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Rod groups and their settings as special geometric realisations of line groups

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Rod groups (monoperiodic subgroups of the 3-periodic space groups) are considered as a special case of the commensurate line groups (discrete symmetry groups of the three-dimensional objects translationally periodic along a line). Two different factorizations of line groups are considered: (1) The standard $\mathbf{L} = \mathbf{T}(a)\mathbf{F}$ used in crystallography for rod groups; $\mathbf{F}$ is a finite system of representatives of line-group decomposition in cosets of 1-periodic translation group $\mathbf{T}(a)$; (2) $\mathbf{L} = \mathbf{ZP}$ used in the theory of line groups; $\mathbf{Z}$ is a cyclic generalized translation group and $\mathbf{P}$ is a finite point group. For symmorphic line groups (five line-group families of 13 families) the two factorizations are equivalent: the cyclic group $\mathbf{Z}$ is a monoperiodic translation group and $\mathbf{P}$ is the point group defining the crystal class. For each of the remaining eight families of non-symmorphic line groups the explicit correspondence between rod groups and relevant geometric realisations of the corresponding line groups is established. The settings of rod groups and line groups are taken into account. The results are presented in a table of 75 rod groups listed (in international and factorized notation) by families of the line groups according to the order of the principal axis q (q = 1, 2, 3, 4, 6) of the corresponding isogonal point group.

1. Introduction

Rod groups appear in crystallography as 1-periodic subgroups of space groups with orders of principal rotation axes equal to 1, 2, 3, 4 and 6. There are 75 rod groups and relevant transformations are explicitly tabulated in Kopský & Litvin (2002). Independent study of polymers, or, in more rigorous terms, general 1-periodic three-dimensional objects, stimulated the analysis of 1-periodic symmetry groups that could include rotation axes of arbitrary order. Such groups received the collective name 'line groups'. There are infinitely many line groups and their classification may be performed in a number of ways (Šijački *et al.*, 1972; Vujičić *et al.*, 1977; Damnjanović & Milosěvić, 2010). Rod groups constitute a subset of the set of line groups, but, due to their origin the enumeration, notations and geometric realisations of rod groups possess certain specifics as compared with the line groups. The major task of this paper is to establish the explicit correspondence between rod groups and relevant geometric realisations of the corresponding line groups to lay a bridge between crystallography and the symmetry description of stereoregular polymers. This seems to be of increasing importance due to the very fast developments in the field of nanotubes, nanorods and nanowires. These 1-periodic objects originate from solids, but their symmetry elements may include rotation axes of arbitrary order.

2. Notations and basic definitions

Line groups, being discrete subgroups of the Euclidean group $\mathbf{E}^3 = \mathbb{R}^3 \rtimes \mathbf{O}(3)$, are divided into two classes: commensurate and incommensurate (Damnjanović & Milosěvić, 2010). By definition, commensurate line groups are discrete symmetry groups of three-dimensional objects translationally periodic along a line. Incommensurate line groups contain transformations $(C_\varphi|f)$ with rotation angles φ that are not commensurate with π. In the present work, only commensurate line groups are considered. Normally the z axis is chosen as a line-group principal axis and with such a convention subgroups of pure translations are of the form $\mathbf{T}(a) = \{(e|n(0,0,a)) : n \in \mathbb{Z}\}$. Here a is a translation period defined as a smallest positive real number such that $(e|(0,0,a))$ belongs to the group under consideration. With some abuse of the notation for elements of $\mathbf{T}(a)$, the symbol $(e|a)$ instead of $(e|(0,0,a))$ will be used. The symbol $\mathbf{T}$ will be used for the discrete group of pure translations along the z axis when $a = 1$.

From the definition of commensurate line groups it immediately follows that any such group can be included in short exact sequences $0 \to \mathbf{T}(a) \to \mathbf{L} \to \mathbf{G} \to 1$, where $\mathbf{G}$ is a finite point group (called isogonal). For the classification of short exact sequences [or, in other terminology, extensions of $\mathbf{G}$ by $\mathbf{T}(a)$] there exists a general procedure based on the cohomological theory of group extensions (Brown, 1982). For commensurate line groups such a classification can be performed in full analogy with the classification of space groups (Asher & Janner, 1965, 1968; Mozrzymas, 1974). However, the relatively simple structure of line groups allows one to suggest less general but simpler classification methods. One such method is based on the generalization of the notion of semi-direct group products and is outlined in Šijački *et al.* (1972) and Vujičić *et al.* (1977). An alternative method suggested in Milošević *et al.* (1997) and Damnjanović & Milošević (2010) exploits elementary group-theoretical means (with quite a bit of number theory), but embraces both commensurate and incommensurate line groups.

It is well known that some subgroups of the group of Euclidean transformations admit different geometric realisations. An example is the group $\mathbf{C}_{nv}(\alpha) = \mathbf{C}_n \cup \sigma_\alpha \mathbf{C}_n$, where σ_α is a reflection in the vertical plane passing through the z axis and a line in the xy plane with the direction vector $(\cos\alpha, \sin\alpha, 0)$ is a geometric realisation of the $\mathbf{C}_{nv}$ group defined by the setting angle α. The setting angle is usually taken to be equal to zero, which corresponds to choosing xz as a benchmark reflection plane. In particular, in the theory of line groups the setting angle is usually chosen equal to zero. On the other hand, groups $\mathbf{C}_n$ stipulate a unique geometric realisation as soon as the axis and direction of rotations are chosen. Rod groups, being a special case of the line groups, arise as 1-periodic subgroups of space groups, and it comes as no surprise that space groups may contain different geometric realisations of the same line group. In crystallography different realisations of the same rod group are called *settings*. In the theory of line groups crystallographic settings manifest themselves as geometric realisations with specially chosen setting angles. Besides infinitely many geometric realisations of line groups containing reflections in vertical planes or *Umklapp* transformations, there exist realisations that differ in the choice of a horizontal reflection plane. For example, instead of the point group $\mathbf{C}_{nh} = \mathbf{C}_n \cup \sigma_h \mathbf{C}_n$ it is possible to take the group $\mathbf{C}'_{nh} = \mathbf{C}_n \cup (\sigma_h|a/2)\mathbf{C}_n$, which corresponds to selecting as the reflection plane the affine plane parallel to the xy plane but passing through the point $(0, 0, a/4)$.

