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Decomposition of Sohncke space groups into products of Bieberbach and symmorphic parts

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Abstract: Point groups consist of rotations, reflections, and roto-reflections and are foundational in crystallography. Symmorphic space groups are those that can be decomposed as a semi-direct product of pure translations and pure point subgroups. In contrast, Bieberbach groups consist of pure translations, screws, and glides. These "torsion-free" space groups are rarely mentioned as being a special class outside of the mathematics literature. Every space group can be thought of as lying along a spectrum with the symmorphic case at one extreme and Bieberbach space groups at the other. The remaining nonsymmorphic space groups lie somewhere in between. Many of these can be decomposed into semi-direct products of Bieberbach subgroups and point transformations. In particular, we show that those 3D Sohncke space groups most populated by macromolecular crystals obey such decompositions. We tabulate these decompositions for those Sohncke groups that admit such decompositions. This has implications to the study of packing arrangements in macromolecular crystals. We also observe that every Sohncke group can be written as a product of Bieberbach and symmorphic subgroups, and this has implications for new nomenclature for space groups.

Keywords: Bieberbach groups; crystallographic space groups; point groups.

Introduction

In any space group Γ there exist Bieberbach (torsion-free) subgroups (consisting only of translations, screw displacements, and glides) and subgroups which contain only the identity and torsion elements (roto-reflections).[1] In the symmorphic case, the Bieberbach subgroup Γ_B with smallest index in Γ is simply T, the translation group of the primitive lattice. And in this case it is well known that $\Gamma_P = T \rtimes \mathbb{P}$ (the semi-direct product of T and $\mathbb{P}$) where $\mathbb{P}$ is the point group. We have observed that for many nonsymmorphic subgroups there is a Bieberbach group Γ_B such that $[\Gamma{:}\Gamma_B] < [\Gamma{:}T]$ (where $[G{:}H]$ denotes the index of H in G) and

$$\Gamma = \Gamma_B \rtimes \mathbb{S} \text{ where } \mathbb{S} < \mathbb{P}. \tag{1}$$

(Here $<$ denotes "is a proper subgroup of".) In particular, in this paper we focus on the 65 Sohncke space groups that preserve the chirality of crystallographic motifs.

In our calculations we work in the factor group Γ/Σ where $\Sigma \leq T$ is the translation group of a sublattice of the primitive lattice that is normal in Γ, and we arrive at statements such as[2]

$$\frac{\Gamma}{\Sigma} = \mathbb{B} \rtimes \mathbb{S} \text{ where } \mathbb{B} := \frac{\Gamma_B}{\Sigma} \tag{2}$$

(which we call a *semi-decomposition*), and we show that the equalities in (1) and (2) are equivalent. The fraction notation is used to emphasizes that $\Gamma/\Sigma = \Sigma\backslash\Gamma$, which holds when Σ is a normal subgroup. (Normality of a subgroup is denoted as $\Sigma \lhd \Gamma$.)

The primary goal of this paper is to identify which Sohncke groups can be decomposed as in (1) and to identify Γ_B and $\mathbb{S}$ in these cases. We have found that all but four Sohncke groups can be decomposed in this way. As a secondary goal for these four we seek a weaker decomposition of the form

$$\Gamma = \Gamma_B S \tag{3}$$

where Γ_B need not be normal. We find that two of these four can be decomposed in this way, and that (3) is backwards

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1 In general, an element g of a discrete group G is called a torsion element if $g^n = e$ (the group identity) for some finite natural number n. That is, a torsion element is an element of finite order. For any space group together with an appropriate choice of origin, each torsion element generates a cyclic subgroup of $S := \{\mathbf{0}\} \rtimes \mathbb{S} < \Gamma$ where $\mathbb{S}$ is a subgroup of the point group, $\mathbb{P}$.

2 In fact, most of the time it is possible to take $\Sigma = T$, but there are a few cases where taking $\Sigma < T$ enables the decomposition to be performed when it would not be possible otherwise, as will be described later in the paper. (An example of this is $P4_2$.)

compatible with (1). That is, whenever (1) holds, so must (3), but not the other way around.

We also observe that *every* Sohncke space group can be written as a product of the form

$$\Gamma = \Gamma_B \Gamma_S \tag{4}$$

where Γ_B and Γ_S are respectively Bieberbach and symmorphic subgroups, regardless of whether or not there is a normal Γ_B, and (4) need not correspond to the above decompositions, though it is backwards compatible with them. That is, whenever (3) holds it must also be true that (4) holds, but not vice versa.

The remainder of this paper is structured as follows. The section "Motivation: the molecular replacement problem" describes our motivation in pursuing these decompositions. The section "Literature review" reviews the literature to explain where the current work fits in the broader world of mathematical crystallography. In the section "Definitions and core theorems" a small subset of the fundamental definitions and concepts from group theory most relevant to our study are reviewed. The section "Theory behind the decomposability of space groups" presents a new theorem to assist in our calculations. The section "Outline of decomposition algorithms for Sohncke groups" outlines the algorithmic approach that we take to performing these decompositions. In the section "Table of semi-decomposable nonsymmorphic Sohncke space groups" tables describing the complete results of these calculations are given.

