

Appendix B Symmetry

B0 Origin $\langle 0,0,0 \rangle$

The symmetry group is \mathbf{Z}_2^2

$$T_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = T_0^{-1}$$

$$T_0 : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,0 \rangle$$

d, a, b, c	$d, +a, +b, +c$
o, p, q, r, s	o, p, q, r, s

$$T_c = \frac{1}{624} \begin{bmatrix} +538 & +172 & -344 \\ +79 & +466 & +316 \\ -251 & +502 & -380 \end{bmatrix} = T_c^{-1}$$

$$T_c : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,0 \rangle$$

d, a, b, c	$d, +a, +b, -c$
--------------	-----------------

$$T_{ab} = \frac{1}{208} \begin{bmatrix} +98 & -196 & -24 \\ -165 & -86 & -36 \\ -55 & -98 & +196 \end{bmatrix} = T_{ab}^{-1}$$

$$T_{ab} : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,0 \rangle$$

d, a, b, c	$d, -a, -b, +c$
--------------	-----------------

$$T_{abc} = \frac{1}{3} \begin{bmatrix} +1 & -2 & -2 \\ -2 & -2 & +1 \\ -2 & +1 & -2 \end{bmatrix} = T_{abc}^{-1} \quad \text{rotation by } \pm\pi \text{ about } p = \langle +2, -1, -1 \rangle$$

$$T_{abc} : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,0 \rangle$$

d, a, b, c	$d, -a, -b, -c$
o, p, q, r, s	s, p, r, q, o

B1 Symmetric line $\langle 0,0,0 \rangle + w\langle 0,0,1 \rangle$

The symmetry group is \mathbf{Z}

$$S_{(w)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{10}{117}w \begin{bmatrix} +2 & -4 & +8 \\ +3 & -6 & +12 \\ +1 & -2 & +4 \end{bmatrix} = S_{(-w)}^{-1}$$

$$S_{(w)} : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,+w \rangle$$

d, a, b, c	d, a, b, c
--------------	--------------

$$S_{(w)}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{10}{117}w \begin{bmatrix} +2 & -4 & +8 \\ +3 & -6 & +12 \\ +1 & -2 & +4 \end{bmatrix} = S_{(-w)}$$

$$S_{(w)}^{-1} : \text{packing } \langle 0,0,0 \rangle \rightarrow \text{packing } \langle 0,0,-w \rangle$$

d, a, b, c	d, a, b, c
--------------	--------------

B2 Symmetric line $\langle 0,0,0 \rangle + w\langle 0,0,1 \rangle$

The symmetry group is \mathbf{Z}_2^2

$$S_{(w)} T_0 S_{(w)}^{-1} = T_0$$

$$S_{(w)} T_0 S_{(w)}^{-1} : \text{packing } \langle 0,0,w \rangle \rightarrow \text{packing } \langle 0,0,w \rangle$$

d, a, b, c	$d, +a, +b, +c$
o, p, q, r, s	o, p, q, r, s

$$S_{(w)} T_c S_{(w)}^{-1} = T_c - \frac{20}{117}w \begin{bmatrix} +2 & -4 & +8 \\ +3 & -6 & +12 \\ +1 & -2 & +4 \end{bmatrix}$$

$$S_{(w)} T_c S_{(w)}^{-1} : \text{packing } \langle 0,0,w \rangle \rightarrow \text{packing } \langle 0,0,w \rangle$$

d, a, b, c	$d, +a, +b, -c$
--------------	-----------------

$$S_{(w)} T_{ab} S_{(w)}^{-1} = T_{ab} + \frac{20}{117}w \begin{bmatrix} +2 & -4 & +8 \\ +3 & -6 & +12 \\ +1 & -2 & +4 \end{bmatrix}$$

$$S_{(w)} T_{ab} S_{(w)}^{-1} : \text{packing } \langle 0,0,w \rangle \rightarrow \text{packing } \langle 0,0,w \rangle$$

d, a, b, c	$d, -a, -b, +c$
--------------	-----------------

$$S_{(w)} T_{abc} S_{(w)}^{-1} = T_{abc} \quad \text{rotation by } \pm\pi \text{ about } p = \langle +2, -1, -1 \rangle$$

$$S_{(w)} T_{abc} S_{(w)}^{-1} : \text{packing } \langle 0,0,w \rangle \rightarrow \text{packing } \langle 0,0,w \rangle$$

d, a, b, c	$d, -a, -b, -c$
o, p, q, r, s	s, p, r, q, o

B3 Parameter space

For any packing $\langle u, v, w \rangle$

$$R_a = R_a^{-1} : \langle x, y, z \rangle \rightarrow d - \langle x, y, z \rangle + a \quad \text{inversion about } \frac{1}{2}(d+a)$$

$$R_a : \text{packing } \langle u, v, w \rangle \rightarrow \text{packing } \langle u, v, w \rangle$$

d, a, b, c	$a, d, d+a-b, d-c+a$
--------------	----------------------

$$R_b = R_b^{-1} : \langle x, y, z \rangle \rightarrow d - \langle x, y, z \rangle + b \quad \text{inversion about } \frac{1}{2}(d+b)$$

$$R_b : \text{packing } \langle u, v, w \rangle \rightarrow \text{packing } \langle u, v, w \rangle$$

d, b, c, a	$b, d, d+b-c, d-a+b$
--------------	----------------------

$$R_c = R_c^{-1} : \langle x, y, z \rangle \rightarrow d - \langle x, y, z \rangle + c \quad \text{inversion about } \frac{1}{2}(d+c)$$

$$R_c : \text{packing } \langle u, v, w \rangle \rightarrow \text{packing } \langle u, v, w \rangle$$

d, c, a, b	$c, d, d+c-a, d-b+c$
--------------	----------------------

For any 2 packings $\langle u, v, w \rangle, \langle \tilde{u}, \tilde{v}, \tilde{w} \rangle$ related by

