Delaunay Reducing a Niggli Reduced Cell

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1. Notation

- {...} an unordered ensemble
- [...] an ordered list

2. Delaunay Reduction

Given three cell edge vectors $\vec{a}$, $\vec{b}$, $\vec{c}$, that cell is called Delaunay-reduced if the four vectors (the Delaunay tetrahedron(Delaunay, 1933)) $\vec{a}$, $\vec{b}$, $\vec{c}$, $-\vec{a}-\vec{b}-\vec{c}$, numbered 1 through 4, all form right angles or obtuse angles relative to one another. In terms of G^6, (Andrews & Bernstein, 1988) given a cell described by a $[g_1, g_2, g_3, g_4, g_5, g_6]$, converting from the P, Q, R, S, T, U or $s_{23}, s_{13}, s_{12}, s_{14}, s_{24}, s_{34}$ notation for the inner products of (Henry & Lonsdale, 1952), based on (Ito, 1950) and (Delaunay, 1933), the six doubled inner products among the Delaunay tetrahedron vectors are:

$$2P = 2\vec{b}.\vec{c} = 2s_{23} = g_4 \tag{2.1}$$

$$2Q = 2\vec{a}.\vec{c} = 2s_{13} = g_5 \tag{2.2}$$

$$2R = 2\vec{a}.\vec{b} = 2s_{12} = g_6 \tag{2.3}$$

$$2S = 2\vec{a}.(-\vec{a} - \vec{b} - \vec{c}) = -2\vec{a}.\vec{a} - 2\vec{a}.\vec{b} - 2\vec{a}.\vec{c} = 2s_{14} = -2g_1 - g_6 - g_5 \tag{2.4}$$

$$2T = \vec{b}.(-\vec{a} - \vec{b} - \vec{c}) = -2\vec{b}.\vec{a} - 2\vec{b}.\vec{b} - 2\vec{b}.\vec{c} = 2s_{24} - g_6 - 2g_2 - g_4 \tag{2.5}$$

$$2U = 2\vec{c}.(-\vec{a} - \vec{b} - \vec{c}) = -2\vec{c}.\vec{a} - 2\vec{c}.\vec{b} - 2\vec{c}.\vec{c} = 2s_{34} = -g_5 - g_4 - 2g_3 \tag{2.6}$$

For a Delaunay-reduced cell all of expressions 2.1 through 2.6 must be zero or negative.

(**?**) used a slightly different notation and presented a very efficient algorithm for Delaunay-reduction.

3. The Niggli Conditions

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

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

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

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

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

$$\text{require } 0 \leqslant g_1 \leqslant g_2 \leqslant g_3$$

$$\text{if } g_2 = g_3, \text{then require } |g_5| \leqslant |g_6|$$

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

$$\text{or require } \{g_4 \leqslant 0 \text{ and } g_5 \leqslant 0 \text{ and } g6 \leqslant 0\}$$

$$\text{require } |g_4| \leqslant g_2$$

$$\text{require } |g_5| \leqslant g_1$$

$$\text{require } |g_6| \leqslant g_1$$

$$\text{require } g_3 \leqslant g_1 + g_2 + g_3 + g_4 + g_5 + g_6$$

$$\text{if } g_4 = g_2, \text{then require } g_6 \leqslant 2g_5$$

$$\text{if } g_5 = g_1, \text{then require } g_6 \leqslant 2g_4$$

$$\text{if } g_6 = g_1, \text{then require } g_5 \leqslant 2g_4$$

$$\text{if } g_4 = -g_2, \text{then require } g_6 = 0$$

$$\text{if } g_5 = -g_1, \text{then require } g_6 = 0$$

$$\text{if } g_6 = -g_1, \text{then require } g_5 = 0$$

$$\text{if } g_3 = g_1 + g_2 + g_3 + g_4 + g_5 + g_6, \text{then require } 2g_1 + 2g_5 + g_6 \leqslant 0$$

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

4. Converting from the $\boldsymbol{G}^6$ or $\boldsymbol{E}^3$ representation of a Niggli-reduced cell to Delaunay-reduced