Motivation: the molecular replacement problem

In a series of papers [1–3] we are developing new methods for molecular replacement (MR) [4] for use in the field of macromolecular crystallography. This motivated the kind of decomposition proposed in this paper for certain of the Sohncke groups (i.e. the 65 of the 230 types that preserve chirality). Though the methodology presented here is applicable to many non-Sohncke groups as well, we limit the current presentation for issues of brevity and relevance to the MR application.

In MR, a diffraction pattern (or equivalently, the Patterson function) for a macromolecular crystal is presented, and a model for the hypothesized shape of the macromolecule (which is typically a protein) is constructed from information in the Protein Data Bank [5]. The problem is that the diffraction pattern does not contain phase information. Such information is often provided by additional experiments in which heavy metal atoms are introduced. The spirit of molecular replacement is that if the model is a good shape match for the actual protein molecule of interest, and if it has similar density, then the phase problem can be solved computationally rather than experimentally. Given such a model molecule, it should be possible to find a translation and rotation,[3] $g = (R, \mathbf{t}) \in SE(3) := \mathbb{R}^3 \rtimes SO(3)$ (the group consisting of all special Euclidean motions), to place the model molecule in the unit cell in the same way as the actual molecule. Here $\mathbb{R}^3$ is three-dimensional Euclidean space, $SO(3)$ is the group of rotations (i.e. 3×3 orthogonal matrices with positive determinant, thereby excluding reflections), and $SE(3)$ is the full group of rigid-body motions (which is a six-dimensional Lie group). Of course, the pose sought in MR is not unique because both the symmetry mates within a unit cell and translates in all of the other unit cells are equivalent to this pose. This equivalence is described by them being members of the same right coset Γg where $\Gamma < SE(3)$ is the Sohncke space group of the crystal. The group element $g \in SE(3)$ appears on the right because it is rigid motion relative to the motions described by the globally defined motions describing the crystal symmetry. Therefore, one does not need to search the full space $SE(3)$ in MR. Rather, choosing one representative element of $SE(3)$ from each of the right cosets in the right coset space $\Gamma \backslash SE(3)$ will describe all nonredundant ways to situate a model molecule. We collect all such g's into a connected and bounded six-dimensional subset of $SE(3)$ denoted as $\mathcal{F}_{\Gamma \backslash SE(3)}$. (In general such a set of coset representatives is called a *fundamental domain*.) We then take the closure of this set, which adds some redundancy in the same way that choosing a closed interval with boundary points identified is slightly redundant as a fundamental domain for a the circle group $\mathbb{R}/(2\pi\mathbb{Z})$. We denote this closure of the fundamental domain as $\bar{\mathcal{F}}_{\Gamma \backslash SE(3)} \subset SE(3)$.

Explicit choices for $\bar{\mathcal{F}}_{\Gamma \backslash SE(3)}$ are described in [2]. For example if

$$\Gamma_P := T \rtimes \mathbb{P}, \tag{5}$$

then we can choose

$$\bar{\mathcal{F}}_{\Gamma_P \backslash SE(3)} = \bar{\mathcal{F}}_{T \backslash \mathbb{R}^3} \times \bar{\mathcal{F}}_{\mathbb{P} \backslash SO(3)}$$

[where here $\times$ is the Cartesian product, rather than direct product, and $\bar{\mathcal{F}}_{\mathbb{P} \backslash SO(3)} \subset SO(3)$]. This makes sense because $\mathbb{P} < SO(3)$. Alternatively we can always make the choice for any Sohncke space group Γ

$$\bar{\mathcal{F}}_{\Gamma \backslash SE(3)} = \bar{\mathcal{F}}_{\Gamma \backslash \mathbb{R}^3} \times SO(3).$$

Since the choice of fundamental domain can be made in a number of ways based on properties of Γ, this motivates us

3 The combination of which is called "pose" for brevity.

to investigate the structure of Γ. For example, if $\Gamma = \Gamma_B \rtimes \mathbb{S}$ where $\mathbb{S} < \mathbb{P}$, then we can make the additional choice

$$\bar{\mathcal{F}}_{\Gamma\backslash SE(3)} = \bar{\mathcal{F}}_{\Gamma_B\backslash\mathbb{R}^3} \times \bar{\mathcal{F}}_{\mathbb{S}\backslash SO(3)}.$$

This is potentially interesting because the space $\Gamma_B\backslash\mathbb{R}^3$ is an "orientable flat manifold" and the coset space $\mathbb{S}\backslash SO(3)$ can be identified with a "spherical space form," which is also orientable.

Though the non-Sohncke case is not relevant to macromolecular crystals, one can ask analogous questions about how the fundamental domains corresponding to $\Gamma\backslash E(3)$ can be defined where

$$E(3) := \mathbb{R}^3 \rtimes O(3)$$

is the full Euclidean group (as opposed to the "Special" Euclidean group), including reflections and glides. But in the current paper we focus only on the case of Sohncke groups.

Literature review

In recent years there appears to be a renaissance in the field of mathematical crystallography, as described in [6–8].

Mathematical and computational crystallography has many facets including algebraic structure theory of space groups [9–13], geometric approaches [13–24] and topological approaches [12, 25]. And the representation theory of space groups has long been known to play an important role in solid state physics and therefore has been studied intensively [26–29].

