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Supporting information for article:

The intrinsic group–subgroup structures of the diamond and gyroid minimal surfaces in their conventional unit cells

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Supporting Information - The intrinsic group-subgroup structures of the Diamond and Gyroid minimal surfaces in their conventional unit cells

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SI.1 Groups, translations, and fundamental domains

SI.1.1 The group with orbifold symbol $*246$

We begin by describing the group labelled $*246$, as it is the most symmetric group of our TPMS. The group is generated by three generators. These are reflections, and we label them R_2, R_4, and R_6. These generators obey the "usual" relations of a *triangle group*:

$$R_2^2 = R_4^2 = R_6^2 = (R_2R_4)^6 = (R_6R_2)^4 = (R_4R_6)^2 = I, \tag{SI.1}$$

where I is the identity element of the group. See Figure SI.1 for a graphical and geometric explanation of this notation. Note that R_2 is the reflection in the geodesic opposite of the $*2$ point in the fundamental domain and similarly for R_4 and R_6.

SI.1.2 The Primitive surface

As the conventional unit cell of the primitive surface is identical to the primitive unit cell, the generators of the translational group are well known and readily expressed using the generators in Equation (SI.1) [1]:

$$\begin{aligned}
t_1 &= R_2R_4R_2R_4R_2R_6R_2R_4R_2R_4R_2R_6 \\
t_2 &= R_4R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2 \\
t_3 &= R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_4 \\
\tau_1 &= R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4 \\
\tau_2 &= R_4R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_6 \\
\tau_3 &= R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2
\end{aligned} \tag{SI.2}$$

as is the relation they obey:

$$I = \tau_1 t_2 \tau_3^{-1} t_1^{-1} \tau_2 t_3 \tau_1^{-1} t_2^{-1} \tau_3 t_1 \tau_2^{-1} t_3^{-1}$$

The notation is graphically explained in Figure SI.1. These translations are readily associated to three lattice vectors in a Euclidean lattice, which we denote a, b, and c:

$$\begin{aligned}
t_1 &\to a & \qquad \tau_1 &\to c - b \\
t_2 &\to b & \qquad \tau_2 &\to a - c \\
t_3 &\to c & \qquad \tau_3 &\to b - a
\end{aligned}$$