$$\langle \tilde{u}, \tilde{v}, -\frac{1}{2}\tilde{u} + \tilde{v} + \tilde{w} \rangle = \langle -u, -v, -\frac{1}{2}u + v + w \rangle$$

$$T_{abc} = \frac{1}{3} \begin{bmatrix} +1 & -2 & -2 \\ -2 & -2 & +1 \\ -2 & +1 & -2 \end{bmatrix} \quad \text{rotation by } \pm\pi \text{ about } p = \langle +2, -1, -1 \rangle$$

$$T_{abc} : \text{packing } \langle u, v, w \rangle \rightarrow \text{packing } \langle \tilde{u}, \tilde{v}, \tilde{w} \rangle$$

d, a, b, c	$d, -a, -b, -c$
o, p, q, r, s	s, p, r, q, o

Appendix C Computations

C0_{vec} Vector space $\langle x, y, z \rangle$

The cluster vertices are

$$\begin{aligned} o &= \langle +2, +2, +2 \rangle \\ p &= \langle +2, -1, -1 \rangle \\ q &= \langle -1, +2, -1 \rangle \\ r &= \langle -1, -1, +2 \rangle \\ s &= \langle -2, -2, -2 \rangle \end{aligned}$$

The cluster volume is

$$U = \frac{1}{6} \det[o - p, o - q, o - r] + \frac{1}{6} \det[s - p, s - q, s - r] = 18$$

The lattice vectors are

$$\begin{aligned} a &= \langle a_x, a_y, a_z \rangle \\ b &= \langle b_x, b_y, b_z \rangle \\ c &= \langle c_x, c_y, c_z \rangle \\ d &= \langle d_x, d_y, d_z \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= 2 \det[a, b, c] = \det[a + b, b + c, c + a] \\ \phi &= 2U/V = 36/V \end{aligned}$$

C0_{pac} Packing parameter space $\langle u, v, w \rangle$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b} \\ \langle a_x, b_y, c_z \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20}, w + \frac{753}{320} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} - v, -\frac{3}{20} + 2u + v \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} + v, \frac{27}{20} - 2u - v \rangle \\ c &= \langle \frac{129}{160} - 2u + 4v + 2w, -\frac{237}{320} - u + 2v + 3w, \frac{753}{320} + w \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u + v, -\frac{1}{20} + u - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= 2 \det[a, b, c] = \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2) \\ \phi &= 36/V = 100/(117 + 60u^2 - 80uv - 80v^2) \end{aligned}$$

C1_{∂V}/C1_{opt} Optimal plane $u = \frac{2}{5}v$

The lattice volume function is a rotated parabolic hyperboloid

$$V = \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2)$$

The contours (of constant V) are rotated hyperbolas

$$\frac{3}{5}u^2 - \frac{4}{5}uv - \frac{4}{5}v^2 = \frac{1}{36}V - \frac{117}{100}$$

The asymptotes (of the hyperbolas) are

$$\begin{aligned} u &= +2v \\ u &= -\frac{2}{3}v \end{aligned}$$

The 2 maximal lines have slope $du/dv = -6$

$$\begin{aligned} \langle +\frac{3}{160}, +\frac{3}{64}, -\frac{3}{80} \rangle + u \langle 1, -\frac{1}{6}, +\frac{5}{6} \rangle \\ \langle -\frac{3}{160}, -\frac{3}{64}, +\frac{3}{80} \rangle + u \langle 1, -\frac{1}{6}, +\frac{1}{2} \rangle \end{aligned}$$

The contours have slope $du/dv = -6$ when

$$u = +\frac{2}{5}v$$

C1_{a-b}/C1_{cen} Central plane $u = 0$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{a-b} \\ \langle b_y, c_z \rangle = \langle v + \frac{51}{20}, w + \frac{753}{320} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10}, \frac{21}{20} - v, -\frac{3}{20} + v \rangle \\ b &= \langle -\frac{3}{10}, \frac{51}{20} + v, \frac{27}{20} - v \rangle \\ c &= \langle \frac{129}{160} + 4v + 2w, -\frac{237}{320} + 2v + 3w, \frac{753}{320} + w \rangle \\ d &= \langle \frac{1}{10}, -\frac{1}{20} + v, -\frac{1}{20} - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 - 80v^2) \\ \phi &= 100/(117 - 80v^2) \end{aligned}$$

C1_{b+c} Boundary plane $+u + v - w = \frac{33}{320}$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c} \\ \langle a_x, b_y \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} - v, -\frac{3}{20} + 2u + v \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} + v, \frac{27}{20} - 2u - v \rangle \\ c &= \langle \frac{3}{5} + 6v, -\frac{21}{20} + 2u + 5v, \frac{9}{4} + u + v \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u + v, -\frac{1}{20} + u - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2) \\ \phi &= 100/(117 + 60u^2 - 80uv - 80v^2) \end{aligned}$$

C1_{c+a} **Boundary plane** $-3v - w = \frac{33}{320}$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{c+a} \\ \langle a_x, b_y \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} - v, -\frac{3}{20} + 2u + v \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} + v, \frac{27}{20} - 2u - v \rangle \\ c &= \langle \frac{3}{5} - 2u - 2v, -\frac{21}{20} - u - 7v, \frac{9}{4} - 3v \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u + v, -\frac{1}{20} + u - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2) \\ \phi &= 100/(117 + 60u^2 - 80uv - 80v^2) \end{aligned}$$

C1_{b-c} **Boundary plane** $-u + 2w = \frac{3}{32}$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c} \\ \langle a_x, b_y \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} - v, -\frac{3}{20} + 2u + v \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} + v, \frac{27}{20} - 2u - v \rangle \\ c &= \langle \frac{9}{10} - u + 4v, -\frac{3}{5} + \frac{1}{2}u + 2v, \frac{12}{5} + \frac{1}{2}u \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u + v, -\frac{1}{20} + u - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2) \\ \phi &= 100/(117 + 60u^2 - 80uv - 80v^2) \end{aligned}$$

