}^7 . To avoid the case where all the cells reduce to the same Niggli-reduced cell, a small perturbation of .01 was applied to entries *u* or *w* in ii – v so that the vector did not sit precisely on the relevant boundaries.*

| 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 |

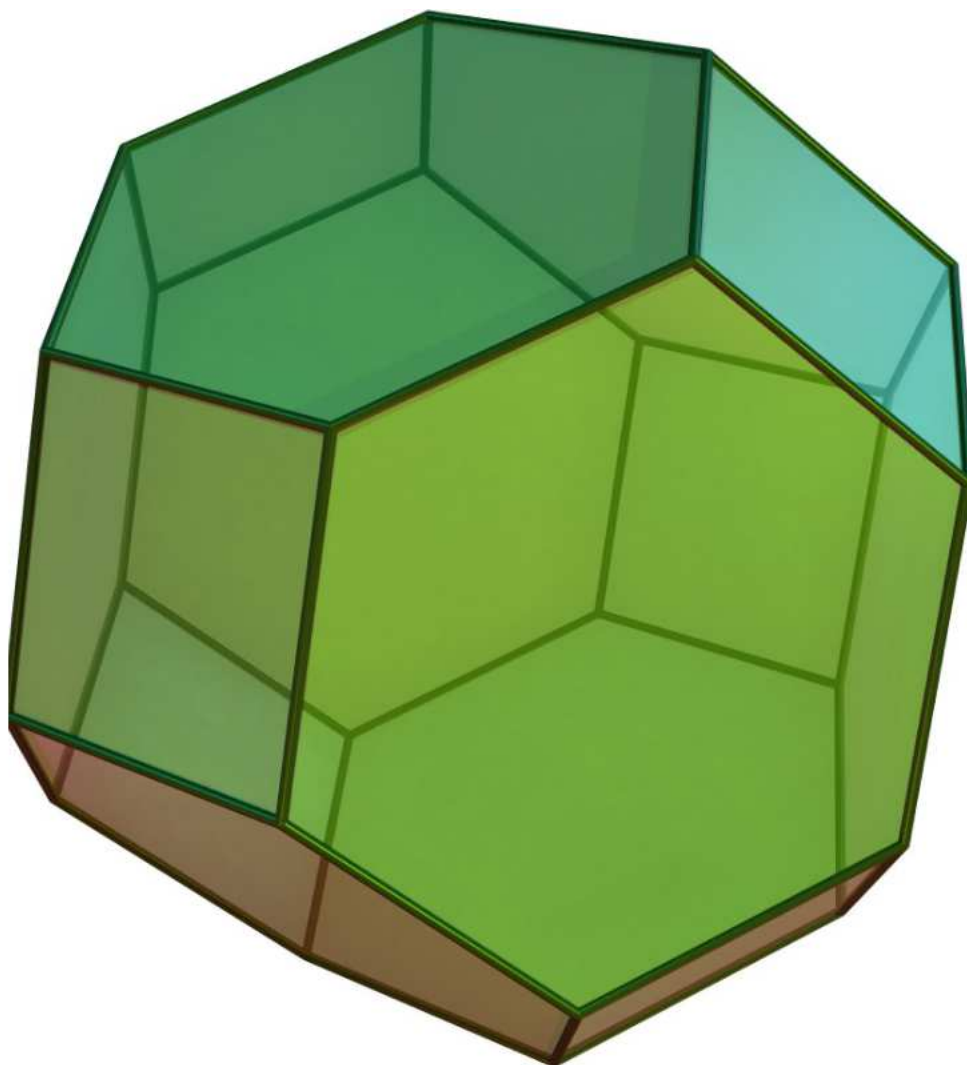


Fig. 1. Truncated octahedron (Wikipedia, 2017). Image licensed under the Creative Commons Attribution-Share Alike 3.0 Unported license. Subject to disclaimers. See web site.

