

P-cages from Mozaic Graphs

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1 Graphs

In this supplementary material we consider the p-cages generated from 3 graphs which lead only to very deformed p-cages. The graphs considered are

p-cage name	graph name	Description
TTM3	56_F44_4-0-3_4-3-0_12-2-1_24-1-2_V12_12	Truncated tetrahedron where the hexagons become 3-mosaic.
TOM3	56_F86_6-0-4_8-3-0_24-2-1_48-1-2_V24_24	Truncated octahedron where the hexagons are 3-mosaic.
TCM4	56_F86_6-4-0_8-0-3_24-2-1_48-1-2_V24_24	Truncated cube where the octagons are 4-mosaic.

Table 1: Bi-symmetric hole polyhedron graphs with valency 5 and 6 nodes as well as triangular and square faces and which include mosaics sub-graphs[Piette2024]. The first column is the label describing the p-cages derived from the graph, the second column is the label for the graph used in [Piette2024] and the third column describes a solid for which the planar graph corresponds to the hole polyhedron graph.

The hole-edge mappings for these graphs are presented on Figure 1 for the TTM3 p-cages and on Figure 2.a and 2.b for respectively the TOM3 and TCM4 p-cages.

2 Parametrisation

In what follows we use the same notations as in the main paper: $R_{\mathbf{w}}(\theta)$ denotes a rotation of angle θ around the vector \mathbf{w} while $R_x(\theta)$, $R_y(\theta)$ and $R_z(\theta)$ correspond to rotations of an angle θ around respectively the x , y and z axes.

$\mathbf{u}_{j_1,i;j_2,k}$ is a unit length vector parallel to the intersection line between face i of type j_1 and face k of type j_2 . $\mathbf{Q}_{j_1,i;j_2,k}$ is the intersection point between the reference face of type 2, face i of type j_1 and face k of type j_2 . $\mathbf{P}_{j_1,i;j_2,k}$ is the intersection point between the reference face of type 1, the type j_1 face i and type j_2 face k .

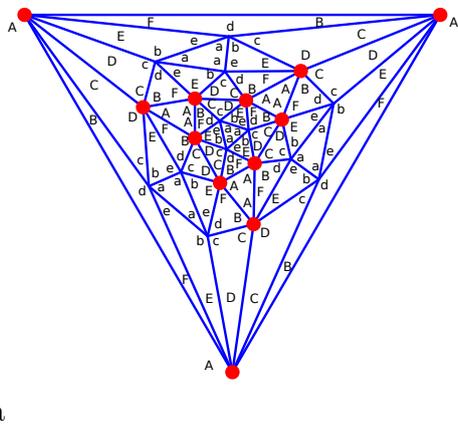


Figure 1: Hole edges mapping for the hole polyhedron graphs: a) **56_F44_4-0-3_4-3-0_12-2-1_24-1-2_V12_12**