C1_{c-a} **Boundary plane** $-u + 4v + 2w = \frac{3}{32}$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{c-a} \\ \langle a_x, b_y \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20} \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} - v, -\frac{3}{20} + 2u + v \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} + v, \frac{27}{20} - 2u - v \rangle \\ c &= \langle \frac{9}{10} - u, -\frac{3}{5} + \frac{1}{2}u - 4v, \frac{12}{5} + \frac{1}{2}u - 2v \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u + v, -\frac{1}{20} + u - v \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 60u^2 - 80uv - 80v^2) \\ \phi &= 100/(117 + 60u^2 - 80uv - 80v^2) \end{aligned}$$

C2_{sym} **Symmetric line** $\langle 0, 0, 0 \rangle + w\langle 0, 0, 1 \rangle$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{a-b}, \partial V \\ \langle b_y, c_z \rangle = \langle v + \frac{51}{20}, w + \frac{753}{320} \rangle, v = 0 \text{ [min } V] \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10}, \frac{21}{20}, -\frac{3}{20} \rangle \\ b &= \langle -\frac{3}{10}, \frac{51}{20}, \frac{27}{20} \rangle \\ c &= \langle \frac{129}{160} + 2w, -\frac{237}{320} + 3w, \frac{753}{320} + w \rangle \\ d &= \langle \frac{1}{10}, -\frac{1}{20}, -\frac{1}{20} \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{1053}{25} \\ \phi &= \frac{100}{117} \end{aligned}$$

C2_{min}⁺ **Minimal line** $\langle 0, 0, +\frac{3}{64} \rangle + u\langle 1, 0, +\frac{1}{2} \rangle$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c}, \mathbf{H}_{c-a} \\ a_x = u + \frac{27}{10} \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20}, -\frac{3}{20} + 2u \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20}, \frac{27}{20} - 2u \rangle \\ c &= \langle \frac{9}{10} - u, -\frac{3}{5} + \frac{1}{2}u, \frac{12}{5} + \frac{1}{2}u \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + u, -\frac{1}{20} + u \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 60u^2) \\ \phi &= 100/(117 + 60u^2) \end{aligned}$$

C2_{min}⁻ **Minimal line** $\langle 0, 0, -\frac{33}{320} \rangle + u\langle 1, -\frac{1}{4}, +\frac{3}{4} \rangle$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c}, \mathbf{H}_{c+a} \\ a_x = u + \frac{27}{10} \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{21}{20} + \frac{1}{4}u, -\frac{3}{20} + \frac{7}{4}u \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{51}{20} - \frac{1}{4}u, \frac{27}{20} - \frac{7}{4}u \rangle \\ c &= \langle \frac{3}{5} - \frac{3}{2}u, -\frac{21}{20} + \frac{3}{4}u, \frac{9}{4} + \frac{3}{4}u \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{20} + \frac{3}{4}u, -\frac{1}{20} + \frac{5}{4}u \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{25}(117 + 75u^2) \\ \phi &= 100/(117 + 75u^2) \end{aligned}$$

$$\mathbf{C2}_{\max}^+ \quad \mathbf{Maximal\ line} \langle 0, +\frac{1}{20}, -\frac{17}{320} \rangle + u \langle 1, -\frac{1}{6}, +\frac{5}{6} \rangle$$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c}, \mathbf{H}_{c-a} \\ a_x = u + \frac{27}{10} \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, 1 + \frac{1}{6}u, -\frac{1}{10} + \frac{11}{6}u \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{13}{5} - \frac{1}{6}u, \frac{13}{10} - \frac{11}{6}u \rangle \\ c &= \langle \frac{9}{10} - u, -\frac{4}{5} + \frac{7}{6}u, \frac{23}{10} + \frac{5}{6}u \rangle \\ d &= \langle \frac{1}{10} + u, 0 + \frac{5}{6}u, -\frac{1}{10} + \frac{7}{6}u \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{1000} (4671 + \frac{25600}{9} (u - \frac{3}{160})^2) \\ \phi &= 4000 / (4671 + \frac{25600}{9} (u - \frac{3}{160})^2) \end{aligned}$$

$$\mathbf{C2}_{\max}^- \quad \mathbf{Maximal\ line} \langle 0, -\frac{1}{20}, +\frac{3}{64} \rangle + u \langle 1, -\frac{1}{6}, +\frac{1}{2} \rangle$$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c}, \mathbf{H}_{c+a} \\ a_x = u + \frac{27}{10} \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle \frac{27}{10} + u, \frac{11}{10} + \frac{1}{6}u, -\frac{1}{5} + \frac{11}{6}u \rangle \\ b &= \langle -\frac{3}{10} - u, \frac{5}{2} - \frac{1}{6}u, \frac{7}{5} - \frac{11}{6}u \rangle \\ c &= \langle \frac{7}{10} - \frac{5}{3}u, -\frac{7}{10} + \frac{1}{6}u, \frac{12}{5} + \frac{1}{2}u \rangle \\ d &= \langle \frac{1}{10} + u, -\frac{1}{10} + \frac{5}{6}u, 0 + \frac{7}{6}u \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{9}{1000} (4671 + \frac{25600}{9} (u + \frac{3}{160})^2) \\ \phi &= 4000 / (4671 + \frac{25600}{9} (u + \frac{3}{160})^2) \end{aligned}$$

$$\mathbf{C3}_{\text{orig}} \quad \mathbf{Origin} \langle 0, 0, 0 \rangle$$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b} \\ \langle a_x, b_y, c_z \rangle = \langle u + \frac{27}{10}, v + \frac{51}{20}, w + \frac{753}{320} \rangle, \langle u, v, w \rangle = \langle 0, 0, 0 \rangle \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{27}{10}, +\frac{21}{20}, -\frac{3}{20} \rangle \\ b &= \langle -\frac{3}{10}, +\frac{51}{20}, +\frac{27}{20} \rangle \\ c &= \langle +\frac{129}{160}, -\frac{237}{320}, +\frac{753}{320} \rangle \\ d &= \langle +\frac{1}{10}, -\frac{1}{20}, -\frac{1}{20} \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= 2 \det[a, b, c] = \frac{1053}{25} \\ \phi &= 36/V = \frac{100}{117} \end{aligned}$$