Many excellent general introductions to mathematical crystallography are available including [29–35] as well as introductions to group theory [36, 37] and books on solid-state physics and phase transitions [38–40] that have detailed mathematical introductions to crystallography. Of course, the most complete source for knowledge about mathematical properties of space groups is the International Tables, and particularly Vols A and A1 [41, 42].

The space-group decompositions derived here originated in our study of the molecular replacement problem in protein crystallography, as described in [1–3]. In particular, in that problem the quotient space in which copies of proteins are packed is $\Gamma\backslash\mathbb{R}^3$. When $\Gamma = \Gamma_B$ (a Bieberbach group), it acts properly discontinuously and freely on $\mathbb{R}^3$ and so $\Gamma_B\backslash\mathbb{R}^3$ is a flat manifold [14, 24, 43] which is orientable if and only if Γ_B is Sohncke . More generally, the space $\Gamma\backslash\mathbb{R}^3$ is a Euclidean orbifold [22, 44]. Regardless of whether Γ is Bieberbach or not, the fundamental domain $\bar{\mathcal{F}}_{\Gamma\backslash\mathbb{R}^3} \subset \mathbb{R}^3$ can be identified with the crystallographic asymmetric unit. When faces of $\bar{\mathcal{F}}_{\Gamma\backslash\mathbb{R}^3}$ are glued appropriately, the result is $\Gamma\backslash\mathbb{R}^3$. For this reason, the modern geometric approaches to crystallography have relevance to structural biology. Moreover, if $E(3)$ denotes the noncompact noncommutative six-dimensional Lie group of all Euclidean motions and Γ is any space group drawn from the 230 types, then each $\Gamma\backslash E(3)$ is a compact six-dimensional manifold. These manifolds (and their generalizations in higher dimensions) were mentioned by Hilbert in the formulation of his "18th problem," but other than the fact that they are known to be compact, they appear not to have been studied since. In the Sohncke case, $\Gamma\backslash SE(3)$ is the configuration space of a rigid-protein molecule moving in $\Gamma\backslash\mathbb{R}^3$. The decompositions presented in this paper allow us to better understand the structure of this configuration space to address the molecular replacement problem with new computational tools.

In our work, we use two theorems given later in the paper in combination with functions that we use in the Bilbao Crystallographic Server [45–47] (particularly the COSET, MAXSUB, SUBGROUPGRAPH, IDENTIFY GROUP, and HERMANN functions). We have made extensive use of this valuable community tool to both refine our theory and to do computations.

Definitions and core theorems

We begin with a few basic definitions in order to establish notation, under the assumption that the reader is already familiar with the basic concepts of group theory.

The most basic definitions

Let G denote a group. If G is finite, then $|G|$ denotes the number of elements in it. The product of two elements g, $h \in G$ is denoted by simply writing the elements next to each other, gh. In general $gh \neq hg$. The identity element is denoted as $e \in G$, and the inverse of an element $g \in G$ is denoted as $g^{-1} \in G$.

Given a group G, two elements a and b are called conjugate if there exists an element g such that

$$a^g := gag^{-1} = b. \tag{6}$$

The notation $H < G$ indicates that H is a proper subgroup, i.e. a subgroup for which $H \neq G$. In contrast, the notation $H \leq G$ indicates that H is a subgroup, leaving open the possibility that $H = G$.

Two subgroups $H, K < G$ are called conjugate if there exists an element $g \in G$ such that

$$H^g := gHg^{-1} = K. \quad (7)$$

If in the above expression $H^g = H$ for all $g \in G$, then $H < G$ is called a normal subgroup of G and we write $H \lhd G$.

Given a subgroup $H < G$, and any element $g \in G$, the *left coset gH* is defined as

$$gH := \{gh \mid h \in H\}.$$

Similarly, the right coset Hg is defined as

$$Hg := \{hg \mid h \in H\}.$$

A group is divided into cosets (left or right) all of the same size. And the set of all cosets is called a coset space. The left coset space

$$G/H := \{gH \mid g \in G\}$$

and the right coset space

$$H \backslash G := \{Hg \mid g \in G\}$$

are generally different from each other. But when $H \lhd G$, then $gH = Hg$ for all $g \in G$ and $G/H = H \backslash G$. In this special case we can denote both as $\frac{G}{H}$, and this space forms a group under the operation $(g_1H)(g_2H) = (g_1g_2)H$.

Given a left coset decomposition, it is possible to define (in a non-unique way) a fundamental domain

$$\mathcal{F}_{G/H} \subset G$$

consisting of exactly one element per left coset:[4]

$$|\mathcal{F}_{G/H} \cap gH| = 1$$

for every $g \in G$. (And similarly for right-coset decompositions.) Since a group is partitioned into disjoint cosets,

$$\bigcup_{g \in \mathcal{F}_{G/H}} gH = G.$$

In the case when $H \lhd G$, this fundamendamental domain is a group with respect to the original group operation mod H. And this group is isomorphic with G/H. The utility of this concept is that we can use it to perform set-theoretic calculations inside of G.

When G is a Lie group such as $SE(3)$ and H is a discrete subgroup, the fundamental domain $F_{G/H}$ will have the same dimensionality as G. But when G is a space group and H is a space subgroup, the fundamental domain $F_{G/H}$ will be a finite set.