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

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

$$g_1 \leqslant g_2 \leqslant g_3$$

$$|g_4| \leqslant g_2 \leqslant g_3$$

$$|g_5| \leqslant g_1 \leqslant g_2 \leqslant g_3$$

$$|g_6| \leqslant g_1 \leqslant g_2 \leqslant g_3$$

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

4.1. The Niggli-reduced $---$ case

If we have $g_{\{4,5,6\}}$ all less than or equal to zero, examine each element of expressions 2.1 through 2.6:

$$g_6 \leqslant 0$$

$$g_5 \leqslant 0$$

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

$$g_4, \leqslant 0$$

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

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

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

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

$$-g_2 \leqslant g_4 \leqslant 0$$

$$-g_1 \leqslant g_5 \leqslant 0$$

$$-g_1 \leqslant g_6 \leqslant 0$$

4.2. The Niggli-reduced $+++$ cases

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

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

$$0 \leqslant g_4 \leqslant g_2$$

$$0 \leqslant g_5 \leqslant g_1$$

$$0 \leqslant g_6 \leqslant g_1$$

One of $g_{\{4,5,6\}}$ is smallest.

4.2.1. The Niggli-reduced $+++$, g_6 smallest case Suppose $g_6 \leqslant g_4$, $g_6 \leqslant g_5$. In this case consider the Delaunay tetrahedron

$$\vec{a},\ \ -\vec{b},\ \ -\vec{c}+\vec{b},\ \ \vec{c}-\vec{a} \tag{4.1}$$

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

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

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

which are $---$ vectors in this case, and the elements of expressions 2.1 through 2.6

are

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

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

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

4.2.2. The Niggli-reduced $+++$, g_5 smallest case Suppose $g_5 \leqslant g_4$, $g_5 \leqslant g_6$. In this case consider the Delaunay tetrahedron

$$\vec{a},\ \ \vec{b}-\vec{a},\ \ -\vec{c},\ \ \vec{c}-\vec{b} \tag{4.2}$$

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

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

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

which are $---$ vectors in this case, and the elements of expressions 2.1 through 2.6

are

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

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

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

4.2.3. The Niggli-reduced $+++$, g_4 smallest case Suppose $g_4 \leqslant g_5$, $g_4 \leqslant g_6$. In this case consider the Delaunay tetrahedron

$$\vec{b}-\vec{a},\ \ -\vec{b},\ \ \vec{c},\ \ \vec{a}-\vec{c} \tag{4.3}$$

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

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

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

which are $---$ vectors in this case, and the elements of expressions 2.1 through 2.6

are

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

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

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

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

5. The effects of perturbations

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

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

will use the additive face and body diagonals

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

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

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

6. The 7-Dimensional Delaunay Space $\boldsymbol{D}^7$

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

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

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

Taking squares of these lengths gives a seven-vector in a space we call $\boldsymbol{D}^7$ for Delaunay 7-space:

$$[d_1 = ||\vec{a}||^2,\ \ d_2 = ||\vec{b}||^2,\ \ d_3 = ||\vec{c}||^2,\ \ d_4 = ||\vec{d}||^2,\ \ d_5 = ||\vec{b}+\vec{c}||^2,\ \ d_6 = ||\vec{a}+\vec{c}||^2,\ \ d_7 = ||\vec{a}+\vec{b}||^2]$$

$$= [d_1 = ||\vec{a}||^2,\ \ d_2 = ||\vec{b}||^2,\ \ d_3 = ||\vec{c}||^2,\ \ d_4 = ||\vec{d}||^2,\ \ d_5 = ||\vec{a}+\vec{d}||^2,\ \ d_6 = ||\vec{b}+\vec{d}||^2,\ \ d_7 = ||\vec{c}+\vec{d}||^2]$$