$$\mathbf{C3}_{\text{opt}}^+ \quad \mathbf{Optimal\ point} \langle +\frac{3}{160}, +\frac{3}{64}, -\frac{3}{80} \rangle$$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c}, \mathbf{H}_{c-a}, \partial V \\ a_x = u + \frac{27}{10}, u = +\frac{3}{160} [\min V] \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{87}{32}, +\frac{321}{320}, -\frac{21}{320} \rangle = \langle +2.71875, +1.003125, -0.065625 \rangle \\ b &= \langle -\frac{51}{160}, +\frac{831}{320}, +\frac{81}{64} \rangle = \langle -0.31875, +2.596875, +1.265625 \rangle \\ c &= \langle +\frac{141}{160}, -\frac{249}{320}, +\frac{741}{320} \rangle = \langle +0.88125, -0.778125, +2.315625 \rangle \\ d &= \langle +\frac{19}{160}, +\frac{1}{64}, -\frac{5}{64} \rangle = \langle +0.11875, +0.015625, -0.078125 \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{42039}{1000} = 42.039 \\ \phi &= \frac{4000}{4671} \approx .856347677156 \end{aligned}$$

$$\mathbf{C3}_{\text{opt}}^- \quad \mathbf{Optimal\ point} \langle -\frac{3}{160}, -\frac{3}{64}, +\frac{3}{80} \rangle$$

The linear incidence conditions are

$$\begin{aligned} \mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c}, \mathbf{H}_{c+a}, \partial V \\ a_x = u + \frac{27}{10}, u = -\frac{3}{160} [\min V] \end{aligned}$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{429}{160}, +\frac{351}{320}, -\frac{15}{64} \rangle = \langle +2.68125, +1.096875, -0.234375 \rangle \\ b &= \langle -\frac{9}{32}, +\frac{801}{320}, +\frac{459}{320} \rangle = \langle -0.28125, +2.503125, +1.434375 \rangle \\ c &= \langle +\frac{117}{160}, -\frac{45}{64}, +\frac{153}{64} \rangle = \langle +0.73125, -0.703125, +2.390625 \rangle \\ d &= \langle +\frac{13}{160}, -\frac{37}{320}, -\frac{7}{320} \rangle = \langle +0.08125, -0.115625, -0.021875 \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{42039}{1000} = 42.039 \\ \phi &= \frac{4000}{4671} \approx .856347677156 \end{aligned}$$

$$\mathbf{C3}_{\text{cen}}^+ \quad \mathbf{Central\ point} \langle 0, +\frac{1}{20}, -\frac{17}{320} \rangle$$

The linear incidence conditions are

$$\mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c}, \mathbf{H}_{c-a}, \mathbf{H}_{a-b}$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{27}{10}, +1, -\frac{1}{10} \rangle \\ b &= \langle -\frac{3}{10}, +\frac{13}{5}, +\frac{13}{10} \rangle \\ c &= \langle +\frac{9}{10}, -\frac{4}{5}, +\frac{23}{10} \rangle \\ d &= \langle +\frac{1}{10}, 0, -\frac{1}{10} \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{5256}{125} \\ \phi &= \frac{125}{146} \end{aligned}$$

C3_{cen}⁻ Central point $\langle 0, -\frac{1}{20}, +\frac{3}{64} \rangle$

The linear incidence conditions are

$$\mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c}, \mathbf{H}_{c+a}, \mathbf{H}_{a-b}$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{27}{10}, +\frac{11}{10}, -\frac{1}{5} \rangle \\ b &= \langle -\frac{3}{10}, +\frac{5}{2}, +\frac{7}{5} \rangle \\ c &= \langle +\frac{7}{10}, -\frac{7}{10}, +\frac{12}{5} \rangle \\ d &= \langle +\frac{1}{10}, -\frac{1}{10}, 0 \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{5256}{125} \\ \phi &= \frac{125}{146} \end{aligned}$$

C3_{sym}⁺ Symmetric point $\langle 0, 0, +\frac{3}{64} \rangle$

The linear incidence conditions are

$$\mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b-c}, \mathbf{H}_{c-a}, \mathbf{H}_{a-b}, \partial V$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{27}{10}, +\frac{21}{20}, -\frac{3}{20} \rangle \\ b &= \langle -\frac{3}{10}, +\frac{51}{20}, +\frac{27}{20} \rangle \\ c &= \langle +\frac{9}{10}, -\frac{3}{5}, +\frac{12}{5} \rangle \\ d &= \langle +\frac{1}{10}, -\frac{1}{20}, -\frac{1}{20} \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{1053}{25} \\ \phi &= \frac{100}{117} \end{aligned}$$

C3_{sym}⁻ Symmetric point $\langle 0, 0, -\frac{33}{320} \rangle$

The linear incidence conditions are

$$\mathbf{G}_a^\pm, \mathbf{G}_b^\pm, \mathbf{G}_c^\pm, \mathbf{G}_{abc}^\pm, \mathbf{G}_{a+b}, \mathbf{H}_{b+c}, \mathbf{H}_{c+a}, \mathbf{H}_{a-b}, \partial V$$

The lattice vectors are

$$\begin{aligned} a &= \langle +\frac{27}{10}, +\frac{21}{20}, -\frac{3}{20} \rangle \\ b &= \langle -\frac{3}{10}, +\frac{51}{20}, +\frac{27}{20} \rangle \\ c &= \langle +\frac{3}{5}, -\frac{21}{20}, +\frac{9}{4} \rangle \\ d &= \langle +\frac{1}{10}, -\frac{1}{20}, -\frac{1}{20} \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \frac{1053}{25} \\ \phi &= \frac{100}{117} \end{aligned}$$