As we already mentioned, the rod groups are distinguished among general line groups by the orders q of the principal axes of the isogonal groups, which can take the values q = 1, 2, 3, 4, 6. For q = 3, 6 in tables of rod groups (Kopský & Litvin, 2002) the *hexagonal* coordinate system is used. The hexagonal coordinate system is obtained by the rotation of the y axis counter-clockwise by an angle of $\pi/6$ in the xy plane. The basis vectors of the hexagonal coordinate system are connected with the Cartesian ones by the relations

$$h_1 = e_1, \quad h_2 = -(1/2)e_1 + (3^{1/2}/2)e_2, \quad h_3 = e_3. \qquad (1)$$

To compare line- and rod-group realisations, one should be able to proceed from the usual mathematical notation of affine transformations to that accepted in crystallography (Kopský & Litvin, 2002).

Symmetry elements (reflection planes, axes *etc.*) are defined in crystallography *parametrically*. For example, in Cartesian coordinates a triplet $x, 0, z$ defines a plane as a locus $\{xe_1 + ze_3 : x, z \in \mathbb{R}\}$. It is clear that the normal vector of this plane is $e_2 = (0, 1, 0)$. A triplet $x + s, -x, z$ defines the affine plane $\{(x + s)e_1 - xe_2 + ze_3 : x, z \in \mathbb{R}\}$ passing through the point $(s, 0, 0)$ and with the normal vector $e_1 + e_2 = (1, 1, 0)$. A triplet $x, -x, 0$ defines a line $\{xe_1 - xe_2 : x \in \mathbb{R}\}$ in the xy plane. A triplet $x, -x, a/4$ is a line in the affine plane passing through the point $(0, 0, a/4)$ parallel with the xy plane. The analogous convention is used in the case where the hexagonal coordinate system is used. For example, lines in the xy plane having angles with the x axis of $-\pi/3, -\pi/6, 0, \pi/6, \pi/3, \pi/2, 2\pi/3$ and passing through the origin have the following parametric presentation in the hexagonal coordinate system: $0, y, 0$; $x, -x, 0$; $x, 0, 0$; $2x, x, 0$; $x, x, 0$; $x, 2x, 0$; $0, y, 0$.

Basic symmetry operations of rod groups in crystallography have the following designations: rotation $(C_{\pm 2\pi/n}|0)$ around the z axis is designated as $n^{\pm}\ 0, 0, z$, screw rotation $(C_{\pm 2\pi/n}|f)$ as $n^{\pm}(f)\ 0, 0, z$, reflection $(\sigma_0|0)$ with respect to the xz plane as $m\ x, 0, z$, reflection $(\sigma_{\pi/4}|0)$ as $m\ x, x, z$, reflection $(\sigma_h|0)$ as $m\ x, y, 0$. Glide-plane reflections of the type $(\sigma_0|a/2)$ are designated as $c\ x, 0, z$, transformations $(\sigma_h|a/2)$ as $m\ x, y, a/4$. *Umklapp* transformations are interpreted as rotations: for example, transformation $(u_{\pi/2}|0)$ is designated as $2\ 0, y, 0$, and transformation $(u_{\pi/2}|a/2)$ as $2\ 0, y, a/4$. The notation for transformations of the type $(\sigma_h C_{\pm 2\pi/n}|f)$ is slightly more cumbersome and not unique: operation $(\sigma_h C_{\pm 2\pi/n}|0)$ is designated as $\overline{n}^{\pm}\ 0, 0, z; 0, 0, 0$, and operation $(\sigma_h C_{\pm 2\pi/n}|a/2)$ either as $\overline{n}^{\pm}(a/2)\ 0, 0, z; 0, 0, 0$ or as $\overline{n}^{\pm}\ 0, 0, z; 0, 0, a/4$. In the last example the ambiguity is connected with the existence of two equivalent presentations of the transformation under consideration: $(\sigma_h C_{\pm 2\pi/n}|a/2) = (\sigma_h|a/2)(C_{\pm 2\pi/n}|0) = (C_{\pm 2\pi/n}|a/2)(\sigma_h|0)$. Inversion at the origin is encoded as $\overline{1}\ 0, 0, 0$.

3. Different factorization of line groups

Under the standard approach, any commensurate line group may be presented in the form

$$\mathbf{L} = \mathbf{T}(a)\mathbf{F}, \qquad (2)$$

where $\mathbf{F}$ is a finite system of coset representatives of line-group decomposition in cosets of $\mathbf{T}(a)$. The choice of representatives is not unique and any specific set $\mathbf{F}$ is, in general, not a subgroup of $\mathbf{L}$. However, since $\mathbf{L}$ is the extension of $\mathbf{G}$ by $\mathbf{T}(a)$, $\mathbf{F}$ can be interpreted as a group with multiplication modulo pure translations. Factorization (2) of line group $\mathbf{L}$ will be referred to as standard. The Damnjanović approach (Damnjanović & Milošević, 2010) is based on the factorization

$$\mathbf{L} = \mathbf{Z}\mathbf{P}, \qquad (3)$$

where $\mathbf{Z}$ is a cyclic generalized translation group and $\mathbf{P}$ is a finite point group. The requirement that $\mathbf{Z}$ contains a subgroup of pure translations immediately implies that $\mathbf{Z}$ must be of one of the following two forms:

$$\mathbf{Z} = \mathbf{T}^k_q(f) = \langle (C_{2\pi k/q}|f) \rangle \quad \text{or} \quad \mathbf{Z} = \mathbf{T}'(a) = \langle (\sigma_v|a/2) \rangle, \quad (4)$$

where f is a *fractional* translation.

If the factorization (3) is used, then the structure of line groups may be studied in several steps. As the first step it is reasonable to analyze the discrete point groups operating on cylindrical surfaces. Such an analysis is not complicated and gives seven families of the point groups which leave a cylinder invariant (the so-called axial point groups):

$$\mathbf{C}_n, \quad \mathbf{S}_{2n}, \quad \mathbf{C}_{nh}, \quad \mathbf{D}_n, \quad \mathbf{C}_{nv}, \quad \mathbf{D}_{nd}, \quad \mathbf{D}_{nh}. \tag{5}$$

Then step-by-step it is necessary to consider the products **ZP** to find out when each concrete product is a group, and to ascertain that it has not occurred at previous steps, probably in a different guise. In Table 2.2 from Damnjanović & Milosěvić (2010) the result of such an analysis is presented: all line groups are divided into 13 families, each family includes infinitely many line groups. Among these families there are five symmorphic ones for which factorization (3) coincides with the standard one.

4. Rod groups as a special case of line groups

In the theory of line groups the first family, being one of the simplest, plays nevertheless the most important role. The reason is in the structure of axial groups **P** in (3): any such group contains $\mathbf{C}_n$ as its subgroup and, consequently, admits decomposition in cosets of $\mathbf{C}_n$.