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

In $\boldsymbol{D}^7$ the Delaunay reduced cells are defined by:

$$d_1,\ \ d_2,\ \ d_3,\ \ d_4,\ \ d_5,\ \ d_6,\ \ d_7 > 0$$

$$d_1 + d_2 + d_3 + d_4 - d_5 - d_6 - d_7 = 0 \tag{6.1}$$

$$d_1 \leqslant d_2 \leqslant d_3 \leqslant d_4 \tag{6.2}$$

$$d_5 \leqslant d_2 + d_3 \tag{6.3}$$

$$d_5 \leqslant d_1 + d_4 \tag{6.4}$$

$$d_6 \leqslant d_1 + d_3 \tag{6.5}$$

$$d_6 \leqslant d_2 + d_4 \tag{6.6}$$

$$d_7 \leqslant d_1 + d_2 \tag{6.7}$$

$$d_7 \leqslant d_3 + d_4 \tag{6.8}$$

$$d_5 \geqslant d_2 - d_3 \tag{6.9}$$

$$d_5 \geqslant d_1 - d_4 \tag{6.10}$$

$$d_6 \geqslant d_1 - d_3 \tag{6.11}$$

$$d_6 \geqslant d_2 - d_4 \tag{6.12}$$

$$d_7 \geqslant d_1 - d_2 \tag{6.13}$$

$$d_7 \geqslant d_3 - d_4 \tag{6.14}$$

Boundaries may be defined by equalities in the above relationships.

7. The 5-D Boundaries Polytopes of $\boldsymbol{D}^7$

The full 7-dimensional space is projected to a 6-dimensional space by the linear constraint 6.1. We start the exploration of this space by identifying the 5-dimensional boundary polytopes that result from considering one equality in the above relationships at a time.

7.1. Cases 1, 2 and 3: Equal Delaunay Tetrahedron Edge Lengths

These cases arise when two Delaunay tetrahedron edges have equal lengths, the equality cases in expression 6.2. Consider for example $d_1 = d_2$. The boundary transformation would be based on exchanging $\vec{a}$ and $\vec{b}$, but that simple exchange would reverse the handedness of the cell, so we also negate all resulting edges to restore the handedness.

7.1.1. Case 1 $d_1 = d_2$, $||\vec{a}||^2 = ||\vec{b}||^2$, $\vec{a} \to -\vec{b}$, $\vec{b} \to -\vec{a}$, $\vec{c} \to -\vec{c}$, $\vec{d} \to \vec{a} + \vec{b} + \vec{b} = -\vec{d}$

$$MD_1 = (\mathbf{01}00000/\mathbf{10}00000/0010000/0001000/0000\mathbf{01}0/0000\mathbf{10}0/0000001)$$

$$PD_1 =$$
$$\left(\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{5}{14}\frac{5}{14}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{6}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{6}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{6}{7}\right)$$

$$PD_1^{\perp} =$$
$$\left(\frac{9}{14}\frac{\bar{5}}{14}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{5}}{14}\frac{9}{14}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}/\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{\bar{1}}{7}\frac{1}{7}\frac{1}{7}\frac{1}{7}\right)$$

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

7.1.2. Case 2 $d_2 = d_3$, $||\vec{b}||^2 = ||\vec{c}||^2$, $\vec{a} \to -\vec{a}$, $\vec{b} \to -\vec{c}$, $\vec{c} \to -\vec{b}$, $\vec{d} \to \vec{a} + \vec{b} + \vec{b} = -\vec{d}$

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

$$PD_2 =$$

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

$PD_2^{\perp} =$

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

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

7.1.3. Case 3 $d_3 = d_4$, $||\vec{c}||^2 = ||\vec{d}||^2 = ||\vec{a} + \vec{b} + \vec{c}||^2$, $\vec{a} \to -\vec{a}$, $\vec{b} \to -\vec{b}$, $\vec{c} \to \vec{a} + \vec{b} + \vec{c}$, $\vec{d} \to -\vec{c}$,

$MD_3 =$ (1000000/0100000/00**01**000/00**10**000/0000**01**0/0000**10**0/0000001)