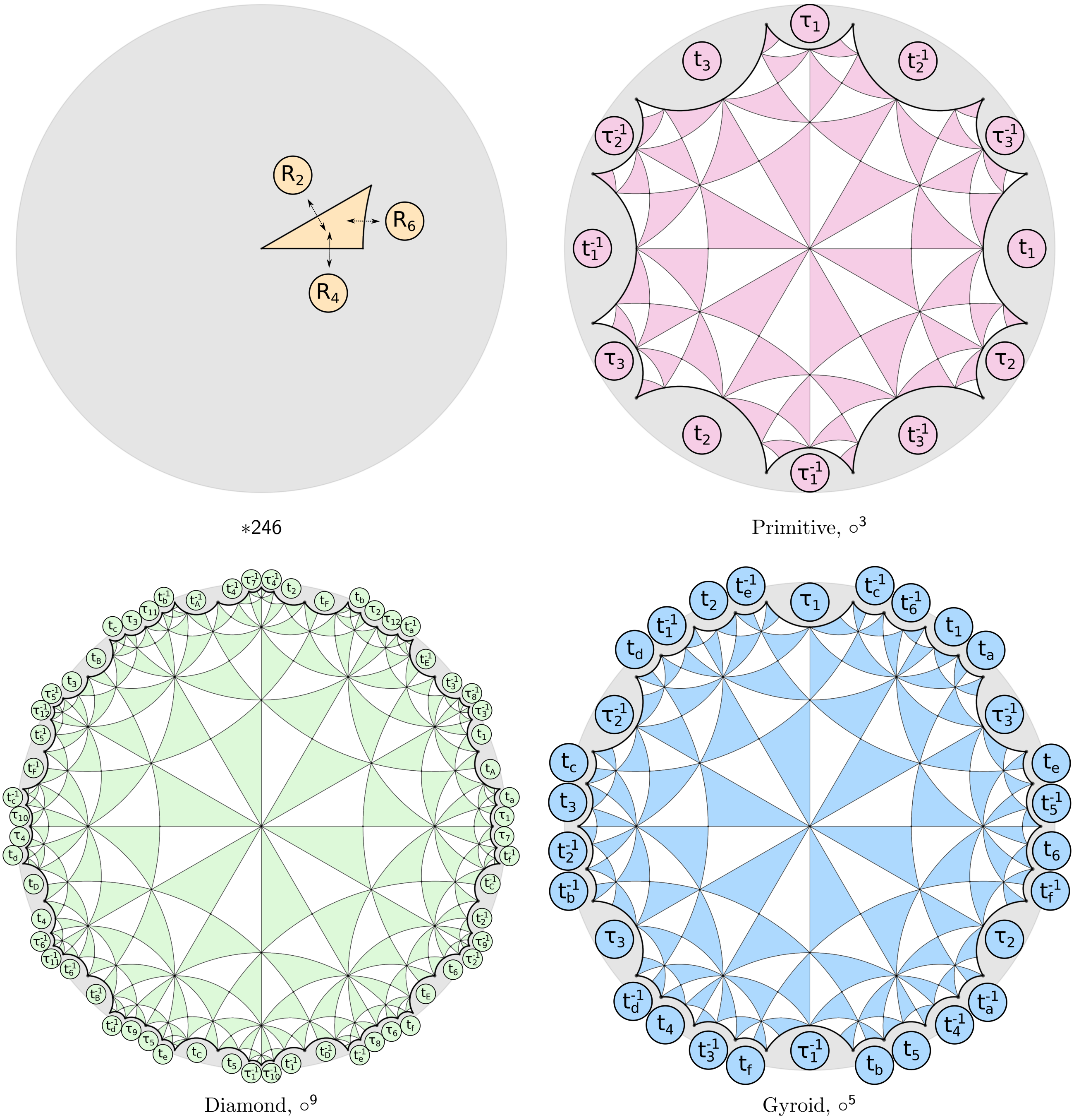

Figure SI.1: Graphical/geometrical explanations of our naming conventions for the groups labelled $*246$, $\circ^3$, $\circ^9$, and $\circ^5$. For $*246$, the annotated operations are reflections, whereas they are translations in the other cases.

SI.1.3 The Diamond surface

When compactified, the unit cell of the Diamond surface shown in Figure 1 in the main text forms a 9-torus. We choose to represent the fundamental domain of this as the 60-gon shown in Figure SI.1. Thus, we need a total of 30 words in the group with orbifold symbol $*246$; the words presented here are reduced by GAP:

$$\begin{aligned}
t_A &= R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2\\
t_B &= R_2R_4R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_2R_4\\
t_C &= R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6\\
t_D &= R_2R_4R_2R_4R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4\\
t_E &= R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2\\
t_F &= R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_2\\
t_1 &= R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4\\
t_2 &= R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6\\
t_3 &= R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_6\\
t_4 &= R_2R_4R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4R_6R_2\\
t_5 &= R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2\\
t_6 &= R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4\\
t_a &= R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2\\
t_b &= R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2\\
t_c &= R_2R_4R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_4R_2\\
t_d &= R_2R_4R_2R_4R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_2R_4\\
t_e &= R_4R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4\\
t_f &= R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6\\
\tau_1 &= R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4\\
\tau_2 &= R_2R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6\\
\tau_3 &= R_2R_4R_2R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_6\\
\tau_4 &= R_2R_4R_2R_4R_2R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2\\
\tau_5 &= R_4R_2R_4R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2\\
\tau_6 &= R_4R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4\\
\tau_7 &= R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2\\
\tau_8 &= R_4R_2R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_6\\
\tau_9 &= R_4R_2R_4R_2R_4R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6\\
\tau_{10} &= R_2R_4R_2R_4R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4\\
\tau_{11} &= R_2R_4R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4\\
\tau_{12} &= R_2R_6R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2
\end{aligned}$$