4 For any finite set, X, the number of elements in X is denoted as $|X|$.

Space groups

In our study, we are interested in space groups, denoted as Γ, acting on three-dimensional Euclidean space. These discrete groups are subgroups of $E(3)$, the group consisting of the continuum of all possible rigid-body motions of three-dimensional Euclidean space. In turn, $E(3) < Aff(3)$, the group of affine transformations. All three groups $\Gamma < E(3) < Aff(3)$ can be thought of as consisting of elements that are pairs of the form $(A, \mathbf{a})$ where $A \in GL(3, \mathbb{R})$ (the general linear group consisting of 3×3 invertible matrices with real entries) and $\mathbf{a} \in \mathbb{R}^3$. And the group operation is[5]

$$(A_1, \mathbf{a}_1)(A_2, \mathbf{a}_2) = (A_1A_2, A_1\mathbf{a}_2 + \mathbf{a}_1). \quad (8)$$

This is equivalent to expressing group elements as 4×4 homogeneous transformation matrices of the form

$$\mathcal{H}(A, \mathbf{a}) = \begin{pmatrix} A & \mathbf{a} \\ \mathbf{0}^t & 1 \end{pmatrix}$$

(where $\mathbf{0}^t$ is the transpose of the 3-dimensional zero vector), and describing the group operation as matrix multiplication.

The relationship between $(A, \mathbf{a})$ and $\mathcal{H}(A, \mathbf{a})$ is an example of an isomorphism. That is, there is a bijective correspondence between the set of all pairs of the form $(A, \mathbf{a})$ and of all matrices of the form $\mathcal{H}(A, \mathbf{a})$, and the group operation is preserved by this correspondence in the sense that

$$\mathcal{H}((A_1, \mathbf{a}_1)(A_2, \mathbf{a}_2)) = \mathcal{H}(A_1, \mathbf{a}_1)\mathcal{H}(A_2, \mathbf{a}_2).$$

When two groups G and G' are related by an isomorphism they are called isomorphic, and this is written symbolically as $G \cong G'$.

Throughout this paper we describe three-dimensional crystallographic group operations by their actions on an arbitrary point $x \in \mathbb{R}^3$. That is, instead of writing $\gamma \in \Gamma$ explicitly as a pair of the form $(A, \mathbf{a})$ or as a matrix $\mathcal{H}(A, \mathbf{a})$ we will often write the row vector $(\gamma \cdot x)^t$. This is consistent with the way space group operations are reported in the crystallography literature. Explicitly,

$$\gamma = (R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma))$$

5 Various other notations for $(A, \mathbf{a})$ include $(A|\mathbf{a})$, $\{A|\mathbf{a}\}$ and versions of these with A and $\mathbf{a}$ written in reverse order.

and

$$\gamma \cdot \mathbf{x} = R_\gamma \mathbf{x} + \mathbf{t}_\gamma + \mathbf{v}(R_\gamma).$$

Here $R_\gamma \in \mathbb{P}$ (the point group), $t_\gamma \in \mathbb{L}$ (the lattice) and $\mathbf{v}: \mathbb{P} \to \mathbb{R}^n$ is a translation by a fraction of a lattice motion such as those that can appear in screw or glide motions, and the mapping $\mathbf{v}$ observes the co-cycle condition

$$\mathbf{v}(R_{\gamma_1} R_{\gamma_2}) = R_{\gamma_1} \mathbf{v}(R_{\gamma_2}) + \mathbf{v}(R_{\gamma_1}) \bmod T. \tag{9}$$

The "mod T" effectively removes any component in the sum that is in T, in analogy with the way $3+4=2 \bmod 5$ in modulo 5 arithmetic. If there exists a point $\boldsymbol{p} \in \mathbb{R}^3$ such that $\gamma \cdot \mathbf{p} = \mathbf{p}$ for some $\gamma \in \Gamma$ other than the identity element, then γ is called a *torsion element* of Γ. If it is possible to choose a coordinate system in $\mathbb{R}^3$ with $\mathbf{p}$ as the origin such that $\mathbf{v}(R_\gamma) = \mathbf{0}$ for all $\gamma \in \Gamma$, then Γ can be decomposed as a product of translations and torsion elements (rotations, reflections, and roto-translations). That is, $\Gamma = T \cdot P$ where all of the elements of

$$P := \{\mathbf{0}\} \rtimes \mathbb{P} \tag{10}$$

preserve the location of the origin. The distinction between P and $\mathbb{P}$ is that $P < \Gamma$ whereas $\mathbb{P}$ is not. $\Gamma = T \cdot P$ is the symmorphic case in which the group is decomposed into a product of translations and point-preserving transformations, $\mathbb{P}$. Of the 230 types of 3D space groups, 73 can be decomposed in this way. These are the *symmorphic* space groups. Some space groups have no torsion elements. These are the *Bieberbach* groups. For them it is not possible to define an origin such that $\mathbf{v}(R_\gamma) = \mathbf{0}$ for any $\gamma \in \Gamma$ other than the identity element.