$PD_3 =$

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

$PD_3^{\perp} =$

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

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

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

$$d_1 = d_3 \tag{7.1}$$

$$d_1 = d_4 \tag{7.2}$$

$$d_1 = d_5 \tag{7.3}$$

$$d_1 = d_6 \tag{7.4}$$

$$d_1 = d_7 \tag{7.5}$$

$$d_2 = d_4 \tag{7.6}$$

$$d_2 = d_5 \tag{7.7}$$

$$d_2 = d_6 \tag{7.8}$$

$$d_2 = d_7 \tag{7.9}$$

$$d_3 = d_5 \tag{7.10}$$

$$d_3 = d_6 \tag{7.11}$$

$$d_3 = d_7 \tag{7.12}$$

$$d_4 = d_5 \tag{7.13}$$

$$d_4 = d_6 \tag{7.14}$$

$$d_4 = d_7 \tag{7.15}$$

$$d_5 = d_6 \tag{7.16}$$

$$d_5 = d_7 \tag{7.17}$$

$$d_6 = d_7 \tag{7.18}$$

The boundary polytopes 7.1, 7.2, 7.6 are of dimensions 4, 3 and 4 respectively because they imply additional equalties from the ordering in 6.2. Many of the others arise in mapping Niggli characacters into Delaunay conditions.

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

There are six cases in which edges of the Delaunay tetrahedron meet at right angles. They are given by expressions 6.3 through 6.8 when the inequalities are replaced by equality. Consider for example

$$d_5 = d_2 + d_3$$

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

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

The full set of resulting equations in the same ordering as expressions 6.3 through 6.8 are

$$2\vec{b}.\vec{c} = g_4 = 0; \tag{7.19}$$

$$2\vec{a}.\vec{d} = 2\vec{a}.(-\vec{a} - \vec{b} - \vec{c}) = -2g_1 - g_6 - g_5 = 0; \tag{7.20}$$

$$2\vec{a}.\vec{c} = g_5 = 0; \tag{7.21}$$

$$2\vec{b}.\vec{d} = 2\vec{b}.(-\vec{a} - \vec{b} - \vec{c}) = -g_6 - 2g_2 - g_4 = 0; \tag{7.22}$$

$$2\vec{a}.\vec{b} = g_6 = 0; \tag{7.23}$$

$$2\vec{c}.\vec{d} = 2\vec{c}.(-\vec{a} - \vec{b} - \vec{c}) = -g_5 - g_4 - 2g_3 = 0; \tag{7.24}$$

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

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

for which $2\vec{b}_{orig}.\vec{c}_{orig} = 0$. Impose a slight perturbation on $\vec{b}_{orig}$ to form $\vec{b}_{ptrb}$ such that $\vec{b}_{ptrb}.\vec{c}_{orig} = \epsilon > 0$, all other inner products are non-positive. If we define $\vec{a}_{ptrb} = -\vec{a}_{orig}$ with a small additional perturbation to guarantee that

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

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

then we are starting from a $+++$ case with a small g_4 and can apply the transformation in expression 4.3 to return to the $---$ case using the tetrahedron

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

which says, up to reordering, the boundary transform takes the tetrahedron to

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

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

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

7.2.1. Case 4 Case 4: $d_5 = d_2 + d_3$ (see equation 6.3). This is equivalent to $g_4 = 0$. The Delaunay tetrahedron edges to be ordered are

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

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

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

$$||\vec{a}||^2 + 2\vec{a}.\vec{b} \leqslant 0 \tag{7.25}$$

From the ordering constraint $||\vec{c}||^2 \leqslant ||\vec{d}||^2$ and equation 7.25 it follows that

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

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

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

i.e.

$$|| - \vec{a} - \vec{c}|| \geqslant ||\vec{c}||^2$$

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

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

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

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

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

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

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

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

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

$$PD_4 =$$

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

$$PD_4^{\perp} =$$

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

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

7.2.2. Case 4 Internal Boundaries The eight permutations that constitute the case 4 five-dimensional case in terms of D^7 components are

d_2, d_3, d_6, d_7

d_2, d_3, d_7, d_6

d_2, d_6, d_3, d_7

d_2, d_6, d_7, d_3

d_2, d_7, d_3, d_6

d_2, d_7, d_6, d_3

d_6, d_2, d_3, d_7

d_7, d_2, d_3, d_6

so the internal boundaries are:

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

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

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

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

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

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

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

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

The projectors onto the 4-dimensional internal boundaries are:

$PD_{4\_67} =$

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

$PD_{4\_36} =$

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

$PD_{4\_37} =$

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

$PD_{4\_26} =$

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

$PD_{4\_27} =$

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

7.2.3. Case 5 case 5: $d_5 = d_1 + d_4$ (see equation 6.4). The Delaunay tetrahedron edges to be ordered are

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

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

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

$$MD_{5.1} = (1000000/0001000/0000010/0000001/0100000/0010000/0\bar{2}\bar{2}0122)$$

$$MD_{5.2} = (1000000/0001000/0000001/0000010/0010000/0100000/0\overline{2}\overline{2}0122)$$

$$MD_{5.3} = (1000000/0000010/0001000/0000001/0100000/0\overline{2}\overline{2}0122/0010000)$$

$$MD_{5.4} = (1000000/0000010/0000001/0001000/0\overline{2}\overline{2}0122/0100000/0010000)$$

$$MD_{5.5} = (1000000/0000001/0001000/0000010/0010000/0\overline{2}\overline{2}0122/0100000)$$

$$MD_{5.6} = (1000000/0000001/0000010/0001000/0\overline{2}\overline{2}0122/0010000/0100000)$$

$$MD_{5.7} = (0000010/1000000/0001000/0000001/0\overline{2}\overline{2}0122/0100000/0010000)$$

$$MD_{5.8} = (0000001/1000000/0001000/0000010/0\overline{2}\overline{2}0122/0010000/0100000)$$

$$PD_5 =$$

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

$$PD_5^{\perp} =$$

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

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

7.2.4. Case 6 $d_6 = d_1 + d_3$, (see equation 6.5). The Delaunay tetrahedron edges to be ordered are

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

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

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

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

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

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

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

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

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

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

$$PD_6 =$$

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

$$PD_6^{\perp} =$$

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

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

7.2.5. Case 7 case 7: $d_6 = d_2 + d_4$ (see equation 6.6). The Delaunay tetrahedron edges to be ordered are

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

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

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

with the ordering

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

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

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

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

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

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

and

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

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

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

$$PD_7 = \frac{(77\overline{33}242/77\overline{33}242/\overline{33}77242/\overline{33}77242/2222C4\overline{8}/4444484/2222\overline{8}4C)}{20}$$
$$PD_7^\perp = \frac{(D\overline{7}33\overline{242}/\overline{7}D33\overline{242}/33D\overline{7242}/33D\overline{7}\overline{242}/\overline{2222}8\overline{4}8/\overline{44444}C\overline{4}/\overline{2222}8\overline{4}8)}{20}$$

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

7.2.6. Case 8 case 8: $d_7 = d_1 + d_2$ (see equation 6.7). The Delaunay tetrahedron edges to be ordered are

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

As with cases 4 and 6, there are potentially 8 feasible permutations, but in this case, two of them would have $||\vec{b}||^2 \leqslant ||\vec{a}||^2$, reducing the dimension in those two cases, leaving 6 feasible permutations that result in 5-dimensional polytopes.

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

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

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

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

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

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

$$PD_8 =$$

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

$$PD_8^{\perp} =$$

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

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

7.2.7. Case 9 case 9: $d_7 = d_3 + d_4$ (see equation 6.8). The Delaunay tetrahedron edges to be ordered are

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

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

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

with the ordering

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

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

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

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

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

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

and

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

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

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

$$MD_{9.1} = (0010000/0000010/0000100/0001000/\overline{22}00221/0100000/1000000)$$

The 2-dimensional projector for case 9 is

$$PD_9 = \frac{(1111112/1111112/1111112/1111112/1111 6\overline{4}2/1111\overline{4}62/2222224)}{10}$$

$$PD_9^{\perp} = \frac{(9\overline{111112}/\overline{1}9\overline{11112}/\overline{11}9\overline{112}/\overline{111}9\overline{12}/\overline{1111}44\overline{2}/\overline{1111}44\overline{2}/\overline{22222}26)}{10}$$