The main result concerning the line groups of the first family may be formulated as follows (Damnjanović & Milosěvić, 2010):

For a fixed translation period a, *commensurate* line groups of the first family are parametrized by triplets $(\tilde{q}, n, k) \in \mathbb{N}^+ \times \mathbb{N}^+ \times K$,

$$\mathbf{L} = \mathbf{T}^k_{\tilde{q}n}\left(\frac{a}{\tilde{q}}\right)\mathbf{C}_n = \mathbf{T}(a)\mathbf{F}, \tag{6}$$

where $K = \{k : 0 \le k \le \tilde{q} \text{ and } \mathrm{GCD}(\tilde{q}, k) = 1\}$, GCD is the abbreviation for the greatest common divisor and $\mathbb{N}^+$ is the set of positive natural numbers. Here

$$\mathbf{F} = \bigcup_{t=0}^{\tilde{q}-1}\left(C_{(2\pi k/q)t}\left|\frac{a}{\tilde{q}}t\right.\right)\mathbf{C}_n, \quad q = \tilde{q}n. \tag{7}$$

Note that, by definition, $\mathrm{GCD}(l, 0) = 1 \Leftrightarrow l = 1$ and, consequently, $k = 0$ corresponds to the case $\mathbf{T}^0_n(a) = \mathbf{T}(a)$. It is pertinent to emphasize as well that a [for fixed $(\tilde{q}, n, k)$] is a translation period of the maximal free 1-periodic subgroup $\mathbf{T}(a)$ of the line group (6). The analogous subgroup of the generalized group **Z** of translations has, in general, greater period (Damnjanović & Milosěvić, 2010).

Line groups of the first family do not depend on the setting angle, because their geometric realisation is uniquely defined by the choice of the rotation axis and a convention about the direction of rotation (normally counter-clockwise). Therefore, each rod group of the first family should appear in the unique setting. We consider as an example rod groups of the first family with $q = 3$. From equation (6) it readily follows that

$$q = 3 \Rightarrow \begin{cases} \tilde{q} = 1 \text{ and } n = 3 \text{ gives line group} & \mathbf{T}(a)\mathbf{C}_3 \\ \tilde{q} = 3 \text{ and } n = 1 \text{ gives line groups} & \begin{cases}\mathbf{T}^1_3(a/3)\mathbf{C}_1 \\ \mathbf{T}^2_3(a/3)\mathbf{C}_1\end{cases} \end{cases}. \tag{8}$$

Symmetry operations corresponding to these three cases are

$$\mathbf{F} = \begin{cases} \mathbf{C}_3 = \{1;\ 3^+\ 0,0,z;\ 3^-\ 0,0,z\}, \\ \mathbf{C}_1 \cup (C_{2\pi/3}|a/3)\mathbf{C}_1 \cup (C_{-2\pi/3}|2a/3)\mathbf{C}_1 \\ \quad = \{1;\ 3^+(a/3)\ 0,0,z;\ 3^-(2a/3)\ 0,0,z\}, \\ \mathbf{C}_1 \cup (C_{-2\pi/3}|a/3)\mathbf{C}_1 \cup (C_{2\pi/3}|2a/3)\mathbf{C}_1 \\ \quad = \{1;\ 3^-(a/3)\ 0,0,z;\ 3^+(2a/3)\ 0,0,z\}. \end{cases} \tag{9}$$

and, using the tables from Kopský & Litvin (2002), it is easy to conclude that we have the rod groups $\not{p}3, \not{p}3_1$ and $\not{p}3_2$.

Line groups of the second and the third families are symmorphic and do not depend on the setting angle.

Now let us turn to the fourth family. In this case, the dependence on the setting angle is also absent, but relevant geometric realisations may require a shift of the horizontal reflection plane. The general expression for the line groups of the fourth family in the two factorizations is

$$\mathbf{L} = \mathbf{T}^1_{2n}\left(\frac{a}{2}\right)\mathbf{C}_{nh} = \mathbf{T}(a)\mathbf{F}, \tag{10}$$

where

$$\mathbf{F} = \mathbf{C}_{nh}\bigcup\left(C_{\pi/n}\left|\frac{a}{2}\right.\right)\mathbf{C}_{nh}. \tag{11}$$

Rod groups from this family correspond to $q = 2, 4, 6$. To get their standard realisation it it necessary to replace $\mathbf{C}_{nh}$ by $\mathbf{C}'_{nh}$ for $q = 2$ and $q = 6$. Indeed, if $q = 2$ then

$$\begin{aligned}\mathbf{F} &= \{(e|0), (\sigma_h|0), (C_\pi|a/2), (\sigma_h C_\pi|a/2)\} \\ &= \{1;\ m\ x,y,0;\ 2(a/2)\ 0,0,z;\ \bar{2}(a/2)\ 0,0,z;\ 0,0,0\}.\end{aligned} \tag{12}$$

This realisation is not standard. Replacing $\mathbf{C}_{nh}$ by $\mathbf{C}'_{nh}$ gives

$$\begin{aligned}\mathbf{F}' &= \{(e|0), (\sigma_h|a/2), (C_\pi|a/2), (\sigma_h C_\pi|0)\} \\ &= \{1;\ m\ x,y,a/4;\ 2(a/2)\ 0,0,z;\ \bar{1}\ 0,0,0\}\end{aligned} \tag{13}$$

and this realisation corresponds to the rod group $\not{p}112_1/m$. Analogous arguments lead to the conclusion that $\mathbf{T}^1_4(a/2)\mathbf{C}_{2h} = \not{p}4_2/m$ and $\mathbf{T}^1_6(a/2)\mathbf{C}'_{3h} = \not{p}6_3/m$.