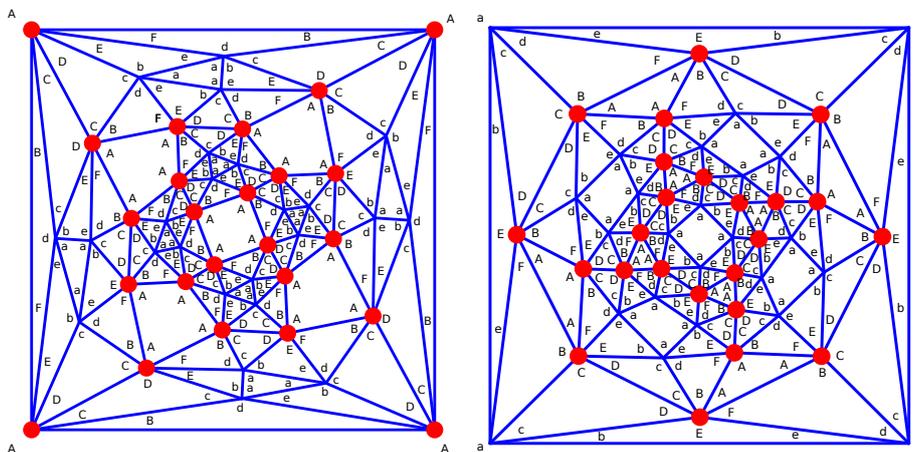


Figure 2: Hole edges mapping for the hole polyhedron graphs: a) **56_F86_6-0-4_8-3-0_24-2-1_48-1-2_V24_24** b) **56_F86_6-4-0_8-0-3_24-2-1_48-1-2_V24_24**

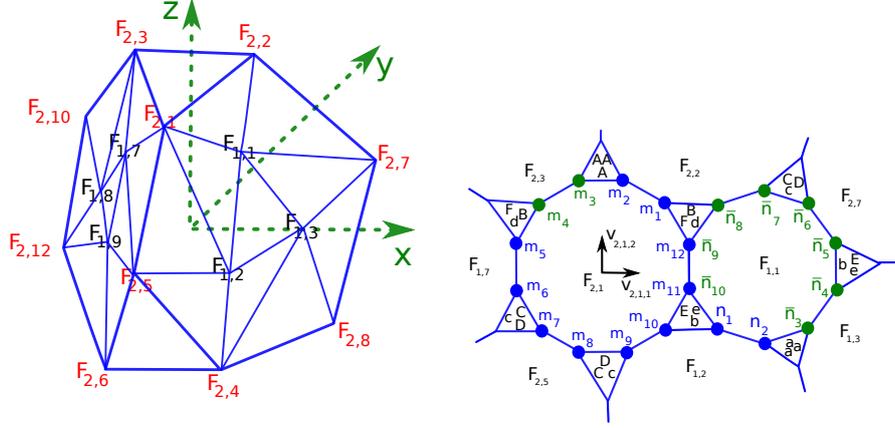


Figure 3: Parametrisation of the truncated tetrahedron with a 3-mosaic p-cage. a) Truncated tetrahedron with a 3-mosaic vectors. b) Mapping of vertices.

2.1 TTM3

The underlying symmetry of these p-cages is that of the truncated tetrahedron. We orient the truncated tetrahedron so that the centre of the top triangle face is in the direction $(0, 0, 1)$ and the centre of the side hexagon is in the direction $(1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3})$. This is illustrated in figure 3.

The vertices of the underlying tetrahedron are

$$\begin{aligned} \mathbf{G}_1 &= (0, 0, 1), & \mathbf{G}_2 &= \left(0, -\frac{\sqrt{8}}{3}, -\frac{1}{3}\right) \\ \mathbf{G}_3 &= \left(\sqrt{\frac{2}{3}}, \frac{\sqrt{2}}{3}, -\frac{1}{3}\right), & \mathbf{G}_4 &= \left(-\sqrt{\frac{2}{3}}, \frac{\sqrt{2}}{3}, -\frac{1}{3}\right) \end{aligned} \quad (1)$$

The centre of the top three faces of the tetrahedron, also the centre of the top three hexagons, are

$$\mathbf{H}_1 \left(\sqrt{\frac{2}{27}}, -\frac{\sqrt{2}}{9}, \frac{1}{9} \right), \quad \mathbf{H}_2 = R_z \left(\frac{4\pi}{3} \right) \mathbf{H}_1, \quad \mathbf{H}_3 = R_z \left(\frac{2\pi}{3} \right) \mathbf{H}_1. \quad (2)$$