In the theory of space groups, perhaps the most well-known isomorphism originates from the fact that the translation group of the primitive lattice is always normal, $T \lhd \Gamma$, and

$$\frac{\Gamma}{T} \cong \mathbb{P}. \tag{11}$$

Isomorphism vs. equality of fundamental domains

Though the concept of isomorphism is critically important in group theory, we stress the difference between isomorphism and true equality by considering fundamental domains of the form $\mathcal{F}_{\Gamma/T}$ constructed by choosing one element per coset in Γ/T. In the case when coset representatives are chosen with minimal translational part, a stronger version of (11) can be written by defining

$$\mathcal{F}_{\Gamma/T} := \{(R_p, \mathbf{v}(R_p)) \mid R_p \in \mathbb{P}\} \tag{12}$$

where $\mathbf{v}(R_p)$ is a translation by a fraction of the unit-cell dimensions corresponding to a screw displacement or glide. The $\cong$ notation hides $\mathbf{v}(R_p)$ from view, and therefore should not be misinterpreted as equality.

When $\mathbf{v}(R_p) \neq \mathbf{0}$ for at least one $R_p \in \mathbb{P}$, then $\mathcal{F}_{\Gamma/T}$ is not a group under the original operation of Γ. However, it does become a group under the rule

$$(R_{p_1}, \mathbf{v}(R_{p_1}))(R_{p_2}, \mathbf{v}(R_{p_2})) := (R_{p_1} R_{p_2}, \mathbf{v}(R_{p_1} R_{p_2}))$$

where (9) is used to evaluate $\mathbf{v}(R_{p_1} R_{p_2})$.

But since the group operation of $\mathcal{F}_{\Gamma/T}$ is not that of Γ, it follows that $\mathcal{F}_{\Gamma/T}$ cannot be a subgroup of Γ in the nonsymmorphic case.

With the above defined group operation, the following isomorphism holds

$$\mathcal{F}_{\Gamma/T} \cong \frac{\Gamma}{T} \tag{13}$$

and this is somewhat more descriptive of Γ than is (11) because the set $\mathcal{F}_{\Gamma/T}$ can be used to reconstruct Γ as

$$\Gamma = T \cdot \mathcal{F}_{\Gamma/T} \tag{14}$$

where the product in the above expression simply means that every $\gamma \in \Gamma$ can be decomposed as

$$(R_\gamma, \mathbf{t}_\gamma + \mathbf{v}(R_\gamma)) = (\mathbb{I}, \mathbf{t}_\gamma)(R_\gamma, \mathbf{v}(R_\gamma)).$$

Note that even in the symmorphic case where $\mathbf{v}(R_p) = \mathbf{0}$ for all $R_p \in \mathbb{P}$, (13)–(14) and (11) are not the same in the strictest possible sense. But at least in this case $\mathcal{F}_{\Gamma_p/T} := P$ is a subgroup of Γ_p. Here we have used the definitions in (5) and (10).

To illustrate further the difference between isomorphism and equality, consider the following. If $H \lhd G$ and $K < G$ such that $H \cap K = \{e\}$, and $HK = G$ then $G = H \rtimes K$. Corresponding to the coset space $G/H = H \backslash G$ is the fundamental domain constructed from one representative element of G per coset: $\mathcal{F}_{\frac{G}{H}} \subset G$. There is no unique way to construct this fundamental domain, but a natural choice is

$$\mathcal{F}_{\frac{G}{H}} := K,$$

which is consistent with the isomorphism $\frac{G}{H} \cong K$, but is stronger than isomorphism in the sense that it is an equality.

If in addition there is a supergroup $A > G$, then for any $\alpha \in A$ we can write

$$\alpha G\alpha^{-1}=(\alpha H\alpha^{-1})(\alpha K\alpha^{-1})$$

in which case we can choose

$$\mathcal{F}_{\frac{\alpha G\alpha^{-1}}{\alpha H\alpha^{-1}}}:=\alpha K\alpha^{-1}.$$

In the context of symmorphic space groups $G:=\Gamma_P$, if $H:=T$ and $K:=\{0\}\rtimes\mathbb{P}$ and if $A=Aff(3)$, then it is possible to find $\alpha\in A$ such that $\Sigma=\alpha T\alpha^{-1}$ is the translation group of a sublattice. Moreover, it can be the case that $\alpha K\alpha^{-1}=K$ when $\alpha\neq e$. For example, if

$$\alpha=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&a&0\\0&0&0&1\end{pmatrix}$$

and

$$\gamma=\begin{pmatrix}c\theta&-s\theta&0&v_1x+w_1y\\s\theta&c\theta&0&v_2x+w_2y\\0&0&1&z\\0&0&0&1\end{pmatrix}$$

where θ takes discrete values consistent with the 2D lattice spanned by $\mathbf{v}=[v_1, v_2]^t$ and $\mathbf{w}=[w_1, w_2]^t$ and $x, y, z\in\mathbb{Z}$, and $a\in\mathbb{Z}_{>0}$, then

$$\alpha\gamma\alpha^{-1}=\begin{pmatrix}c\theta&-s\theta&0&v_1x+w_1y\\s\theta&c\theta&0&v_2x+w_2y\\0&0&1&az\\0&0&0&1\end{pmatrix}.$$