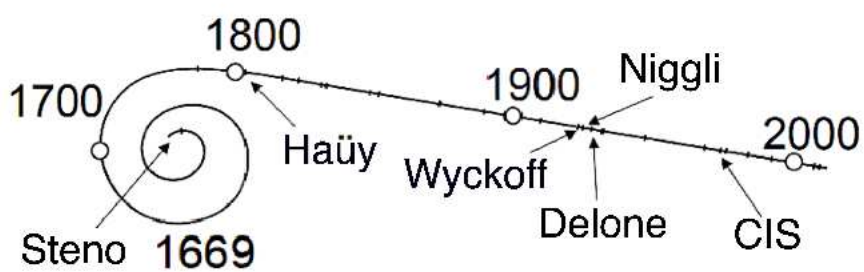


Fig. 2. Historical timeline of studies of crystallographic lattice characterization. Figure drawn by E. Kincaid. Used with permission of the artist.

Table 7. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type, unsorted DC⁷ subspace, boundary polytope. Note that the variables r , s and t are non-negative, and u , v and w may be positive, negative or zero as constrained below.*

| Roof/ Niggli Symbol | IT Lattice Char | Bravais Lattice Type | Unsorted DC ⁷ Subspace | Bound- ary Polytope |
|---------------------------|-----------------------|----------------------------|---|---|
| 44A | 3 | cP | $(r, r, r, 2r, 2r, 2r, 3r)$ | $12345 = 12\hat{3} = 12\hat{4} = 12\hat{5}$ |
| 44C | 1 | cF | $(r, r, r, r, r, 2r)$ | 12679ACD |
| 44B | 5 | cI | $(r, r, r, 4r/3, 4r/3, 4r/3, r)$ | $12F2'F' = 12\hat{F}$ |
| 45A | 11 | tP | $(r, r, t, r + t, r + t, 2r, 2r + t)$ | $1345 = 1\hat{3} = 1\hat{4} = 1\hat{5}$ |
| 45B | 21 | tP | $(r, s, s, 2s, r + s, r + s, r + 2s)$ | $2345 = 2\hat{3} = 2\hat{4} = 2\hat{5}$ |
| 45D | 6 | tI | $(r, r, r, r - w/2, r - w/2, 2r + w, r),$ $-r \leq w \leq 0$ | $12FF' = 12\hat{F}$ |
| 45D | 7 | tI | $[r, r, r, 2 * r + u, r - u/2, r - u/2, r],$ $-r \leq u \leq 0$ | $12F2' = 12\hat{F}$ |
| 45C | 15 | tI | $(r, r, t, t, t, 2r, t)$ | 158BF |
| 45E | 18 | tI | $(r, s, s, -r/2 + 2s, s, s, -r/2 + 2s)$ | $2ADA' = 2\hat{A}\hat{D}$ |
| 48A | 12 | hP | $(r, r, t, r + t, r + t, r, r + t)$ | 134E |
| 48B | 22 | hP | $(r, s, s, s, r + s, r + s, r + s)$ | 2458 |
| 49C | 2 | hR | $(r, r, r, 2r - u, 2r - u, 2r - u, 3r - u),$ $0 < u \leq r$ | $121'2' = \hat{1}\hat{2}$ |
| 49D | 4 | hR | $(r, r, r, 2r + u, 2r + u, 2r + u, 3r + 3u),$ $-r \leq u \leq 0$ | $121'2' = \hat{1}\hat{2}$ |
| 49B | 9 | hR | $(r, r, t, t, t, r, r + t)$ | 1679ACD |
| 49E | 24 | hR | $(r, s, s, s + r/3, s + r/3, s + r/3, s)$ | $2F2'F' = 2\hat{F}$ |
| 50C | 32 | oP | $(r, s, t, s + t, r + t, r + s, r + s + t)$ | $345 = \hat{3} = \hat{4} = \hat{5}$ |
| 50D | 13 | oC | $(r, r, t, r + t, r + t, 2r + w, 2r + t + w),$ $-r \leq w \leq 0$ | 134 |
| 50E | 23 | oC | $(r, s, s, u + 2 * s, s + r, s + r, u + 2 * s + r),$ $-s \leq u \leq 0$ | 245 |
| 50A | 36 | oC | $(r, s, t, s + t, t, r + s, s + t)$ | 35B |
| 50B | 38 | oC | $(r, s, t, s + t, r + t, s, s + t)$ | 34E |
| 50F | 40 | oC | $[r, s, t, t, r + t, r + s, r + t)$ | 458 |
| 51A | 16 | oF | $(r, r, s, r + s + u, r + s + u, -2u, s),$ $-r \leq u \leq 0$ | $1F1' = \hat{1}F$ |
| 51B | 26 | oF | $(r, s, t, -r/2 + s + t, t, s, -r/2 + s + t)$ | $ADA' = \hat{A}\hat{D}$ |
| 52A | 8 | oI | $(r, r, r, 2r + u, 2r + v, -u - v, r),$ $-r \leq u \leq 0, -r \leq v \leq 0$ | 12F |
| 52B | 19 | oI | $(r, s, s, 2s - u, s, s, -r + 2s + u),$ $0 < u \leq r$ | |
| | | | $(r, s, s, 2s - u, s, s, r + 2s - u),$ $r < u \leq s$ | 29C = 2AD |
| 52C | 42 | oI | $r, s, t, t, t, r + s, t$ | 58BF |