The general expression for the line groups of the fifth family in the two factorizations is

$$\mathbf{L} = \mathbf{T}^k_{\tilde{q}n}\left(\frac{a}{\tilde{q}}\right)\mathbf{D}_n(\alpha) = \mathbf{T}(a)\mathbf{F}(\alpha), \tag{14}$$

where

$$\mathbf{F}(\alpha) = \bigcup_{t=0}^{\tilde{q}-1}\left(C_{(2\pi k/q)t}\left|\frac{a}{\tilde{q}}t\right.\right)\mathbf{D}_n(\alpha) \tag{15}$$

and

$$\mathbf{D}_n(\alpha) = \mathbf{C}_n \cup (u_\alpha|0)\mathbf{C}_n. \tag{16}$$

Here we have infinitely many geometric realisations, since the dihedral group contains the *Umklapp* transformation $u_\alpha = \sigma_h\sigma_\alpha$. Rod groups of this family appear in different settings only for $q = 3$ and it is this case that will be analyzed here. We have

$$q = 3 \Rightarrow \begin{cases} \tilde{q} = 1 \text{ and } n = 3 \text{ gives line group} & \mathbf{T}(a)\mathbf{D}_3(\alpha) \\ \tilde{q} = 3 \text{ and } n = 1 \text{ gives line groups} & \begin{cases} \mathbf{T}_3^1(a/3)\mathbf{D}_1(\alpha) \\ \mathbf{T}_3^2(a/3)\mathbf{D}_1(\alpha) \end{cases} \end{cases}. \tag{17}$$

In the first case ($\tilde{q} = 1$ and $n = 3$)

$$\mathbf{F}(\alpha) = \{(e|0), (C_{2\pi/3}|0), (C_{-2\pi/3}|0), (u_\alpha|0), (u_{\alpha-\pi/3}|0), (u_{\alpha+\pi/3}|0)\}. \tag{18}$$

For $\alpha = 0$ in hexagonal coordinates we have

$$\mathbf{F}_{\rm hex}(0) = \{1;\ 3^+\ 0,0,z;\ 3^-\ 0,0,z;\ 2\ x,0,0;\ 2\ 0,y,0;\ 2\ x,x,0\} \tag{19}$$

and this is the second setting $\not{p}321$ of rod group No. 46.

Substitution of $\alpha = \pi/6$ into the right-hand side of equation (18) gives

$$\mathbf{F}_{\rm hex}(\pi/6) = \{1;\ 3^+\ 0,0,z;\ 3^-\ 0,0,z;\ 2\ 2x,x,0;\ 2\ x,-x,0;\ 2\ x,2x,0\} \tag{20}$$

and this realisation corresponds to the first setting $\not{p}312$ of rod group No. 46. From equation (18) it is easy to see that the choice of the proper setting angle is not unique: $\mathbf{F}(0) = \mathbf{F}(\pi/3)$ and $\mathbf{F}(\pi/6) = \mathbf{F}(-\pi/6)$.

In the second case ($\tilde{q} = 3$, $n = 1$ and $k = 1$)

$$\mathbf{F}(\alpha) = \{(e|0), (C_{2\pi/3}|a/3), (C_{-2\pi/3}|2a/3), (u_\alpha|0), (u_{\alpha+\pi/3}|a/3), (u_{\alpha-\pi/3}|2a/3)\}. \tag{21}$$

For $\alpha = 0$ in hexagonal coordinates we have

$$\mathbf{F}_{\rm hex}(0) = \{1;\ 3^+(a/3)\ 0,0,z;\ 3^-(2a/3)\ 0,0,z;\ 2\ x,0,0;\ 2\ x,x,a/6;\ 2\ 0,y,a/3\}, \tag{22}$$

but this realisation is not found in Kopský & Litvin (2002). The standard realisations correspond to $\alpha = \pi/3$ and $\alpha = \pi/6$:

$$\mathbf{F}_{\rm hex}(\pi/3) = \{1;\ 3^+(a/3)\ 0,0,z;\ 3^-(2a/3)\ 0,0,z;\ 2\ x,x,0;\ 2\ 0,y,a/6;\ 2\ x,0,a/3\}, \tag{23a}$$

$$\mathbf{F}_{\rm hex}(\pi/6) = \{1;\ 3^+(a/3)\ 0,0,z;\ 3^-(2a/3)\ 0,0,z;\ 2\ 2x,x,0;\ 2\ x,2x,a/6;\ 2\ x,-x,a/3\}. \tag{23b}$$

These two sets of transformations correspond to the settings $\not{p}3_121$ and $\not{p}3_112$, respectively (rod group No. 47).

In exactly the same manner the third case ($\tilde{q} = 3$, $n = 1$ and $k = 2$) is analyzed to give $\mathbf{T}_3^2(a/3)\mathbf{D}_1(\pi/3) = \not{p}3_221$ and $\mathbf{T}_3^2(a/3)\mathbf{D}_1(\pi/6) = \not{p}3_212$ (rod group No. 48).

Realisations of rod groups of the fifth family with $q = 1, 2, 4, 6$ correspond to the setting angle $\alpha = 0$.

Line groups of the sixth family are symmorphic and it is easy to ascertain that standard realisations correspond to $\alpha = \pi/2$ for $q = 1$ (rod group $\not{p}m11$), $\alpha = 0$ for $q = 2$ (rod group $\not{p}mm2$), $\alpha = 0, \pi/6$ for $q = 3$ (settings $\not{p}31m$ and $\not{p}3m1$, respectively), and $\alpha = 0$ for $q = 4, 6$ (rod groups $\not{p}4mm$ and $\not{p}6mm$).

Line groups of the seventh family, being nonsymmorphic, are organized nevertheless in a way analogous to that of the sixth family. Standard realisations of the corresponding rod groups are obtained from the groups of the sixth family simply by replacing m by c in each group symbol.

Now let us consider line groups of the eighth family:

$$\mathbf{L} = \mathbf{T}_{2n}^1\left(\frac{a}{2}\right)\mathbf{C}_{nv}(\alpha) = \mathbf{T}(a)\mathbf{F}(\alpha), \tag{24}$$

where

$$\mathbf{F}(\alpha) = \mathbf{C}_{nv}(\alpha) \bigcup \left(C_{\pi/n}\middle|\frac{a}{2}\right)\mathbf{C}_{nv}(\alpha). \tag{25}$$

Relevant rod groups correspond to $q = 2, 4, 6$. We have

$$\mathbf{F}(\alpha) = \begin{cases} \{(e|0), (\sigma_\alpha|0), (C_\pi|a/2), (\sigma_{\alpha+\pi/2}|a/2)\} \text{ for } q = 2, \\ \{(e|0), (C_\pi|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/2}|0), (C_{\pi/2}|a/2), \\ (C_{-\pi/2}|a/2), (\sigma_{\alpha+\pi/4}|a/2), (\sigma_{\alpha-\pi/4}|a/2)\} \text{ for } q = 4, \\ \{(e|0), (C_{2\pi/3}|0), (C_{-2\pi/3}|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/3}|0), \\ (\sigma_{\alpha-2\pi/3}|0), (C_{\pi/3}|a/2), (C_\pi|a/2), (C_{-\pi/3}|a/2), \\ (\sigma_{\alpha+\pi/6}|a/2), (\sigma_{\alpha-\pi/6}|a/2), (\sigma_{\alpha-\pi/2}|a/2)\} \text{ for } q = 6. \end{cases} \tag{26}$$

For $q = 2$ and $\alpha = 0$ the standard rod-group realisation is not found in the tables of Kopský & Litvin (2002) but $\alpha = \pi/2$ readily gives rod group $\not{p}mc2_1$. For $q = 4$ the setting angle $\alpha = 0$ gives the second setting $\not{p}4_2mc$ of rod group No. 35, and $\alpha = \pi/4$ gives the first setting $\not{p}4_2cm$ of this group. For $q = 6$ we have $\mathbf{T}_6^1(a/2)\mathbf{C}_{3v}(0) = \not{p}6_3cm$ and $\mathbf{T}_6^1(a/2)\mathbf{C}_{3v}(\pi/6) = \not{p}6_3mc$, the second and the first settings of rod group No. 70, respectively.