If $\mathbb{P}$ denotes the point group and P denotes the subgroup of Γ defined in (10) consisting of all transformations of the form of γ given above when $x=y=z=0$, then for the present example it is clear that

$$\alpha P\alpha^{-1}=P.$$

Therefore, similar to how for any natural number, n, $n\mathbb{Z}$ can be both a subgroup of $\mathbb{Z}$ and isomorphic with it, both of the following statements can be true simultaneously: $\alpha G\alpha^{-1}\cong G$ and $\alpha G\alpha^{-1}<G$ (which is an example illustrating how isomorphism is weaker than equality). In the case of symmorphic space groups it can be the case that

$$\mathcal{F}_{\frac{\alpha G\alpha^{1}}{\alpha H\alpha^{-1}}}=K=\mathcal{F}_{\frac{G}{H}}$$

if K is normal in A. And when K is not normal in A,

$$\mathcal{F}_{\frac{\alpha G\alpha^{-1}}{\alpha H\alpha^{-1}}}=\alpha\mathcal{F}_{\frac{G}{H}}\alpha^{-1}.$$

But either way,

$$\frac{\alpha G\alpha^{-1}}{\alpha H\alpha^{-1}}\cong\frac{G}{H}.$$

Classification of space groups

A space group is called *Sohncke* if $\det R_\gamma=+1$ for all $\gamma\in\Gamma$. In the table below we classify space group types. Since the translation group T is both Bieberbach and symmorphic (with trivial point group) it can be classified as both symmorphic and Bieberbach. We include T with the symmorphic space groups and call the remainder of the Bieberbach groups "nontrivial."

	Symmorphic	Nontrivial Bieberbach	NonSymmorphic+ nonBieberbach	Total
Sohncke	24	8 (5)	33 (25)	65 (54)
Non-Sohncke	49	4	112	165
Total	73	12 (9)	145 (137)	230 (219)

The number in parenthesis is for types classified according to equivanence under conjugation by general affine (rather than proper affine) transformations. That is, when counting the space group types in parenthesis, the following enantiomorphic pairs are each considered as being of the same type: ($P3_1$, $P3_2$), ($P4_1$, $P4_3$), ($P6_1$, $P6_5$), ($P6_2$, $P6_4$), ($P3_112$, $P3_212$), ($P3_121$, $P3_221$), ($P4_122$, $P4_322$), ($P4_12_12$, $P4_32_12$), ($P4_132$, $P4_332$), ($P6_122$, $P6_522$), ($P6_222$, $P6_422$). Note that this distinction is only important in the case of Sohncke space groups.

Theory behind the decomposability of space groups

The main goal of this paper is to determine which space groups can be decomposed as

$$\Gamma=\Gamma_B S \text{ where } S<P \tag{15}$$

with $\Gamma_B\lhd\Gamma$. It follows from the third isomorphism theorem of group theory that a necessary condition for (15) to hold is

$$[\Gamma:\Gamma_B]=|S|. \tag{16}$$

Moreover, using the theorems presented below together with Lagrange's theorem, it is possible to show that given a lattice translation subgroup $\Sigma < \Gamma_B$ such that $\Sigma \lhd \Gamma$ and $\Gamma_S = \Sigma S < \Gamma$, then another necessary condition for (15) to hold is

$$[\Gamma:\Sigma] = [\Gamma_B:\Sigma] \cdot |S|. \tag{17}$$

The conditions (16) and (17) impose constraints on the search for compatible Γ_B and Γ_S. Moreover, in the spirit of simplicity, if Γ admits multiple decompositions of the form (15) (due to the existence of multiple Σ's), we retain only the solution for which $[\Gamma:\Sigma]$ is minimal.

We note also that if $[G:H]=2$ then H is simultaneously maximal, minimal index, and normal in G. And this facilitates our search, since many Bieberbach subgroups have index two in their supergroup.

In the remainder of this section a combination of known definitions and properties are reviewed and a new theorem is presented to assist in the computation of these decompositions.

Definitions involving internal products

Suppose G is a group with identity element e and H and K are two normal subgroups of G. If

– $G = HK$
– $H \cap K = \{e\}$

then, G is called the *(internal) direct product* of H by K and is denoted by $G = H \times K$, and this product is symmetrical in the sense that we can also write $G = K \times H$.

Suppose G is a group and H is a normal subgroup of G but K need not be. If

– $G = HK$
– $H \cap K = \{e\}$

then, G is called the *(internal) semidirect product* of H by K and is denoted by $G = H \rtimes K$. Here H is normal in G and $K \cong G/H$ is called the *complement* of H in G. In a semidirect product, $H \rtimes K$, the complement K acts by conjugation on H. By definition of $\ltimes$ this can also be written as $G = K \ltimes H$. In general the order matters here, with the triangular part of $\rtimes$ or $\ltimes$ pointing toward the normal subgroup. Note that

$$G = H \rtimes K = H \ltimes K \Leftrightarrow G = H \times K.$$

And so a direct product is always also a semi-direct product, but not vice versa. In the case of a direct product, then for every $h \in H$ and every $k \in K$, $hk = kh$, whereas this is not true in the case of semi-direct products. As a result, for a direct product the conjugation action of K on H is the trivial action.