Appendix D Small unit cell packings

D1 The clusters are

$$+\mathbf{B}_1 = +B[o, p, q, r]$$

The cluster vertices are

$$\begin{aligned} o &= \langle +1, +1, +1 \rangle \\ p &= \langle +1, -1, -1 \rangle \\ q &= \langle -1, +1, -1 \rangle \\ r &= \langle -1, -1, +1 \rangle \end{aligned}$$

The neighbors of \mathbf{B}_1 are

$$\begin{array}{lll} \mathbf{B}_1+a & \mathbf{B}_1+b & \mathbf{B}_1+c \\ \mathbf{B}_1-a & \mathbf{B}_1-b & \mathbf{B}_1-c \\ \mathbf{B}_1+a+b & \mathbf{B}_1+b+c & \mathbf{B}_1+c+a \\ \mathbf{B}_1-a-b & \mathbf{B}_1-b-c & \mathbf{B}_1-c-a \\ \mathbf{B}_1+a+b+c & & \\ \mathbf{B}_1-a-b-c & & \end{array}$$

The linear incidence conditions are

$$\begin{aligned} E[o, p] \cap (E[q, r] + a) &\neq \emptyset \\ E[o, q] \cap (E[r, p] + b) &\neq \emptyset \\ E[o, r] \cap (E[p, q] + c) &\neq \emptyset \\ F[o, p, q] \cap (V[r] + a + b) &\neq \emptyset \\ F[o, q, r] \cap (V[p] + b + c) &\neq \emptyset \\ F[o, r, p] \cap (V[q] + c + a) &\neq \emptyset \\ V[o] \cap (F[p, q, r] + a + b + c) &\neq \emptyset \end{aligned}$$

optimize (3 free parameters)

The lattice vectors are

$$\begin{aligned} a &= \langle +2, -\frac{1}{3}, -\frac{1}{3} \rangle \\ b &= \langle -\frac{1}{3}, +2, -\frac{1}{3} \rangle \\ c &= \langle -\frac{1}{3}, -\frac{1}{3}, +2 \rangle \end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned} V &= \det[a, b, c] = \frac{196}{27} \\ \phi &= 1 \cdot \frac{8}{3} / V = \frac{18}{49} \end{aligned}$$

D2 The clusters are

$$\begin{aligned} +\mathbf{B}_1 &= +B[o, p, q, r] \\ -\mathbf{B}_1 &= -B[o, p, q, r] \end{aligned}$$

The cluster vertices are

$$\begin{aligned} o &= \langle +1, +1, +1 \rangle \\ p &= \langle +1, -1, -1 \rangle \\ q &= \langle -1, +1, -1 \rangle \\ r &= \langle -1, -1, +1 \rangle \end{aligned}$$

The neighbors of \mathbf{B}_1 are

$$\begin{aligned}
& \mathbf{B}_1 + a + b \quad \mathbf{B}_1 + b + c \quad \mathbf{B}_1 + c + a \\
& \mathbf{B}_1 - a - b \quad \mathbf{B}_1 - b - c \quad \mathbf{B}_1 - c - a \\
& \mathbf{B}_1 + 2a + b + c \quad \mathbf{B}_1 + 2b + c + a \quad \mathbf{B}_1 + 2c + a + b \\
& \mathbf{B}_1 - 2a - b - c \quad \mathbf{B}_1 - 2b - c - a \quad \mathbf{B}_1 - 2c - a - b \\
& \mathbf{B}_1 + 2a + 2b + 2c \\
& \mathbf{B}_1 - 2a - 2b - 2c \\
& d - \mathbf{B}_1 + a \quad d - \mathbf{B}_1 + b \quad d - \mathbf{B}_1 + c \\
& d - \mathbf{B}_1 - a \quad d - \mathbf{B}_1 - b \quad d - \mathbf{B}_1 - c \\
& d - \mathbf{B}_1 + a + b + c \\
& d - \mathbf{B}_1 - a - b - c
\end{aligned}$$

The linear incidence conditions are

$$\begin{aligned}
& E[o, r] \cap (E[p, q] + a + b) \neq \emptyset \\
& E[o, p] \cap (E[q, r] + b + c) \neq \emptyset \\
& E[o, q] \cap (E[r, p] + c + a) \neq \emptyset \\
& F[o, q, r] \cap (V[p] + 2a + b + c) \neq \emptyset \\
& E[o, r, p] \cap (V[q] + 2b + c + a) \neq \emptyset \\
& F[o, p, q] \cap (V[r] + 2c + a + b) \neq \emptyset \\
& V[o] \cap (F[p, q, r] + 2a + 2b + 2c) \neq \emptyset \\
& F[o, q, r] \cap (d - F[o, q, r] + a) \neq \emptyset \\
& F[o, p, q] \cap (d - F[o, p, q] - b) \neq \emptyset \\
& F[o, r, p] \cap (d - F[o, r, p] - c) \neq \emptyset \\
& F[o, p, q] \cap (d - F[o, p, q] + a + b + c) \neq \emptyset \\
& F[p, q, r] \cap (d - F[p, q, r] - a - b - c) \neq \emptyset
\end{aligned}$$

optimize (2 free parameters)