Table 8. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type, unsorted DC⁷ subspace, boundary polytope, continued. Note that the variables r , s and t are non-negative, and u , v and w may be positive, negative or zero as constrained below.*

| Roof/ Niggli Symbol | IT Lattice Char | Bravais Lattice Type | Unsorted DC ⁷ Subspace | Bound- ary Polytope |
|---------------------------|-----------------------|----------------------------|--|---------------------------|
| 53A | 33 | mP | $(r, s, t, t + s, v + t + r, s + r, v + t + s + r),$ $-r \leq v \leq 0$ | 35 |
| 53B | 35 | mP | $(r, s, t, u + t + s, t + r, s + r, u + t + s + r),$ $-r \leq u \leq 0$ | 45 |
| 53C | 34 | mP | $(r, s, t, t + s, t + r, w + s + r, w + t + s + r), 4$ $-r \leq w \leq 0$ | 34 |
| 55A | 10, 14 | mC | $(r, r, t, t + r - u, t + r - u, 2r - w,$ $t + 2r - w), 0 < u \leq w \leq r$ | $11' = \hat{1}$ |
| 57B | 17 | mC | $(r, r, t, t + r - u, t + r - u, 2r - w,$ $t + 2r - 2u + w), 0 < w < u \leq r$ | |
| 55B | 20, 25 | mC | $(r, r, t, u + t + r, v + t + r, -u - v, t),$ $-r \leq u \leq 0$ | 1F |
| 57C | 27 | mC | $(r, s, s, 2s - u, s + r - v, s + r - v,$ $2s + r + u - 2v), -s \leq u \leq v \leq 0$ | $22' = \hat{2}$ |
| | | | $(r, s, s, 2s - u, s + r - v, s + r - v,$ $2s + r - u), -r \leq v < u \leq 0$ | |
| | | | $(r, s, s, 2s - u, s, s, -r + 2s + u)$ $0 < u \leq r$ | 9C = AD |
| | | | $(r, s, s, 2s - u, s, s, r + 2s - u)$ $r < u \leq s$ | |
| 56A | 28 | mC | $(r, s, t, t + s - u, t, s + r - 2u, t + s - u)$ $0 < u \leq r$ | $AA' = \hat{A}$ |
| 56C | 29 | mC | $(r, s, t, t + s - u, t + r - 2u, s, t + s - u)$ $0 < u \leq r$ | $DD' = \hat{D}$ |
| 56B | 30 | mC | $(r, s, t, t, t + r - v, s + r - 2v, +t - v) + r)$ $0 < v \leq r$ | $77' = \hat{7}$ |
| 54C | 37 | mC | $(r, s, t, t + s + u, t, s + r, t + s + u), -r \leq u \leq 0$ | 5B |
| 54A | 39 | mC | $(r, s, t, t + s + u, t + r, s, t + s + u), -r \leq u \leq 0$ | 4E |
| 54B | 41 | mC | $(r, s, t, t, v + t + r, s + r, v + t + r),$ $-r \leq v \leq 0;$ | 58 |
| 57A | 43 | mC | $(r, s, t, t - w/2, t - w/2, w + s + r, t),$ $-r \leq w \leq 0$ | $FF' = \hat{F}$ |

Synopsis

Starting from a Niggli-reduced cell, a crystallographic lattice may be characterized by seven parameters describing the Dirichlet cell: the three shortest non-coplanar lattice vector 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.