Line groups of the ninth family are symmorphic and $\mathbf{F}(\alpha) = \mathbf{D}_{nd}(\alpha) = \mathbf{C}_n \cup (\sigma_\alpha|0)\mathbf{C}_n \cup (\sigma_h C_{\pi/n}|0)\mathbf{C}_n \cup (u_{\alpha+\pi/2n}|0)\mathbf{C}_n$. Rod groups correspond to $q = 1, 2, 3$ and

$$\mathbf{F}(\alpha) = \begin{cases} \{(e|0), (\sigma_\alpha|0), (I|0), (u_{\alpha+\pi/2}|0)\} \text{ for } q = 1, \\ \{(e|0), (C_\pi|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/2}|0), (\sigma_h C_{\pi/2}|0), \\ (\sigma_h C_{-\pi/2}|0), (u_{\alpha+\pi/4}|0), (u_{\alpha-\pi/4}|0)\} \text{ for } q = 2, \\ \{(e|0), (C_{2\pi/3}|0), (C_{-2\pi/3}|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/3}|0), \\ (\sigma_{\alpha+\pi/3}|0), (\sigma_h C_{\pi/3}|0), (I|0), (\sigma_h C_{-\pi/3}|0), \\ (u_{\alpha+\pi/6}|0), (u_{\alpha-\pi/6}|0), (u_{\alpha+\pi/2}|0)\} \text{ for } q = 3. \end{cases} \tag{27}$$

The line-group realisation with $q = 1$ and $\alpha = \pi/2$ corresponds to the rod group $\not{p}2/m11$. For $q = 2$ and $\alpha = 0, \pi/4$ we have the second ($\not{p}\bar{4}m2$) and the first ($\not{p}\bar{4}2m$) setting of rod group No. 37, respectively. For $q = 3$ setting angles $\alpha = 0, \pi/6$ of line group $\mathbf{T}(a)\mathbf{D}_{nd}$ give rod group No. 51 settings $\not{p}\bar{3}1m$ and $\not{p}\bar{3}m1$.

Family ten contains non-symmorphic line groups

$$\mathbf{L} = \mathbf{T}'\left(\frac{a}{2}\right)\mathbf{S}_{2n}(\alpha) = \mathbf{T}(a)\mathbf{F}(\alpha), \tag{28}$$

where

$$\mathbf{F}(\alpha) = \mathbf{S}_{2n} \bigcup \left(\sigma_\alpha\middle|\frac{a}{2}\right)\mathbf{S}_{2n}. \tag{29}$$

Rod groups from this family correspond to $q = 1, 2, 3$ and

Table 1
Rod groups (international and factorized notation) listed by families F of the line groups according to the order q of the principal axis of the corresponding isogonal group.