These obey the following relations for the compactified surface:

$$\begin{aligned}
I = t_1\tau_{10}^{-1}t_c^{-1}\tau_3 &= t_2\tau_9^{-1}t_d^{-1}\tau_4 = t_3\tau_8^{-1}t_e^{-1}\tau_5 = t_4\tau_7^{-1}t_f^{-1}\tau_6 = t_5\tau_{12}^{-1}t_a^{-1}\tau_1 = t_6\tau_{11}^{-1}t_b^{-1}\tau_2 = t_At_4^{-1}t_Dt_1^{-1}\\
&= t_Bt_6^{-1}t_Et_3^{-1} = t_Ct_2^{-1}t_Ft_5^{-1} = \tau_7\tau_4^{-1}\tau_{10}\tau_1^{-1} = \tau_8\tau_3^{-1}\tau_{11}\tau_6^{-1} = \tau_9\tau_2^{-1}\tau_{12}\tau_5^{-1} = t_at_E^{-1}t_ft_C^{-1}t_et_D^{-1}t_dt_B^{-1}t_ct_F^{-1}t_bt_A^{-1}
\end{aligned}$$

GAP confirms that the group is indeed an index-4 subgroup of the group outlined in Eqn (SI.2). As for the primitive surface, each of these can be associated Euclidean lattice translations, a, b, and c, or 0 which we assign to non-trivial loops in the surface:

$$
\begin{array}{lllll}
t_A \to a & t_1 \to 0 & t_a \to 0 & \tau_1 \to -c & \tau_7 \to a \\
t_B \to b & t_2 \to 0 & t_b \to 0 & \tau_2 \to b & \tau_8 \to -b \\
t_C \to c & t_3 \to 0 & t_c \to 0 & \tau_3 \to -a & \tau_9 \to c \\
t_D \to -a & t_4 \to 0 & t_d \to 0 & \tau_4 \to c & \tau_{10} \to -a \\
t_E \to -b & t_5 \to 0 & t_e \to 0 & \tau_5 \to -b & \tau_{11} \to b \\
t_F \to -c & t_6 \to 0 & t_f \to 0 & \tau_6 \to a & \tau_{12} \to -c
\end{array}
$$

SI.1.4 The Gyroid surface

Upon compactification, the unit cell of the Gyroid surface shown in Figure 1 in the main text resembles a 5-torus. We choose to represent the surface of this object by the 30-gon in Figure SI.1. We need a total of 15 translations to describe this shape:

$$
\begin{aligned}
\tau_1 &= R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4 \\
\tau_2 &= R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2 \\
\tau_3 &= R_4R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_6 \\
t_1 &= R_2R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_2 \\
t_2 &= R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_2R_4R_2 \\
t_3 &= R_2R_4R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_4 \\
t_4 &= R_4R_2R_4R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6R_2R_4 \\
t_5 &= R_4R_2R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_6 \\
t_6 &= R_4R_6R_2R_4R_2R_4R_6R_2R_4R_6R_2R_4R_2R_4R_6R_2 \\
t_a &= R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4 \\
t_b &= R_4R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_2R_4R_2 \\
t_c &= R_2R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2 \\
t_d &= R_2R_4R_2R_4R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6R_2R_4R_2R_4 \\
t_e &= R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2 \\
t_f &= R_4R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_6R_2R_4R_2R_4R_6
\end{aligned}
$$

The relationships between these for the compactified Gyroid surface are readily identified from Figure SI.1:

$$
I = t_1t_2t_3t_4t_5t_6 = t_at_4^{-1}t_d^{-1}t_1^{-1} = t_bt_2^{-1}t_e^{-1}t_5^{-1} = t_ct_6^{-1}t_f^{-1}t_3^{-1} = t_d\tau_3t_e\tau_1t_f\tau_2 = \tau_1^{-1}t_c^{-1}\tau_2^{-1}t_a^{-1}\tau_3^{-1}t_b^{-1}
$$

As in the previous section, GAP confirms that the group is an index-2 subgroups of the group outlined in Eqn (SI.2). These relations can once again be associated to three translations, a, b, and c in a Euclidean lattice:

$$
\begin{array}{lll}
\tau_1 \to a & t_1 \to c & t_a \to -b \\
\tau_2 \to c & t_2 \to -b & t_b \to -a \\
\tau_3 \to b & t_3 \to a & t_c \to -c \\
 & t_4 \to -c & t_d \to -b \\
 & t_5 \to b & t_e \to -a \\
 & t_6 \to -a & t_f \to -c
\end{array}
$$

SI.2 Crystallographic information for the net in Figure 2

The canonical equilibrium placement embedding as computed by Systre [2] using the default edge length weight of 3 for the net in Figure 2 can be found below:

Space group	$P4_332$
Unit cell lattice	$(5.51748, 5.51748, 5.51748)$
Unit cell angles, degrees	$(90.0, 90.0, 90.0)$
Coordinates, node 1	$(0.24683, 0.25317, 0.74683)$
Coordinates, node 2	$(0.00015, 0.13368, 0.37736)$
Coordinates, node 3	$(0.08621, 0.28466, 0.32575)$
Coordinates, node 4	$(0.01801, 0.01801, 0.01801)$
Coordinates, edge 1	$(0.08621, 0.28466, 0.32575) \leftrightarrow (0.07575, 0.46534, 0.33621)$
Coordinates, edge 2	$(0.01801, 0.01801, 0.01801) \leftrightarrow (0.16379, -0.07575, -0.03466)$
Coordinates, edge 3	$(0.00015, 0.13368, 0.37736) \leftrightarrow (-0.12736, 0.11632, 0.24985)$
Coordinates, edge 4	$(0.00015, 0.13368, 0.37736) \leftrightarrow (-0.00317, 0.00317, 0.50317)$
Coordinates, edge 5	$(0.00015, 0.13368, 0.37736) \leftrightarrow (0.08621, 0.28466, 0.32575)$
Shortest edge length	0.99950
Average edge length	1.00036
Longest edge length	1.00000
Shortest non-bonded distance	1.55776
Smallest angle between edges, degrees	102.33270
Average angle between edges, degrees	119.99968
Largest angle between edges, degrees	143.68166

Systre-key:

```
3 1 2 0 0 0 1 3 0 0 0 1 4 0 0 0 2 5 0 0 0 2 6 0 0 0 3 7 0 0 0 3 8 0 0 0 4 9 0 0 0 4 10 0 0 0 5
11 0 0 0 5 12 0 0 0 6 13 0 0 0 6 14 0 0 0 7 15 0 0 0 7 16 0 0 0 8 17 0 0 0 8 18 0 0 0 9 19 0 0
0 9 20 0 0 0 10 21 0 0 0 10 22 0 0 0 11 23 0 0 0 11 24 0 0 0 12 25 0 0 0 12 26 0 0 0 13 27 0 0
0 13 28 0 0 0 14 29 0 0 0 14 30 0 0 0 15 23 0 0 0 15 31 0 0 0 16 32 0 0 0 16 33 0 0 0 17 26 1 0
0 17 34 0 0 0 18 35 0 0 0 18 36 0 0 0 19 28 0 1 0 19 37 0 0 0 20 35 0 0 0 20 38 0 0 0 21 24 0 0
1 21 39 0 0 0 22 30 0 0 0 22 33 0 0 1 23 40 0 0 0 24 41 0 0 0 25 42 0 0 0 25 43 0 0 0 26 44 0 0
0 27 42 0 0 0 27 45 0 0 0 28 46 0 0 0 29 40 0 0 1 29 47 0 0 0 30 48 0 0 0 31 49 0 0 0 31 50 0 0
0 32 51 0 0 0 32 52 0 0 0 33 53 0 0 0 34 53 0 0 0 34 54 0 0 0 35 50 0 1 0 36 43 1 0 0 36 55 0 0
0 37 41 0 0 1 37 43 0 0 0 38 44 0 0 0 38 45 0 1 0 39 44 0 0 1 39 49 0 1 1 40 56 0 0 0 41 57 0 0
0 42 58 0 0 0 45 59 0 0 0 46 56 0 0 1 46 60 0 0 0 47 61 0 0 0 47 62 0 0 0 48 57 1 0 1 48 58 1 0
0 49 61 0 0 -1 50 63 0 0 0 51 59 1 0 0 51 63 0 0 0 52 56 1 0 0 52 57 1 0 0 53 61 0 1 -1 54 59 1
1 0 54 60 1 1 -1 55 60 1 1 0 55 62 0 1 0 58 64 0 0 0 62 64 1 0 0 63 64 1 0 0
```

SI.3 Group-subgroup tables and lattice graphs

The tables and graphs containing our enumerated subgroups can be found in the online supporting information as well as from:

`https://www.gitlab.com/mcpe/TPMSGroups/`

References

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[2] Olaf Delgado-Friedrichs and Michael O'Keeffe. Identification of and symmetry computation for crystal nets. *Acta Crystallogr. Sect. A*, 59(4):351–360, 2003.