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

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Table 1. *Delaunay Variety, D^7 subspace, G^6 subspace*

Delaunay Variety	D^7 Subspace	G^6 Subspace
cP	$[-s, -s, -s, -3*s, -2*s, -2*s, -2*s]$	$[-s, -s, -s, 0, 0, 0]$
cF	$[-2p, -2p, -2p, -2p, -2p, -2p, -4p]$	$[-2p, -2p, -2p, 2p, 2p, 0]$
cI	$[-3p, -3p, -3p, -3p, -4p, -4p, -4p]$	$[-3p, -3p, -3p, 2p, 2p, 2p]$
tP	$[-s, -s, -u, -u-2s, -u-s, -u-s, -2s]$	$[-s, -s, -u, 0, 0, 0]$ or [-u,-s,-s,0,0,0]
tI	$[-2p, -2p, -t-2p, -t-2p, -t-2p, -t-2p, -4p]$	$[-2p, -2p, -t-2p, 2p, 2p, 0]$
tI	$[-r-2p, -r-2p, -r-2p, -r-2p, -2r-2p, -2r-2p, -4p]$	$[-r-2p, -r-2p, -r-2p, 2p, 2p, 2r]$

Table 2. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type, $\mathbf{G^6}$ subspace (Andrews & Bernstein, 1988), $\mathbf{D^7}$ subspace.*

Roof/ Niggli Symbol	IT Lattice Char	Bravais Lattice Type	G^6 Subspace	D^7 Subspace
44A	3	**cP**	$[r, r, r, 0, 0, 0]$	$[r, r, r, 3r, 2r, 2r, 2r]$
44C	1	*cF*	$[r, r, r, r, r, r]$	$[r, r, r, r, r, r, 2r]$
44B	5	*cI*	$[r, r, r, -2r/3, -2r/3, -2r/3]$	$[r, r, r, r, 4r/3, 4r/3, 4r/3]$
45A	11	**tP**	$[r, r, s, 0, 0, 0]$	$[r, r, s.s+2r, s+r, s+r, 2r]$
45B	21	**tP**	$[r, s, s, 0, 0, 0]$	$[r, s, s, 2s+r, 2s, s+r, s+r]$
45D	6	*tI*	$[r, r, r, -r+s, -r+s, -2s]$	$[r, r, r, r, s+r, s+r, 2r-2s]$
45D	7	*tI*	$[r, r, r, -2s, -r+s, -r+s]$	$[r, r, r, r, 2r-2s, s+r, s+r]$
45C	15	*tI*	$[r, r, s, -r, -r, 0]$	$[r, r, s, s, s, s, 2r]$
45E	18	*tI*	$[r, s, s, r/2, r, r]$	$[r, s, s, 2s-r/2, 2s+r/2, s, s]$
48A	12	**hP**	$(r, r, s, 0, 0, -r)$	$[r, r, s, s+r, s+r, s+r, r]$
48B	22	**hP**	$(r, s, s, -s, 0, 0)$	$[r, s, s, s+r, s, s+r, s+r]$
49C	2	*hR*	(r, r, r, s, s, s)	$[r, r, 2r-s, 2r-s, r, 3r-s, 2r-s]$
49D	4	*hR*	$(r, r, r, -s, -s, -s)$	$[r, r, r, 3r-3s, 2r-s, 2r-s, 2r-s]$
49B	9	*hR*	$[r, r, s, r, r, r]$	$[r, r, s, s, s, s+r, r]$
49E	24	*hR*	$[r, s, s, -s+r/3, -2r/3, -2r/3]$	$[r, s, s, s, s+r/3, s+r/3, s+r/3]$
50C	32	**oP**	$[r, s, t, 0, 0, 0]$	$[r, s, t, t+s+r, t+s, t+r, s+r]$
50D	13	*oC*	$[r, r, s, 0, 0, -t]$	$[r, r, s, -t+s+2r, s+r, s+r, 2r-t]$
50E	23	*oC*	$[r, s, s, -t, 0, 0]$	$[r, s, s, -t+2s+r, 2s-t, s+r, s+r]$
50A	36	*oC*	$[r, s, t, 0, -r, 0]$	$[r, s, t, t+s, t+s, t, s+r]$
50B	38	*oC*	$[r, s, t, 0, 0, -r]$	$[r, s, t, t+s, t+s, t+r, s]$
50F	40	*oC*	$[r, s, t, -s, 0, 0]$	$[r, s, t, t+r, t, t+r, s+r]$
51A	16	*oF*	$[r, r, s, -t, -t, -2r+2t]$	$[r, r, s, s, -t+s+r, -t+s+r, 2t]$
51B	26	*oF*	$[r, s, t, r/2, r, r]$	$[r, s, t, t+s-r/2, t+s+r/2, t, s]$
52A	8	*oI*	$[r, r, r, -s, -t, -2r+s+t]$	$[r, r, r, r, 2r-s, 2r-t, t+s]$
52B	19	*oI*	$[r, s, s, t, r, r]$	$[r, s, s, 2s-t, -t+2s+r, s, s]$
52C	42	*oI*	$[r, s, t, -s, -r, 0]$	$[r, s, t, r, t, r, s+r]$