Defining

$$\mathbf{e}_t = \left(\sin \left(\frac{\pi}{3} \right), \cos \left(\frac{\pi}{3} \right), 0 \right) = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right). \quad (3)$$

the rotations linking the faces are then as follows:

$$\begin{aligned}
\mathcal{R}_{2,2} &= R_z\left(\frac{2\pi}{3}\right), & \mathcal{R}_{2,3} &= R_z\left(\frac{4\pi}{3}\right), \\
\mathcal{R}_{2,3+i} &= R_{\mathbf{H}_1}\left(\frac{2\pi}{3}\right), & \mathcal{R}_{2,6+i} &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right), & \mathcal{R}_{2,9+i} &= R_{\mathbf{H}_2}\left(\frac{2\pi}{3}\right), \quad i = 1 \dots 3, \\
\mathcal{R}_{1,1} &= R_{\mathbf{e}_t}(\sigma), & \mathcal{R}_{1,2} &= R_{\mathbf{H}_1}\left(\frac{2\pi}{3}\right), & \mathcal{R}_{1,3} &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right), \\
\mathcal{R}_{1,3+i} &= R_z\left(\frac{2\pi}{3}\right), & \mathcal{R}_{1,6+i} &= R_z\left(\frac{4\pi}{3}\right), & \mathcal{R}_{1,9+i} &= R_{\mathbf{G}_2}\left(\frac{4\pi}{3}\right), \quad i = 1 \dots 3.
\end{aligned} \tag{4}$$

We then take as basis vectors of the reference faces

$$\begin{aligned}
\mathbf{V}_{1,1} &= S_1 R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_t}(\sigma) \mathbf{H}_1, \\
\mathbf{v}_{1,1,1} &= R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_t}(\sigma) \mathbf{e}_t, & \mathbf{v}_{1,1,2} &= R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_t}(\sigma) \left(-\frac{1}{2\sqrt{3}}, \frac{1}{6}, \frac{2\sqrt{2}}{3} \right), \\
\mathbf{V}_{2,1} &= S_2 R_z(\phi) (0, -\cos(\theta), \sin(\theta)), \\
\mathbf{v}_{2,1,1} &= R_z(\phi) (1, 0, 0), & \mathbf{v}_{2,1,2} &= R_z(\phi) (0, \sin(\theta), \cos(\theta)). \tag{5}
\end{aligned}$$

$$\begin{aligned}
\mathbf{m}_1 &= Q_{1,1;2,2} + k_1 \mathbf{u}_{2,1;2,2}, & \mathbf{m}_2 &= Q_{1,1;2,2} + k_2 \mathbf{u}_{2,1;2,2}, \\
\mathbf{m}_3 &= R_{\mathbf{G}_1}\left(\frac{4\pi}{3}\right) \mathbf{m}_2, & \mathbf{m}_4 &= R_{\mathbf{G}_1}\left(\frac{4\pi}{3}\right) \mathbf{m}_1, \\
\mathbf{m}_5 &= Q_{2,3;1,7} + k_5 \mathbf{u}_{2,1;1,7}, & \mathbf{m}_6 &= Q_{2,3;1,7} + k_6 \mathbf{u}_{2,1;1,7}, \\
\mathbf{m}_7 &= Q_{1,7;2,5} + k_7 \mathbf{u}_{2,1;2,5}, & \mathbf{m}_8 &= Q_{1,7;2,5} + k_8 \mathbf{u}_{2,1;2,5}, \\
\mathbf{m}_9 &= Q_{2,5;1,2} + k_9 \mathbf{u}_{2,1;1,2}, & \mathbf{m}_{10} &= Q_{2,5;1,2} + k_{10} \mathbf{u}_{2,1;1,2}, \\
\mathbf{m}_{11} &= Q_{1,2;1,1} + k_{11} \mathbf{u}_{2,1;1,1}, & \mathbf{m}_{12} &= Q_{1,2;1,1} + k_{12} \mathbf{u}_{2,1;1,1}, \\
\mathbf{n}_1 &= P_{2,1;1,2} + k_{13} \mathbf{u}_{1,1;1,2}, & \mathbf{n}_2 &= P_{2,1;1,2} + k_{14} \mathbf{u}_{1,1;1,2}, \\
\mathbf{n}_3 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{n}_2, & \mathbf{n}_4 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{n}_1, \\
\mathbf{n}_5 &= R_{\mathbf{H}_1}\left(-\frac{2\pi}{3}\right) R_z \mathbf{m}_{10}, & \mathbf{n}_6 &= R_{\mathbf{H}_1}\left(-\frac{2\pi}{3}\right) R_z \mathbf{m}_9, \\
\mathbf{n}_7 &= R_z\left(\frac{2\pi}{3}\right) \mathbf{m}_6, & \mathbf{n}_8 &= R_z\left(\frac{2\pi}{3}\right) \mathbf{m}_5, \\
\mathbf{n}_9 &= \mathbf{m}_{12}, & \mathbf{n}_{10} &= \mathbf{m}_{11},
\end{aligned} \tag{6}$$