F	q = 1	q = 2	q = 3	q = 4	q = 6
1	1 $\mathbf{TC}_1 = p1$	8 $\mathbf{TC}_2 = p112$ 9 $\mathbf{T}_2\mathbf{C}_1 = p112_1$	42 $\mathbf{TC}_3 = p3$ 43 $\mathbf{T}_3\mathbf{C}_1 = p3_1$ 44 $\mathbf{T}_3^2\mathbf{C}_1 = p3_2$	23 $\mathbf{TC}_4 = p4$ 24 $\mathbf{T}_4\mathbf{C}_1 = p4_1$ 25 $\mathbf{T}_4\mathbf{C}_2 = p4_2$ 26 $\mathbf{T}_4^3\mathbf{C}_1 = p4_3$	53 $\mathbf{TC}_6 = p6$ 54 $\mathbf{T}_6\mathbf{C}_1 = p6_1$ 55 $\mathbf{T}_6\mathbf{C}_2 = p6_2$ 56 $\mathbf{T}_6\mathbf{C}_3 = p6_3$ 57 $\mathbf{T}_6^2\mathbf{C}_2 = p6_4$ 58 $\mathbf{T}_6^5\mathbf{C}_1 = p6_5$
2		2 $\mathbf{TS}_2 = p\bar{1}$		27 $\mathbf{TS}_4 = p\bar{4}$	45 $\mathbf{TS}_6 = p\bar{3}$
3	10 $\mathbf{TC}_{1h} = p11m$	11 $\mathbf{TC}_{2h} = p112/m$	59 $\mathbf{TC}_{3h} = p\bar{6}$	28 $\mathbf{TC}_{4h} = p4/m$	60 $\mathbf{TC}_{6h} = p6/m$
4		12 $\mathbf{T}_2\mathbf{C}_{1h} = p112_1/m$		29 $\mathbf{T}_4\mathbf{C}'_{2h} = p4_2/m$	61 $\mathbf{T}_6\mathbf{C}'_{3h} = p6_3/m$
5	3 $[\mathbf{TD}_1](0) = p211$	13 $[\mathbf{TD}_2](0) = p222$ 14 $[\mathbf{T}_2\mathbf{D}_1](0) = p222_1$	46 $[\mathbf{TD}_3](0) = p321$ $[\mathbf{TD}_3](\pi/6) = p312$ 47 $[\mathbf{T}_3\mathbf{D}_1](\pi/3) = p3_112$ $[\mathbf{T}_3\mathbf{D}_1](\pi/6) = p3_121$ 48 $[\mathbf{T}_3^2\mathbf{D}_1](\pi/6) = p3_212$ $[\mathbf{T}_3^2\mathbf{D}_1](\pi/3) = p3_221$	30 $[\mathbf{TD}_4](0) = p422$ 31 $[\mathbf{T}_4\mathbf{D}_1](0) = p4_122$ 32 $[\mathbf{T}_4\mathbf{D}_2](0) = p4_22$ 33 $[\mathbf{T}_4^3\mathbf{D}_2](0) = p4_322$	62 $[\mathbf{TD}_6](0) = p622$ 63 $[\mathbf{T}_6\mathbf{D}_1](0) = p6_122$ 64 $[\mathbf{T}_6\mathbf{D}_2](0) = p6_222$ 65 $[\mathbf{T}_6\mathbf{D}_3](0) = p6_322$ 66 $[\mathbf{T}_6^2\mathbf{D}_2](0) = p6_422$ 67 $[\mathbf{T}_6^5\mathbf{D}_1](0) = p6_522$
6	4 $[\mathbf{TC}_{1v}](\pi/2) = pm11$	15 $[\mathbf{TC}_{2v}](0) = pmm2$	49 $[\mathbf{TC}_{3v}](0) = p31m$ $[\mathbf{TC}_{3v}](\pi/6) = p3m1$	34 $[\mathbf{TC}_{4v}](0) = p4mm$	68 $[\mathbf{TC}_{6v}](0) = p6mm$
7	5 $[\mathbf{T}'\mathbf{C}_1](\pi/2) = pc$	16 $[\mathbf{T}'\mathbf{C}_2](0) = pcc2$	50 $[\mathbf{T}'\mathbf{C}_3](0) = p31c$ $[\mathbf{T}'\mathbf{C}_3](\pi/6) = p3c1$	36 $[\mathbf{T}'\mathbf{C}_4](0) = p4cc$	69 $[\mathbf{T}'\mathbf{C}_6](0) = p6cc$
8		17 $[\mathbf{T}_2\mathbf{C}_{1v}](\pi/2) = pmc2_1$		35 $[\mathbf{T}_4\mathbf{C}_{2v}](\pi/4) = p4_2cm$ $[\mathbf{T}_4\mathbf{C}_{2v}](0) = p4_2mc$	70 $[\mathbf{T}_6\mathbf{C}_{3v}](0) = p6_3cm$ $[\mathbf{T}_6\mathbf{C}_{3v}](\pi/6) = p6_3mc$
9	6 $[\mathbf{TD}_{1d}](\pi/2) = p2/m11$	37 $[\mathbf{TD}_{2d}](0) = p\bar{4}m2$ $[\mathbf{TC}_{2d}](\pi/4) = p\bar{4}2m$	51 $[\mathbf{TD}_{3d}](0) = p\bar{3}1m$ $[\mathbf{TC}_{3d}](\pi/6) = p\bar{3}m1$		
10	7 $[\mathbf{T}'\mathbf{S}_2](\pi/2) = p\bar{2}/c11$	38 $[\mathbf{T}'\mathbf{S}_4](0) = p\bar{4}c2$ $[\mathbf{T}'\mathbf{S}_4](\pi/4) = p\bar{4}2c$	52 $[\mathbf{T}'\mathbf{S}_6](0) = p\bar{3}1c$ $[\mathbf{T}'\mathbf{S}_6](\pi/6) = p\bar{3}c1$		
11	18 $[\mathbf{TD}_{1h}](0) = p2mm$	20 $[\mathbf{TD}_{2h}](0) = pmmm$	71 $[\mathbf{TD}_{3h}](0) = p\bar{6}2m$ $[\mathbf{TD}_{3h}](\pi/6) = p\bar{6}m2$	39 $[\mathbf{TD}_{4h}](0) = p4/mmm$	73 $[\mathbf{TD}_{6h}](0) = p6/mmm$
12	19 $[\mathbf{T}'\mathbf{C}_{1h}](0) = p2cm$	21 $[\mathbf{T}'\mathbf{C}_{2h}](0) = pccm$	72 $[\mathbf{T}'\mathbf{C}_{3h}](0) = p\bar{6}2c$ $[\mathbf{T}'\mathbf{C}_{3h}](\pi/6) = p\bar{6}c2$	40 $[\mathbf{T}'\mathbf{C}_{4h}](0) = p4/mcc$	74 $[\mathbf{T}'\mathbf{C}_{6h}](0) = p6/mcc$
13		22 $[\mathbf{T}_2\mathbf{D}'_{1h}](\pi/2) = pmcm$		41 $[\mathbf{T}_4\mathbf{D}_{2h}](0) = p4_2/mmc$ $[\mathbf{T}_4\mathbf{D}_{2h}](\pi/4) = p4_2/mcm$	75 $[\mathbf{T}_6\mathbf{D}'_{3h}](0) = p6_3/mcm$ $[\mathbf{T}_6\mathbf{D}'_{3h}](\pi/6) = p6_3/mmc$

$$\mathbf{F}(\alpha) = \begin{cases} \{(e|0), (I|0), (\sigma_\alpha|a/2), (u_{\alpha-\pi/2}|a/2)\} \text{ for } q = 1, \\ \{(e|0), (\sigma_h C_{\pi/2}|0), (C_\pi|0), (\sigma_h C_{-\pi/2}|0), (\sigma_\alpha|a/2), \\ (u_{\alpha-\pi/4}|a/2), (\sigma_{\alpha-\pi/2}|a/2), (u_{\alpha+\pi/4}|a/2)\} \text{ for } q = 2, \\ \{(e|0), (\sigma_h C_{\pi/3}|0), (C_{2\pi/3}|0), (I|0), (C_{-2\pi/3}|0), \\ (\sigma_h C_{-\pi/3}|0), (\sigma_\alpha|a/2), (u_{\alpha-\pi/6}|a/2), (\sigma_{\alpha-\pi/3}|a/2), \\ (u_{\alpha-\pi/2}|a/2), (\sigma_{\alpha+\pi/3}|a/2), (u_{\alpha+\pi/6}|a/2)\} \text{ for } q = 3. \end{cases} \tag{30}$$

The standard realisations are $p\bar{2}/c11$ for $q = 1$, $\alpha = \pi/2$, $p\bar{4}c2$ and $p\bar{4}2c$ for q = 2, $\alpha = 0, \pi/4$, and $p\bar{3}1c$, $p\bar{4}c1$ for q = 3, $\alpha = 0, \pi/6$.

Family 11 contains symmorphic line groups with

$$\mathbf{F}(\alpha) = \mathbf{D}_{nh}(\alpha) = \mathbf{C}_n \bigcup (\sigma_\alpha|0)\mathbf{C}_n \bigcup (\sigma_h|0)\mathbf{C}_n \bigcup (u_\alpha|0)\mathbf{C}_n. \tag{31}$$

Here for q = 1, 2, 4, 6 the setting angle $\alpha = 0$ gives the rod groups $p2mm$, $pmmm$, $p4/mmm$ and $p6/mmm$. For q = 3 the first setting $p\bar{6}m2$ of rod group No. 71 corresponds to the angle $\alpha = \pi/6$, the second setting $p\bar{6}2m$ corresponds to $\alpha = 0$.