Table 3. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type,* $\mathbf{G^6}$ *subspace (Andrews & Bernstein, 1988),* $\mathbf{D^7}$ *subspace.*

Roof/ Niggli Symbol	**IT Lattice Char**	**Bravais Lattice Type**	$\boldsymbol{G^6}$ **Subspace**	$\boldsymbol{D^7}$ **Subspace**
44A	3	**cP**	$[r,r,r,0,0,0]$	$[r,r,r,3r,2r,2r,2r]$
44C	1	*cF*	$[r,r,r,r,r,r]$	$[r,r,r,r,r,r,2r]$
44B	5	*cI*	$[r,r,r,-2r/3,-2r/3,-2r/3]$	$[r,r,r,r,4r/3,4r/3,4r/3]$
45A	11	**tP**	$[r,r,s,0,0,0]$	$[r,r,s.s+2r,s+r,s+r,2r]$
45B	21	**tP**	$[r,s,s,0,0,0]$	$[r,s,s,2s+r,2s,s+r,s+r]$
45D	6	*tI*	$[r,r,r,-r+s,-r+s,-2s]$	$[r,r,r,r,s+r,s+r,2r-2s]$
45D	7	*tI*	$[r,r,r,-2s,-r+s,-r+s]$	$[r,r,r,r,2r-2s,s+r,s+r]$
45C	15	*tI*	$[r,r,s,-r,-r,0]$	$[r,r,s,s,s,s,2r]$
45E	18	*tI*	$[r,s,s,r/2,r,r]$	$[r,s,s,2s-r/2,2s+r/2,s,s]$
48A	12	**hP**	$(r,r,s,0,0,-r)$	$[r,r,s,s+r,s+r,s+r,r]$
48B	22	**hP**	$(r,s,s,-s,0,0)$	$[r,s,s,s+r,s,s+r,s+r]$
49C	2	*hR*	(r,r,r,s,s,s)	$[r,r,2r-s,2r-s,r,3r-s,2r-s]$
49D	4	*hR*	$(r,r,r,-s,-s,-s)$	$[r,r,r,3r-3s,2r-s,2r-s,2r-s]$
49B	9	*hR*	$[r,r,s,r,r,r]$	$[r,r,s,s,s,s+r,r]$
49E	24	*hR*	$[r,s,s,-s+r/3,-2r/3,-2r/3]$	$[r,s,s,s,s+r/3,s+r/3,s+r/3]$
50C	32	**oP**	$[r,s,t,0,0,0]$	$[r,s,t,t+s+r,t+s,t+r,s+r]$
50D	13	*oC*	$[r,r,s,0,0,-t]$	$[r,r,s,-t+s+2r,s+r,s+r,2r-t]$
50E	23	*oC*	$[r,s,s,-t,0,0]$	$[r,s,s,-t+2s+r,2s-t,s+r,s+r]$
50A	36	*oC*	$[r,s,t,0,-r,0]$	$[r,s,t,t+s,t+s,t,s+r]$
50B	38	*oC*	$[r,s,t,0,0,-r]$	$[r,s,t,t+s,t+s,t+r,s]$
50F	40	*oC*	$[r,s,t,-s,0,0]$	$[r,s,t,t+r,t,t+r,s+r]$
51A	16	*oF*	$[r,r,s,-t,-t,-2r+2t]$	$[r,r,s,s,-t+s+r,-t+s+r,2t]$
51B	26	*oF*	$[r,s,t,r/2,r,r]$	$[r,s,t,t+s-r/2,t+s+r/2,t,s]$
52A	8	*oI*	$[r,r,r,-s,-t,-2r+s+t]$	$[r,r,r,r,2r-s,2r-t,t+s]$
52B	19	*oI*	$[r,s,s,t,r,r]$	$[r,s,s,2s-t,-t+2s+r,s,s]$
52C	42	*oI*	$[r,s,t,-s,-r,0]$	$[r,s,t,r,t,r,s+r]$