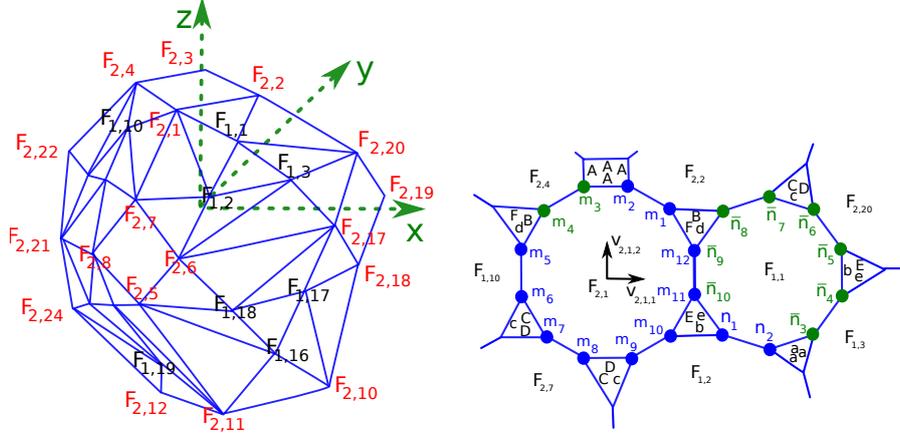


Figure 4: Parametrisation of the truncated octahedron with a 3 mosaic p-cage. a) truncated octahedron vectors. b) Mapping of vertices.

The optimization parameters are θ , ϕ , σ , τ , S_1 , S_2 , k_1 , k_2 , k_5 , k_6 , k_7 , k_8 , k_9 , k_{10} , k_{11} , k_{12} , k_{13} , k_{14} as well as the planar coordinates of the non-shared vertices for both reference faces.

2.2 TOM3

We orient the truncated octahedron so that the centre of the top square face is in the direction $(0, 0, 1)$ and the centre of the side hexagon in the direction $(1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3})$. This is illustrated in figure 4.

The symmetry axes of the truncated octahedron are the centre of the face of the underlying cube

$$\begin{aligned} \mathbf{G}_1 &= (0, 0, 1), & \mathbf{G}_2 &= (0, 0, -1) & \mathbf{G}_3 &= (1, 0, 0), \\ \mathbf{G}_4 &= (-1, 0, 0) & \mathbf{G}_5 &= (0, 1, 0), & \mathbf{G}_6 &= (0, -1, 0). \end{aligned} \quad (7)$$

The centres of the hexagonal faces are then

$$\begin{aligned} \mathbf{H}_1 &= \left(\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right), & \mathbf{H}_2 &= R_z \left(\frac{\pi}{2} \right) \mathbf{H}_1 & \mathbf{H}_3 &= R_z (\pi) \mathbf{H}_1 \\ \mathbf{H}_4 &= R_z \left(\frac{3\pi}{2} \right) \mathbf{H}_1 & \mathbf{H}_{4+i} &= R_x (\pi) \mathbf{H}_i \quad i = 1 \dots 4. \end{aligned} \quad (8)$$