Line groups of family 12 are non-symmorphic and are of the following general form:

$$\mathbf{L} = \mathbf{T}'\left(\frac{a}{2}\right)\mathbf{C}_{nh}(\alpha) = \mathbf{T}(a)\mathbf{F}(\alpha), \tag{32}$$

where

$$\mathbf{F}(\alpha) = \mathbf{C}_{nh} \bigcup \left(\sigma_\alpha \middle| \frac{a}{2} \right) \mathbf{C}_{nh}. \quad (33)$$

Here the usual line-group realisations ($\alpha = 0$) coincide with the rod group ones for q = 1, 2, 4, 6. For q = 3 the first setting $p\bar{6}c2$ corresponds to the setting angle $\pi/6$, the second setting $p\bar{6}c2$ to $\alpha = 0$.

The last, 13th, family contains non-symmorphic line groups of the form

$$\mathbf{L} = \mathbf{T}^1_{2n}\left(\frac{a}{2}\right)\mathbf{D}_{nh}(\alpha) = \mathbf{T}(a)\mathbf{F}(\alpha), \quad (34)$$

where

$$\mathbf{F}(\alpha) = \mathbf{D}_{nh} \bigcup \left(C_{\pi/n} \middle| \frac{a}{2} \right) \mathbf{D}_{nh}. \quad (35)$$

Here the relevant rod groups correspond to q = 2, 4, 6 and in the cases q = 2, 6 the horizontal reflection plane should be shifted up by $a/4$:

$$\begin{cases} \mathbf{F}'(\alpha) = \{(e|0), (\sigma_\alpha|0), (\sigma_h|a/2), (u_\alpha|a/2), (C_\pi|a/2), \\ \quad (\sigma_{\alpha-\pi/2}|a/2), (I|0), (u_{\alpha+\pi/2}|0)\} \text{ for } q = 2, \\ \mathbf{F}(\alpha) = \{(e|0), (C_\pi|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/2}|0), (\sigma_h|0), (I|0), \\ \quad (u_\alpha|0), (u_{\alpha-\pi/2}|0), (C_{\pi/2}|a/2), (C_{-\pi/2}|a/2), \\ \quad (\sigma_{\alpha+\pi/4}|a/2), (\sigma_{\alpha-\pi/4}|a/2), (\sigma_h C_{\pi/2}|a/2), (\sigma_h C_{-\pi/2}|a/2), \\ \quad (u_{\alpha+\pi/4}|a/2), (u_{\alpha-\pi/4}|a/2)\} \text{ for } q = 4, \\ \mathbf{F}'(\alpha) = \{(e|0), (C_{2\pi/3}|0), (C_{-2\pi/3}|0), (\sigma_\alpha|0), (\sigma_{\alpha-\pi/3}|0), \\ \quad (\sigma_{\alpha+\pi/3}|0), (\sigma_h|a/2), (\sigma_h C_{2\pi/3}|a/2), (\sigma_h C_{-2\pi/3}|a/2), \\ \quad (u_\alpha|a/2), (u_{\alpha-\pi/3}|a/2), (u_{\alpha+\pi/3}|a/2), (C_{\pi/3}|a/2), \\ \quad (C_\pi|a/2), (C_{-\pi/3}|a/2), (\sigma_{\alpha+\pi/6}|a/2), (\sigma_{\alpha-\pi/2}|a/2), \\ \quad (\sigma_h C_{\pi/3}|0), (I|0), (\sigma_h C_{-\pi/3}|0), (u_{\alpha+\pi/6}|0), (u_{\alpha-\pi/6}|0), \\ \quad (u_{\alpha+\pi/2}|0)\} \text{ for } q = 6. \end{cases} \quad (36)$$

For q = 2 to get the standard realisation $pmcm$ we must take $\alpha = \pi/2$ and shift the horizontal reflection plane up by $a/4$. For q = 4 two settings, $p4_2/mmc$ and $p4_2/mcm$, are obtained for $\alpha = 0$ and $\alpha = \pi/4$, respectively. For q = 6 to get the standard realisations of the rod groups it is necessary to shift the horizontal reflection plane and take $\alpha = 0, \pi/6$ (settings $p6_3/mcm$ and $p6_3/mmc$, respectively).

In Table 1 the exact correspondence between the rod groups and the relevant realisations of line groups is presented in a compact form.

5. Orbits with respect to line and rod groups

The line groups (with the z axis as the principal one) operate on the cylindrical surface $\mathrm{Cyl}_\rho = \{(x, y, z) : x^2 + y^2 = \rho^2\}$ of a fixed radius ρ and the corresponding orbits also lie on this surface. It is convenient to introduce the notation $\mathbf{x}_\rho(\alpha + \beta, z) = (\rho\cos(\alpha+\beta), \rho\sin(\alpha+\beta), z)$ for a general point belonging to Cyl_ρ, where α is the *setting angle* and the angle β is used for the parametrization of the set of equivalent orbits (along with the z coordinate).

L-orbits and their types do not depend on the line-group factorization. But there exist in a certain sense minimal sets of representatives of the line-group orbits which (i) uniquely define the orbit type, and (ii) can be used for *easy* generation of the whole **L**-orbit, and these sets may depend on the line-group factorization. It is clear that **F**-orbits can play the role of such sets of representatives in the case when the standard factorization is used. If the factorization (3) is exploited, then, as was shown by Damnjanović & Milošević (2010), either **P**- or $\mathbf{P}^+$-orbits satisfy the aforementioned requirements (i) and (ii) in *almost all* situations. Here $\mathbf{P}^+$ is a subgroup of the isogonal group **P** formed by the orthogonal transformations leaving unchanged the z coordinate of any point. Ambiguity may arise in the case when the type of $\mathbf{P}(\mathbf{P}^+)$-orbit depends on the parity of n, but the corresponding **L**-orbits turn out to be equivalent for all values of n.

It is easy to see that $\mathbf{P}(\mathbf{P}^+)$-orbits are always the subsets of the corresponding **F**-orbits. The major difference between them is the following. The **L**-orbit is obtained from the corresponding **F**-orbit by application to its points all possible pure translations along the z axis. If the factorization (3) is used, then either the screw-axis group or the glide-plane group must be applied to the points of the $\mathbf{P}(\mathbf{P}^+)$-orbit to get the whole **L**-orbit.