The lattice vectors are

$$\begin{aligned}
a &= \frac{1}{3} \langle -7 + \sqrt{10}, -19 + 7\sqrt{10}, +16 - 4\sqrt{10} \rangle \\
b &= \frac{1}{3} \langle +7 - 1\sqrt{10}, -7 + 1\sqrt{10}, -10 + 4\sqrt{10} \rangle \\
c &= \frac{1}{3} \langle -1 + 1\sqrt{10}, +25 - 7\sqrt{10}, +2 - 2\sqrt{10} \rangle \\
d &= \frac{1}{3} \langle -1 + 1\sqrt{10}, +9 - 3\sqrt{10}, -8 + 2\sqrt{10} \rangle
\end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned}
V &= 2 \det[a, b, c] = \det[a + b, b + c, c + a] = \frac{16}{27} (139 - 40\sqrt{10}) \\
\phi &= 2 \cdot \frac{8}{3} / V = 9 / (139 - 40\sqrt{10})
\end{aligned}$$

D3 The clusters are

$$\begin{aligned}
+ \mathbf{B}_1 &= +B[o, p, q, r] \\
- \mathbf{B}_1 &= -B[o, p, q, r] \\
T \mathbf{B}_1 &= TB[o, p, q, r]
\end{aligned}$$

The cluster vertices are

$$\begin{aligned}
o &= \langle +1, +1, +1 \rangle \\
p &= \langle +1, -1, -1 \rangle \\
q &= \langle -1, +1, -1 \rangle \\
r &= \langle -1, -1, +1 \rangle
\end{aligned}$$

$$T = \frac{1}{3} \begin{bmatrix} +1 & -2 & -2 \\ -2 & +1 & -2 \\ -2 & -2 & +1 \end{bmatrix}$$

reflection through the plane $+x + y + z = 0$

The neighbors of \mathbf{B}_1 are

$$\begin{aligned}
& \mathbf{B}_1 + a - b \quad \mathbf{B}_1 + b - c \quad \mathbf{B}_1 + c - a \\
& \mathbf{B}_1 - a + b \quad \mathbf{B}_1 - b + c \quad \mathbf{B}_1 - c + a \\
& \mathbf{B}_1 + 2d \\
& \mathbf{B}_1 - 2d \\
& -\mathbf{B}_1 - a \quad -\mathbf{B}_1 - a \quad -\mathbf{B}_1 - c \\
& T\mathbf{B}_1 + d + a \quad T\mathbf{B}_1 + d + b \quad T\mathbf{B}_1 + d + c \\
& T\mathbf{B}_1 - d + a \quad T\mathbf{B}_1 - d + b \quad T\mathbf{B}_1 - d + c
\end{aligned}$$

The linear incidence conditions are

$$\begin{aligned}
& E[r, p] \cap (V[q] + a - b) \neq \emptyset \\
& E[p, q] \cap (V[r] + b - c) \neq \emptyset \\
& E[q, r] \cap (V[p] + c - a) \neq \emptyset \\
& V[o] \cap (F[p, q, r] + 2d) \neq \emptyset \\
& F[o, q, r] \cap (-F[o, q, r] - a) \neq \emptyset \\
& F[o, r, p] \cap (-F[o, r, p] - b) \neq \emptyset \\
& F[o, p, q] \cap (-F[o, p, q] - c) \neq \emptyset
\end{aligned}$$

$$\begin{aligned}
& E[o, p] \cap (TE[o, q] + d + a) \neq \emptyset \\
& E[o, q] \cap (TE[o, r] + d + b) \neq \emptyset \\
& E[o, r] \cap (TE[o, p] + d + c) \neq \emptyset \\
& F[p, q, r] \cap (TF[p, q, r] - d + a) \neq \emptyset \\
& F[p, q, r] \cap (TF[p, q, r] - d + b) \neq \emptyset \\
& F[p, q, r] \cap (TF[p, q, r] - d + c) \neq \emptyset
\end{aligned}$$

The lattice vectors are

$$\begin{aligned}
a &= \langle +1, -1, 0 \rangle \\
b &= \langle 0, +1, -1 \rangle \\
c &= \langle -1, 0, +1 \rangle \\
d &= \langle +\frac{2}{3}, +\frac{2}{3}, +\frac{2}{3} \rangle
\end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned}
V &= 2 \det[d + a, d + b, d + c] = 12 \\
\phi &= 3 \cdot \frac{8}{3} / V = \frac{2}{3}
\end{aligned}$$

D5 The clusters are

$$+\mathbf{B}_5 = +(\mathbf{F}_2 \cup \mathbf{B}_p \cup \mathbf{B}_q \cup \mathbf{B}_r)$$

$$\mathbf{F}_2 = B[o, p, q, r] \cup B[so, p, q, r]$$

$$\mathbf{B}_p = d + T_p B[sp, q, r, o]$$

$$\mathbf{B}_q = e + T_q B[sq, r, o, p]$$

$$\mathbf{B}_r = f + T_r B[sr, o, p, q]$$

The cluster vertices are

$$o = \langle +1, +1, +1 \rangle$$

$$p = \langle +1, -1, -1 \rangle$$

$$q = \langle -1, +1, -1 \rangle$$

$$r = \langle -1, -1, +1 \rangle$$

$$s = -\frac{5}{3}$$

$$T_{\langle i, j, k \rangle}^{\theta} = (\cos \theta) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + (\sin \theta) \begin{bmatrix} 0 & -k & +j \\ +k & 0 & -i \\ -j & +i & 0 \end{bmatrix} + (1 - \cos \theta) \begin{bmatrix} ii & ji & ki \\ ij & jj & kj \\ ik & jk & kk \end{bmatrix}$$

rotation by θ about the unit vector $\langle i, j, k \rangle$

$$T_p = T_{\langle -1, +1, +1 \rangle / \sqrt{3}}^{\alpha}$$

$$T_q = T_{\langle +1, -1, +1 \rangle / \sqrt{3}}^{\beta}$$

$$T_r = T_{\langle +1, +1, -1 \rangle / \sqrt{3}}^{\gamma}$$

The neighbors of \mathbf{B}_5 are

$$\begin{array}{lll} \mathbf{B}_5 + a & \mathbf{B}_5 + b & \mathbf{B}_5 + c \\ \mathbf{B}_5 - a & \mathbf{B}_5 - b & \mathbf{B}_5 - c \\ \mathbf{B}_5 + a - b & \mathbf{B}_5 + b - c & \mathbf{B}_5 + c - a \\ \mathbf{B}_5 - a + b & \mathbf{B}_5 - b + c & \mathbf{B}_5 - c + a \end{array}$$