Defining

$$\mathbf{e}_{xy} = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right), \quad (9)$$

the rotations linking the faces are then as follows:

$$\begin{aligned}
\mathcal{R}_{2,2} &= R_z\left(\frac{\pi}{2}\right), & \mathcal{R}_{2,3} &= R_z(\pi), & \mathcal{R}_{2,4} &= R_z\left(\frac{3\pi}{2}\right), \\
\mathcal{R}_{2,4+i} &= R_x\left(\frac{\pi}{2}\right), & \mathcal{R}_{2,8+i} &= R_x(\pi), & \mathcal{R}_{2,12+i} &= R_x\left(\frac{3\pi}{2}\right), \quad i = 1 \dots 4, \\
\mathcal{R}_{2,16+i} &= R_y\left(\frac{\pi}{2}\right), & \mathcal{R}_{2,20+i} &= R_y\left(\frac{3\pi}{2}\right), & & i = 1 \dots 4, \\
\mathcal{R}_{1,2} &= R_{\mathbf{H}_1}\left(\frac{2\pi}{3}\right), & \mathcal{R}_{1,3} &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right), \\
\mathcal{R}_{1,3+i} &= R_z\left(\frac{\pi}{2}\right), & \mathcal{R}_{1,6+i} &= R_z(\pi), & & i = 1 \dots 4, \\
\mathcal{R}_{1,9+i} &= R_z\left(\frac{3\pi}{2}\right), & \mathcal{R}_{1,12+i} &= R_x(\pi), & & i = 1 \dots 12.
\end{aligned} \tag{10}$$

We then take

$$\begin{aligned}
\mathbf{V}_{1,1} &= S_1 R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_{xy}}(\sigma) \mathbf{H}_1, & \mathbf{v}_{1,1,1} &= R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_{xy}}(\sigma) \mathbf{e}_{xy}, \\
\mathbf{v}_{1,1,2} &= R_{\mathbf{H}_1}(\tau) R_{\mathbf{e}_{xy}}(\sigma) \left(-\frac{\sqrt{2}}{\sqrt{3}}, -\frac{1}{\sqrt{(6)}}, \frac{1}{\sqrt{(6)}} \right), \\
\mathbf{V}_{2,1} &= S_2 R_z(\phi) (0, -\cos(\theta), \sin(\theta)), & \mathbf{v}_{2,1,1} &= R_z(\phi) (1, 0, 0), \\
\mathbf{v}_{2,1,2} &= R_z(\phi) (0, \sin(\theta), \cos(\theta)).
\end{aligned} \tag{11}$$

$$\begin{aligned}
\mathbf{m}_1 &= Q_{1,1;2,2} + k_1 \mathbf{u}_{2,1;2,2}, & \mathbf{m}_2 &= Q_{1,1;2,2} + k_2 \mathbf{u}_{2,1;2,2}, \\
\mathbf{m}_3 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{m}_2, & \mathbf{m}_4 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{m}_1, \\
\mathbf{m}_5 &= Q_{2,4;1,10} + k_5 \mathbf{u}_{2,1;1,10}, & \mathbf{m}_6 &= Q_{2,4;1,10} + k_6 \mathbf{u}_{2,1;1,10}, \\
\mathbf{m}_7 &= Q_{1,10;2,7} + k_7 \mathbf{u}_{2,1;2,7}, & \mathbf{m}_8 &= Q_{1,10;2,7} + k_8 \mathbf{u}_{2,1;2,7}, \\
\mathbf{m}_9 &= Q_{2,7;1,2} + k_9 \mathbf{u}_{2,1;1,2}, & \mathbf{m}_{10} &= Q_{2,7;1,2} + k_{10} \mathbf{u}_{2,1;1,2}, \\
\mathbf{m}_{11} &= Q_{1,2;1,1} + k_{11} \mathbf{u}_{2,1;1,1}, & \mathbf{m}_{12} &= Q_{1,2;1,1} + k_{12} \mathbf{u}_{2,1;1,1}, \\
\mathbf{n}_1 &= P_{2,1;1,2} + k_{13} \mathbf{u}_{1,1;1,2}, & \mathbf{n}_2 &= P_{2,1;1,2} + k_{14} \mathbf{u}_{1,1;1,2}, \\
\mathbf{n}_3 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{n}_2, & \mathbf{n}_4 &= R_{\mathbf{H}_1}\left(\frac{4\pi}{3}\right) \mathbf{n}_1, \\
\mathbf{n}_5 &= R_y\left(\frac{\pi}{2}\right) R_z(\pi) \mathbf{m}_{10}, & \mathbf{n}_6 &= R_y\left(\frac{\pi}{2}\right) R_z(\pi) \mathbf{m}_9, \\
\mathbf{n}_7 &= R_y\left(\frac{\pi}{2}\right) \mathbf{m}_6, & \mathbf{n}_8 &= R_y\left(\frac{\pi}{2}\right) \mathbf{m}_5, \\
\mathbf{n}_9 &= \mathbf{m}_{12}, & \mathbf{n}_{10} &= \mathbf{m}_{11},
\end{aligned} \tag{12}$$