As an example, we consider orbits with respect to the line group $\mathbf{T}^1_4\mathbf{C}_{2v}$ from the eighth family corresponding to rod group No. 35.

According to Damnjanović & Milošević (2010), on the cylindrical surface of a fixed radius there is a 2-parametric set of equivalent $\mathbf{C}_{2v}(\alpha)$-orbits of length 4, two 1-parametric sets of non-equivalent orbits of length 2, and a 1-parametric set of single point orbits situated on the z axis:

$$\mathbf{C}_{2v}(\alpha)\mathbf{x}_\rho(\alpha+\beta, z) = \{\mathbf{x}_\rho(\alpha \pm \beta, z), \mathbf{x}_\rho(\alpha + \pi \pm \beta, z)\} \quad \text{(line group label } a_1\text{)}, \quad (37a)$$

$$\mathbf{C}_{2v}(\alpha)\mathbf{x}_\rho(\alpha, z) = \{\mathbf{x}_\rho(\alpha, z), \mathbf{x}_\rho(\alpha + \pi, z)\} \quad \text{(line group label } b_1\text{)}, \quad (37b)$$

$$\mathbf{C}_{2v}(\alpha)\mathbf{x}_\rho(\alpha + \pi/2, z) = \{\mathbf{x}_\rho(\alpha + \pi/2, z), \mathbf{x}_\rho(\alpha + 3\pi/2, z)\} \quad \text{(line group label } c_1\text{)}, \quad (37c)$$

$$\mathbf{C}_{2v}(\alpha)(0, 0, z) = \{(0, 0, z)\} \quad \text{(line group label } d_1\text{)} \quad (37d)$$

and the screw axis group $\mathbf{T}^1_4(a/2) = \langle (C_{\pi/2}|a/2) \rangle$ must be applied to the points of each of these orbits to generate the whole line-group orbits.

The orbits with respect to $\mathbf{F}(\alpha) = \mathbf{C}_{2v}(\alpha) \cup (C_{\pi/2}|a/2)\mathbf{C}_{2v}(\alpha)$ are

$$\mathbf{F}(\alpha)\mathbf{x}_\rho(\alpha+\beta, z) = \{\mathbf{x}_\rho(\alpha \pm \beta, z), \mathbf{x}_\rho(\alpha + \pi \pm \beta, z), \mathbf{x}_\rho(\alpha + \pi/2 \pm \beta, z + a/2), \mathbf{x}_\rho(\alpha + 3\pi/2 \pm \beta, z + a/2)\} \quad \text{(standard type } c\text{)}, \quad (38a)$$

$$\mathbf{F}(\alpha)\mathbf{x}_\rho(\alpha, z) = \{\mathbf{x}_\rho(\alpha, z), \mathbf{x}_\rho(\alpha + \pi, z), \mathbf{x}_\rho(\alpha + \pi/2, z + a/2), \mathbf{x}_\rho(\alpha + 3\pi/2, z + a/2)\} \quad \text{(standard type } b\text{)}, \quad (38b)$$

$$\mathbf{F}(\alpha)\mathbf{x}_\rho(\alpha+\pi/2, z) = \{\mathbf{x}_\rho(\alpha+\pi/2, z), \mathbf{x}_\rho(\alpha+3\pi/2, z), \mathbf{x}_\rho(\alpha, z+a/2), \mathbf{x}_\rho(\alpha+\pi, z+a/2)\} \quad \text{(standard type } b\text{)}, \tag{38c}$$

$$\mathbf{F}(\alpha)(0, 0, z) = \{(0, 0, z), (0, 0, z+a/2)\} \quad \text{(standard type } a\text{)}. \tag{38d}$$

The corresponding rod group appears in two settings (Kopský & Litvin, 2002): $p4_2cm(\alpha = \pi/4)$ and $p4_2mc(\alpha = 0)$. For $\alpha = \pi/4$ in the Cartesian coordinates after the change of variables $[(x\cos\alpha - y\sin\alpha, x\sin\alpha + y\cos\alpha) \rightarrow (x, y)$ for the orbits of the standard type c and $x\cos\alpha \rightarrow x$ for the orbits of the standard type $b]$ the corresponding $\mathbf{F}(\pi/4)$-orbits have the following standard form:

$$\mathbf{F}(\pi/4)(x, y, z) = \{(x, y, z), (y, x, z), (-y, x, z+a/2), (-x, y, z+a/2), (-x, -y, z), (-y, -x, z), (y, -x, z+a/2), (x, -y, z+a/2)\} \quad \text{(line group label } a_1, \text{ standard label } c\text{)}, \tag{39a}$$

$$\mathbf{F}(\pi/4)(x, x, z) = \{(x, x, z), (-x, x, z+a/2), (-x, -x, z), (x, -x, z+a/2)\} \quad \text{(line group label } b_1, \text{ standard label } b\text{)}, \tag{39b}$$

$$\mathbf{F}(\pi/4)(-x, x, z) = \{(-x, x, z), (x, -x, z), (-x, -x, z+a/2), (x, x, z+a/2)\} \quad \text{(line group label } b_1\text{)}, \tag{39c}$$

$$\mathbf{F}(\pi/4)(0, 0, z) = \{(0, 0, z), (0, 0, z+a/2)\} \quad \text{(line group label } d_1, \text{ standard label } a\text{)}. \tag{39d}$$

Here two sets of equivalent orbits of type b with the representatives (x, x, z) and $(-x, x, z)$ are parametrized by two parameters x, z and the expression (39b) embraces both sets. Indeed, since the parameters x, z are supposed to be free, the replacement $x \rightarrow -x$, $z \rightarrow z + a/2$ applied to the right-hand side of equation (39b) gives the orbit (39c).

In exactly the same manner the case $\alpha = 0$ can be treated.

6. Conclusion

The notion of a setting angle that defines specific geometric realisations of line groups is introduced. This notion turns out to be useful in the case where a line group contains Euclidean transformations that include as their orthogonal parts either reflections in vertical planes or *Umklapp* operations. Introduction of a setting angle leads to the appearance of continuous series of line groups of families 5–13. A thorough analysis of the crystallographic settings of the rod groups and the appropriate geometric realisations of relevant line groups is performed. This analysis results in establishing the explicit correspondence between rod-group settings and the corresponding line groups. More general and detailed descriptions of the interrelation between the rod- and line-group orbits will be considered in a subsequent publication.

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