The linear incidence conditions are

$$F[o, q, r] \cap (d + T_p F[o, q, r]) \neq \emptyset$$

$$F[o, r, p] \cap (e + T_q F[o, r, p]) \neq \emptyset$$

$$F[o, p, q] \cap (f + T_r F[o, p, q]) \neq \emptyset$$

$$(f + T_r E[o, q]) \cap (d + T_p E[o, q]) \neq \emptyset$$

$$(d + T_p E[q, r]) \cap (e + T_q E[o, r]) \neq \emptyset$$

$$(e + T_q E[r, o]) \cap (f + T_r E[o, p]) \neq \emptyset$$

$$E[o, p] \cap (E[so, q] + a) \neq \emptyset$$

$$(d + T_p E[sp, q]) \cap (E[so, r] + b) \neq \emptyset$$

$$(e + T_q E[sq, o, p]) \cap (V[so] + a) \neq \emptyset$$

$$(f + T_r E[o, q]) \cap (E[so, p] + b) \neq \emptyset$$

$$(d + T_p E[sp, r]) \cap (E[so, q] + c) \neq \emptyset$$

$$(e + T_q E[sq, o]) \cap (f + T_r E(sr, p) + c) \neq \emptyset$$

$$(f + T_r E[sr, o]) \cap (e + T_q E[sq, p] + b) \neq \emptyset$$

$$(d + T_p E[r, o]) \cap (f + T_r E[so, q] + c) \neq \emptyset$$

$$(e + T_q V[sq]) \cap (d + T_p F[sp, q, r] + a - b) \neq \emptyset$$

$$(f + T_r E[sr, o]) \cap (e + T_q E[sq, p] + b - c) \neq \emptyset$$

$$(d + T_p E[q, r]) \cap (f + T_r E[sr, o] + c - a) \neq \emptyset$$

$$F[so, q, r] \cap (f + T_r V[sr] + c - a) \neq \emptyset$$

optimize (3 free parameters)

The lattice vectors are

$$a \approx \langle +2.59649957, +0.85417034, +1.06467162 \rangle$$

$$b \approx \langle -0.14944338, +2.53196005, +0.58678219 \rangle$$

$$c \approx \langle -0.02900844, -0.61508232, +2.49547175 \rangle$$

$$d \approx \langle +0.02462012, -0.05626441, +0.08088453 \rangle$$

$$e \approx \langle -0.03576085, -0.12004584, -0.08428499 \rangle$$

$$f \approx \langle -0.04295985, +0.03620318, -0.00675668 \rangle$$

$$\alpha \approx +.07518716$$

$$\beta \approx -.08591647$$

$$\gamma \approx +.04543238$$

The lattice volume and packing density are

$$V = \det[a, b, c] \approx 17.82301085$$

$$\phi = 5 \cdot \frac{8}{3} / V \approx .74809657$$

D6 The clusters are

$$+\mathbf{F}_2 = +(B[o, p, q, r] \cup B[p, q, r, s])$$

$$-\mathbf{F}_2 = -(B[o, p, q, r] \cup B[p, q, r, s])$$

$$-\mathbf{B}_1 = -B[o, p, q, r]$$

$$+\mathbf{B}_1 = +B[o, p, q, r]$$

The cluster vertices are

$$o = \langle +1, +1, +1 \rangle$$

$$p = \langle +1, -1, -1 \rangle$$

$$q = \langle -1, +1, -1 \rangle$$

$$r = \langle -1, -1, +1 \rangle$$

$$s = \langle -\frac{5}{3}, -\frac{5}{3}, -\frac{5}{3} \rangle$$

The neighbors of \mathbf{F}_2 are

$$\mathbf{F}_2 + a - b \quad \mathbf{F}_2 + b - c \quad \mathbf{F}_2 + c - a$$

$$\mathbf{F}_2 - a + b \quad \mathbf{F}_2 - b + c \quad \mathbf{F}_2 - c + a$$

$$\mathbf{F}_2 + d$$

$$\mathbf{F}_2 - d$$

$$e + f - \mathbf{F}_2 - a \quad e + f - \mathbf{F}_2 - b \quad e + f - \mathbf{F}_2 - c$$

$$e - \mathbf{B}_1 + a \quad e - \mathbf{B}_1 + b \quad e - \mathbf{B}_1 + c$$

$$f + \mathbf{B}_1 + a \quad f + \mathbf{B}_1 + b \quad f + \mathbf{B}_1 + c$$

The linear incidence conditions are

$$\begin{aligned}
V[p] \cap (F[o, q, r] + a - b) &\neq \emptyset \\
V[q] \cap (F[o, r, p] + b - c) &\neq \emptyset \\
V[r] \cap (F[s, p, q] + c - a) &\neq \emptyset \\
E[o, p] \cap (E[s, r] + d) &\neq \emptyset \\
F[s, q, r] \cap (e + f - F[s, q, r] - a) &\neq \emptyset \\
F[s, r, p] \cap (e + f - F[s, r, p] - b) &\neq \emptyset \\
F[s, p, q] \cap (e + f - F[s, p, q] - c) &\neq \emptyset \\
F[o, p, q] \cap (e - F[o, p, q] + a) &\neq \emptyset \\
F[o, q, r] \cap (e - F[o, q, r] + b) &\neq \emptyset \\
F[o, r, p] \cap (e - F[o, r, p] + c) &\neq \emptyset \\
E[o, p] \cap (f + E[q, r] + d + a) &\neq \emptyset \\
E[o, q] \cap (f + E[r, p] + d + b) &\neq \emptyset \\
E[o, r] \cap (f + E[p, q] + d + c) &\neq \emptyset \\
(f + F[o, q, r] + d + a) \cap (e - F[o, q, r] + c) &\neq \emptyset
\end{aligned}$$

optimize (1 free parameter)