Table 4. *Roof/Niggli symbol, International Tables (IT) lattice character, Bravais lattice type,* $\mathbf{G^6}$ *subspace,* $\mathbf{G^6}$ *boundary polytope, continued*

Roof/ Niggli Symbol	**IT Lattice Char**	**Bravais Lattice Type**	$\boldsymbol{G^6}$ **Subspace**	$\boldsymbol{D^7}$ **Subspace**
53A	33	**mP**	$[r,s,t,0,-u,0]$	$[r,s,t,-u+t+s+r,t+s,-u+t+r,s+r]$
53B	35	**mP**	$(r,s,t,-u,0,0)$	$[r,s,t,-u+t+s+r,-u+t+s,t+r,s+r]$
53C	34	**mP**	$(r,s,t,0,0,-u)$	$[r,s,t,-u+t+s+r,t+s,t+r,-u+s+r]$
55A	10	mC	(r,r,s,t,t,u)	$[r,2r-u,s,-t+s+r,-u+s+2r,-t+s+r,r]$
55A	14	mC	$(r,r,s,-t,-t,-u)$	$[r,r,s,-u-2t+s+2r,-t+s+r,-t+s+r,2r-u]$
57B	17	mC	$(r,r,s,-t,-u,-2r+t+u)$	$[r,r,s,s,-t+s+r,-u+s+r,u+t]$
55B	20	mC	(r,s,s,t,u,u)	$[r,s,2*s-t,-u+s+r,s,-t+2*s+r,-u+s+r]$
55B	25	mC	(r,s,s,t,u,u)	$[r,s,s,-2u-t+2s+r,2s-t,-u+s+r,-u+s+r]$
57C	27	mC	(r,s,t,u,r,r)	$[r,s,t,-u+t+s,-u+t+s+r,t,s]$
56A	28	mC	$(r,s,t,u,r,2u)$	$[r,s,t,-u+t+s,u+t+s,t,-2*u+s+r]$
56C	29	mC	$(r,s,t,u,2u,r)$	$\mathrm{DD}'=\hat{\mathrm{D}}$
56B	30	mC	$(r,s,t,s,u,2u)$	$77'=\hat{7}$
54C	37	mC	$(r,s,t,-u,-r,0)$	5B
54A	39	mC	$(r,s,t,-u,0,-r)$	4E
54B	41	mC	$(r,s,t,-s,-u,0)$	58
57A	43	mC	$(r,s,t,-s+u,-r+u,-2u)$	$\mathrm{FF}'=\hat{\mathrm{F}}$

abcdefghijklmnopqrstuvwxyz0123456789ABCDEFGHIJKLMNOPQRSTUVWXYZ

abcdefghijklmnopqrstuvwxyz0123456789ABCDEFGHIJKLMNOPQRSTUVWXYZ