The rotations linking the faces are then as follows:

$$\begin{aligned}
\mathcal{R}_{2,2} &= R_{\mathbf{H}_1} \left(\frac{4\pi}{3} \right) & \mathcal{R}_{2,3} &= R_{\mathbf{G}_1} \left(\frac{\pi}{2} \right), & \mathcal{R}_{2,4} &= R_{\mathbf{G}_1} \left(\frac{\pi}{2} \right), \\
\mathcal{R}_{2,5} &= R_{\mathbf{G}_1} (\pi), & \mathcal{R}_{2,6} &= R_{\mathbf{G}_1} (\pi), & \mathcal{R}_{2,7} &= R_{\mathbf{G}_1} \left(\frac{3\pi}{2} \right), \\
\mathcal{R}_{2,8} &= R_{\mathbf{G}_1} \left(\frac{3\pi}{2} \right), & \mathcal{R}_{2,9} &= R_{\mathbf{H}_1} \left(\frac{2\pi}{3} \right), & \mathcal{R}_{2,9+i} &= R_z \left(i \frac{\pi}{2} \right) \quad i = 1, 2, 3, \\
\mathcal{R}_{2,12+i} &= R_x (\pi) & & & & i = 1 \dots 12.
\end{aligned} \tag{15}$$

We then pick the following vectors for the pentavalent faces

$$\begin{aligned}
\mathcal{R}_{1,2} &= R_{\mathbf{G}_1} \left(\frac{\pi}{2} \right), & \mathcal{R}_{1,3} &= R_{\mathbf{G}_1} (\pi), & \mathcal{R}_{1,4} &= R_{\mathbf{G}_1} \left(\frac{3\pi}{2} \right), \\
\mathcal{R}_{1,4+i} &= R_y \left(\frac{\pi}{2} \right) & \mathcal{R}_{1,8+i} &= R_y (\pi) & \mathcal{R}_{1,12+i} &= R_y \left(\frac{3\pi}{2} \right) \quad i = 1, 2, 3, 4 \\
\mathcal{R}_{1,16+i} &= R_x \left(\frac{\pi}{2} \right) & \mathcal{R}_{1,20+i} &= R_x \left(\frac{3\pi}{2} \right) & & i = 1, 2, 3, 4.
\end{aligned} \tag{16}$$

Defining

$$\mathbf{e}_{xy} = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right). \tag{17}$$