The lattice vectors are

$$\begin{aligned}
a &= \frac{1}{4104} \langle -3069 + 11\sqrt{396129}, -2382 + 2\sqrt{396129}, -3369 - 1\sqrt{396129} \rangle \\
b &= \frac{1}{4104} \langle +17694 - 34\sqrt{396129}, +27651 - 37\sqrt{396129}, +3777 - 7\sqrt{396129} \rangle \\
c &= \frac{1}{4104} \langle -14625 + 23\sqrt{396129}, -25269 + 35\sqrt{396129}, -408 + 8\sqrt{396129} \rangle \\
d &= \frac{1}{4104} \langle +22629 - 19\sqrt{396129}, -30903 + 65\sqrt{396129}, +4152 + 8\sqrt{396129} \rangle \\
e &= \frac{1}{4104} \langle +4131 - 5\sqrt{396129}, +2382 - 2\sqrt{396129}, -3777 + 7\sqrt{396129} \rangle \\
f &= \frac{1}{1026} \langle -2838 + 2\sqrt{396129}, +2865 - 7\sqrt{396129}, +1116 - 4\sqrt{396129} \rangle
\end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned}
V &= \det[d + a, d + b, d + c] = \frac{1}{701784} (97802181 - 132043\sqrt{396129}) \\
\phi &= 6 \cdot \frac{8}{3} / V = 11228544 / (97802181 - 132043\sqrt{396129})
\end{aligned}$$

D10 The clusters are

$$\begin{aligned}
+ \mathbf{E}_5 &= +(\mathbf{B}_1 \cup \mathbf{E}_4) \\
- \mathbf{E}_5 &= -(\mathbf{B}_1 \cup \mathbf{E}_4) \\
\mathbf{B}_1 &= B[t, u, v, w] \\
\mathbf{E}_4 &= B[o, p, v, w] \cup B[p, q, v, w] \cup B[q, r, v, w] \cup B[r, s, v, w]
\end{aligned}$$

The cluster vertices are

$$\begin{aligned}
o &= \sqrt{6} \langle -\frac{4}{9}, -\frac{4}{9}, -\frac{7}{9} \rangle \\
p &= \sqrt{6} \langle -\frac{2}{3}, -\frac{2}{3}, +\frac{1}{3} \rangle \\
q &= \sqrt{6} \langle 0, 0, +1 \rangle \\
r &= \sqrt{6} \langle +\frac{2}{3}, +\frac{2}{3}, +\frac{1}{3} \rangle \\
s &= \sqrt{6} \langle +\frac{4}{9}, +\frac{4}{9}, -\frac{7}{9} \rangle
\end{aligned}$$

$$t = \langle +1, +1, -2 \rangle$$

$$u = \langle -1, -1, -2 \rangle$$

$$v = \langle -1, +1, 0 \rangle$$

$$w = \langle +1, -1, 0 \rangle$$

The neighbors of \mathbf{E}_5 are

$$\begin{array}{lll}
\mathbf{E}_5 + a + b & \mathbf{E}_5 + b + c & \mathbf{E}_5 + c + a \\
\mathbf{E}_5 - a - b & \mathbf{E}_5 - b - c & \mathbf{E}_5 - c - a \\
d - \mathbf{E}_5 + a & d - \mathbf{E}_5 + b & d - \mathbf{E}_5 + c \\
d - \mathbf{E}_5 - a & d - \mathbf{E}_5 - b & d - \mathbf{E}_5 - c \\
d - \mathbf{E}_5 + a + b + c & & \\
d - \mathbf{E}_5 - a - b - c & &
\end{array}$$

The linear incidence conditions are

$$\begin{aligned}
V[t] \cap (F[p, q, v] + a + b) &\neq \emptyset \\
E[r, v] \cap (E[p, w] + b + c) &\neq \emptyset \\
F[q, r, w] \cap (V[u] + c + a) &\neq \emptyset \\
F[t, u, v] \cap (d - F[t, u, v] + b) &\neq \emptyset \\
F[t, u, w] \cap (d - F[t, u, w] - c) &\neq \emptyset \\
F[o, p, v] \cap (d - F[o, p, v] - a) &\neq \emptyset \\
F[r, s, w] \cap (d - F[r, s, w] + a) &\neq \emptyset \\
F[q, r, v] \cap (d - F[q, r, v] + c) &\neq \emptyset \\
F[p, q, w] \cap (d - F[p, q, w] - b) &\neq \emptyset \\
F[r, s, v] \cap (d - F[r, s, v] + a + b + c) &\neq \emptyset \\
F[o, p, w] \cap (d - F[o, p, w] - a - b - c) &\neq \emptyset
\end{aligned}$$

optimize (1 free parameter)

The lattice vectors are

$$\begin{aligned}
a &= \frac{1}{21540} \langle +16713 + 14822\sqrt{6}, -25455 + 13840\sqrt{6}, 0 \rangle \\
b &= \frac{1}{7180} \langle -2656 + 561\sqrt{6}, +14440 - 2385\sqrt{6}, -7285 - 4835\sqrt{6} \rangle \\
c &= \frac{1}{7180} \langle -2656 + 561\sqrt{6}, +14440 - 2385\sqrt{6}, +7285 + 4835\sqrt{6} \rangle \\
d &= \frac{1}{7180} \langle 0, 0, -4339 + 1889\sqrt{6} \rangle
\end{aligned}$$

The lattice volume and packing density are

$$\begin{aligned}
V &= 2 \det[a, b, c] = \frac{1}{370146232} (7885808912 + 1639809563\sqrt{6}) \\
\phi &= 10 \cdot \frac{8}{3} / V = 29611698560 / (23657426736 + 4919428689\sqrt{6})
\end{aligned}$$