In contrast to internal (semi-)direct products, it is possible to define *external* products. For example, $Aff(n)$ can be viewed as the internal semi-direct product of the continuous translation subgroup $\mathcal{T}(n) := \{(\mathbb{I}, \mathbf{a}) | \mathbf{a} \in \mathbb{R}^n\}$ and the subgroup $\mathcal{G}(n) := \{(A, \mathbf{0}) | A \in GL(n)\}$ as

$$Aff(n) = \mathcal{T}(n)\mathcal{G}(n) = T(n) \rtimes \mathcal{G}(n). \tag{18}$$

Alternatively, we can write

$$Aff(n) = \mathbb{R}^n \rtimes GL(n). \tag{19}$$

The distinction is that whereas $\mathcal{T}(n)$, $\mathcal{G}(n) < Aff(n)$, in the strictest sense the groups $\mathbb{R}^n$ and GL(n) are not subgroups of $Aff(n)$. Rather, they are groups isomorphic to $\mathcal{T}(n)$ and $\mathcal{G}(n)$, respectively. And so the symbol $\rtimes$ means different things in (18) and (19). Equipped with the isomorphisms $\mathcal{T}(n) \leftrightarrow \mathbb{R}^n$ and $\mathcal{G}(n) \leftrightarrow GL(n)$ this difference between internal and external direct products is small enough to justify the double use of this symbol. And yet, without this understanding, logical problems can arise.

For example, in mathematical crystallography we say that a symmorphic space group, Γ_P, with point group P can be written as (5). When doing so, this is the external product in (19). If so then $\mathbb{P}$ is not a subgroup of Γ_P. Rather, from the definition in (10)

$$P = \{\mathbf{0}\} \rtimes \mathbb{P} = \{(R_p, \mathbf{0}) | R_p \in \mathbb{P}\} < \Gamma_P$$

and we can write

$$\mathcal{F}_{\Gamma_P/T} = P.$$

In contrast to (11), this is an equality. Moreover, $\mathbb{P} \not< \Gamma$ but $P < \Gamma_P$. And so, for example, while it is possible to form an external direct product of T and $\mathbb{P}$ to yield $\Gamma_P = T \rtimes \mathbb{P}$, it is possible to construct the same thing as an internal direct product by simply multiplying T and P to yield $\Gamma_P = TP$.

We note that with the exception of $P1$, symmorphic groups are never direct products of T and $\mathbb{P}$ because

$$(\mathbb{I}, \mathbf{t}_\gamma)(R_\gamma, \mathbf{0})(\mathbb{I}, -\mathbf{t}_\gamma) = (R_\gamma, (\mathbb{I} - R_\gamma)\mathbf{t}_\gamma).$$

And since for nontrivial point group $(\mathbb{I} - R_\gamma)t_\gamma$ cannot be equal to the zero translation for every possible R_γ in the point group and $\mathbf{t}_\gamma$ in the lattice, the subgroup $P < \Gamma_P$ is not closed under conjugation, and hence is not normal.

Since in the context of space groups the subgroups involved in every internal product can be identified with simpler groups (by for example replacing group elements $(A, \mathbf{0})$ with A or $(\mathbb{I}, \mathbf{a})$ with $\mathbf{a}$), it is often convenient to write decompositions in terms of external products. However, when doing so we must be careful to convert these external products to their equivalent internal description before applying statements such as those at the beginning of this section.

We say the group G is *decomposable* if G is the direct product of two normal subgroups, and *semi-decomposable* if it is the semidirect product of a normal and non-normal subgroup.

Identifying Γ_B and S subgroups

For a Sohncke group, there are only three possibilities for the non-identity elements: They can be pure rotations, pure translations, or (nondegenerate) screw motions. That is, every rigid-body transformation can be decomposed as

$$(R, \mathbf{t}) = (R, (I-R)\mathbf{p} + d\mathbf{n})$$

where $\mathbf{n}$ is the unit vector defining the axis of rotation of R, therefore satisfying $R\mathbf{n}=\mathbf{n}$, $\mathbf{p}$ is a point on the screw axis, and d is the amount of translation along the screw axis. Without loss of generality, we can always enforce the orthogonality condition $\mathbf{p}\cdot\mathbf{n}=0$. When $d=0$, the motion is a pure rotation, though it will only be a rotation around the origin when in addition $(I-R)\mathbf{p}=\mathbf{0}$. When $R=I$, the motion is a pure translation, and we can take $\mathbf{n}=\mathbf{t}/\|\mathbf{t}\|$.

In the general case, simply by taking the dot product of $(I-R)\mathbf{p}+d\mathbf{n}=\mathbf{v}(R)$ with $\mathbf{n}$ then gives

$$\mathbf{v}(R)\cdot\mathbf{n} = d. \tag{20}$$

And so, evaluating (20) is a quick tool to identify what kinds of transformations populate fundamental domains of finite coset spaces.

If $\mathcal{F}_{\Gamma/\Sigma}$ can be decomposed as a product of $\mathbb{B}$ and $\mathbb{S}$ subgroups as in (2), then some of those transformations that are identified as screw will populate $\mathbb{B}$ and some of those identified as rotations will populate $\mathbb{S}$. We must first identify which combination of elements exhibit closure with respect to the group operation of the original group, modulo Σ.

Main theorems used in computations

Throughout this paper, we use the following results to do computations.