We then take

$$\begin{aligned}
\mathbf{V}_{1,1} &= S_1 R_z(\phi) R_{\mathbf{e}_{xy}}(\theta) \left(\frac{1}{2}, -\frac{1}{2}, 1 \right), \\
\mathbf{v}_{1,1,1} &= R_z(\phi) R_{\mathbf{e}_{xy}}(\theta) \mathbf{e}_{xy}, & \mathbf{v}_{1,1,2} &= R_z(\phi) R_{\mathbf{e}_{xy}}(\theta) \left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right), \\
\mathbf{V}_{2,1} &= S_2 R_{\mathbf{H}_1}(\tau) R_z(\sigma) \left(\frac{1}{3}, -1, 1 \right), \\
\mathbf{v}_{2,1,1} &= R_{\mathbf{H}_1}(\tau) R_z(\sigma) \left(\frac{3}{\sqrt{10}}, \frac{1}{\sqrt{10}}, 0 \right), & \mathbf{v}_{2,1,2} &= R_{\mathbf{H}_1}(\tau) R_z(\sigma) \left(-\frac{3}{\sqrt{190}}, \frac{9}{\sqrt{190}}, \frac{\sqrt{10}}{\sqrt{19}} \right).
\end{aligned} \tag{18}$$

$$\begin{aligned}
\mathbf{m}_1 &= Q_{1,18;2,9} + k_1 \mathbf{u}_{2,1;2,9}, & \mathbf{m}_2 &= Q_{1,18;2,9} + k_2 \mathbf{u}_{2,1;2,9}, \\
\mathbf{m}_3 &= R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_2, & \mathbf{m}_4 &= R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_1, \\
\mathbf{m}_5 &= Q_{2,2;1,1} + k_5 \mathbf{u}_{2,1;1,1}, & \mathbf{m}_6 &= Q_{2,2;1,1} + k_6 \mathbf{u}_{2,1;1,1}, \\
\mathbf{m}_7 &= Q_{1,1;2,8} + k_7 \mathbf{u}_{2,1;2,8}, & \mathbf{m}_8 &= Q_{1,1;2,8} + k_8 \mathbf{u}_{2,1;2,8}, \\
\mathbf{m}_9 &= Q_{2,8;1,19} + k_9 \mathbf{u}_{2,1;1,19}, & \mathbf{m}_{10} &= Q_{2,8;1,19} + k_{10} \mathbf{u}_{2,1;1,19}, \\
\mathbf{m}_{11} &= Q_{1,19;1,18} + k_{11} \mathbf{u}_{2,1;1,18}, & \mathbf{m}_{12} &= Q_{1,19;1,18} + k_{12} \mathbf{u}_{2,1;1,18}, \\
\mathbf{n}_1 &= P_{2,2;1,2} + k_{13} \mathbf{u}_{1,1;1,2}, & \mathbf{m}_2 &= P_{2,2;1,2} + k_{14} \mathbf{u}_{1,1;1,2}, \\
\mathbf{n}_3 &= R_{G_1} \left(\frac{3\pi}{2} \right) \mathbf{n}_2, & \mathbf{n}_4 &= R_{G_1} \left(\frac{3\pi}{2} \right) \mathbf{n}_1, \\
\mathbf{n}_5 &= R_{G_1} \left(\frac{3\pi}{2} \right) R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_{10}, & \mathbf{n}_6 &= R_{G_1} \left(\frac{3\pi}{2} \right) R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_9, \\
\mathbf{n}_7 &= \mathbf{m}_6, & \mathbf{n}_8 &= \mathbf{m}_5, \\
\mathbf{n}_9 &= R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_{12}, & \mathbf{n}_{10} &= R_{H_1} \left(\frac{4\pi}{3} \right) \mathbf{m}_{11},
\end{aligned} \tag{19}$$

3 Results

The p-cages **TTM3** and **TOM3** do not lead to any p-cages with deformation below 10% and the best **TCM3** p-cages have deformation exceeding 8% and are not good candidate for protein cages.

The **TCM3** p-cages are all presented graphically in the supplementary file `bi_symmetrix_full_list_56_34.pdf`.

References

[Piette2024] Piette BMAG. Biequivalent Planar Graphs. *Axioms* **2024**, *13*, 437 DOI: 10.3390/axioms13070437/.