Theorem 1: If $N \lhd H$ and $N \lhd \Gamma$ then

$$H \trianglelefteq \Gamma \Leftrightarrow \frac{H}{N} \trianglelefteq \frac{\Gamma}{N}. \tag{21}$$

Proof: See [48]. □

By definition, given a group G with $K<G$, a fundamental domain $F_{K\backslash G} \subset G$ is a set consisting of exactly one representative from each right coset. As G is partitioned into right cosets,

$$G = \bigcup_{g\in F_{K\backslash G}} Kg = K\mathcal{F}_{K\backslash G} \tag{22}$$

and the analogous statement is true for left cosets:

$$G = \bigcup_{g\in F_{G\backslash K}} gK = \mathcal{F}_{G/K}K.$$

If $N \lhd G$, then

$$G = \mathcal{F}_{\frac{G}{N}} N = N\mathcal{F}_{\frac{G}{N}} \tag{23}$$

where the product of two subsets (not necessarily subgroups) $A, B \subset G$ is defined as

$$AB = \{ab \,|\, a\in A,\ b\in B\}.$$

The product of subsets in a group inherits the associativity of the group. That is, given $A, B, C \subset G$, then $(AB)C = A(BC)$.

Lemma 2.1: Let $\Sigma \lhd \Gamma$ be a lattice-translation subgroup (i.e. $\Sigma \le T$), and let $\Sigma < \Gamma_B$, $\Gamma_S < \Gamma$ where Γ_B is Bieberbach, $\Gamma_S = \Sigma S = \Sigma \rtimes \mathbb{S}$, and $S := \{\mathbf{0}\} \rtimes \mathbb{S}$ with $\mathbb{S} < \mathbb{P}$ (the point group of Γ). Then the conditions

$$\mathcal{F}_{\frac{\Gamma}{\Sigma}} = \mathcal{F}_{\frac{\Gamma_B}{\Sigma}} S \bmod \Sigma \tag{24}$$

$$\Gamma = \Sigma\mathcal{F}_{\frac{\Gamma_B}{\Sigma}} S \tag{25}$$

$$\Gamma = \Gamma_B S \tag{26}$$

and

$$\frac{\Gamma}{\Sigma} = \frac{\Gamma_B}{\Sigma}\mathbb{S}. \tag{27}$$

are equivalent.

Proof: By definition, $A = B \bmod \Sigma$ means that $\Sigma A = \Sigma B$ and the equality in (25) results from applying (23). Applying (23) again to (25) gives (26).

Also using condition (24), by an appropriate choice of $\mathcal{F}_{\Gamma/\Sigma}$ every $g \in \mathcal{F}_{\Gamma/\Sigma}$ can be decomposed as $g = bs$ where $b \in F_{\Gamma_B/\Sigma}$ and $s \in S$. Therefore, using the associativity of products of subsets in a group, every coset $\Sigma g = g\Sigma$ can be written as $(\Sigma b)s$, which is the same as (27). □

Lemma 2.2: Let Γ_B be a Bieberbach space group containing lattice translation group Σ and let $\Gamma_S = \Sigma S = \Sigma \rtimes \mathbb{S}$ be a symmorphic space group where $S = \{\mathbf{0}\} \rtimes \mathbb{S}$ with $\mathbb{S}$ denoting the point group of Γ_S. Then

$$\Gamma_B \cap \Gamma_S = \Sigma \tag{28}$$

and

$$\frac{\Gamma_B}{\Sigma} \cap \mathbb{S} = \{\Sigma\}. \tag{29}$$

where $e = (I, \mathbf{0})$.

Proof: (28) follows from the fact that elements of a Bieberbach group always have $\mathbf{v}(R) \neq 0$ except for $\mathbf{v}(I) = \mathbf{0}$ whereas by an appropriate choice of origin, $\mathbf{v}(R) = \mathbf{0}$ always. Therefore they can only share the subgroup Σ. Using the modular law for intersections of subgroups, and rewriting (28) as

$$\Gamma_B \cap (\Sigma S) = \Sigma(\Gamma_B \cap S) = \Sigma,$$

and observing that $\Gamma_B \cap S$ is a group that intersects Σ only at e gives

$$\Gamma_B \cap S = \{e\}.$$

Then since $S \cap \Sigma = \{e\}$, for any choice of $\mathcal{F}_{\frac{\Gamma_B}{\Sigma}}$ containing e we get

$$\mathcal{F}_{\frac{\Gamma_B}{\Sigma}} \cap S = \{e\},$$

which is equivalent to (29). □

Theorem 2: Let $\Sigma \lhd \Gamma$, and $\Sigma < \Gamma_B$, $\Gamma_S < \Gamma$ satisfy the conditions in Lemma 2.1. Moreover, if

$$\mathcal{F}_{\frac{\Gamma}{\Sigma}} = \mathcal{F}_{\frac{\Gamma_B}{\Sigma}} S \bmod \Sigma \tag{30}$$

then the following conditions are equivalent:

$$s\mathcal{F}_{\frac{\Gamma_B}{\Sigma}} s^{-1} = F_{\frac{\Gamma_B}{\Sigma}} \bmod \Sigma \, \forall s \in S \tag{31}$$

$$\Gamma_B \lhd \Gamma \tag{32}$$

$$\Gamma = \Gamma_B \rtimes \mathbb{S} \tag{33}$$

and

$$\frac{\Gamma}{\Sigma} = \frac{\Gamma_B}{\Sigma} \rtimes \mathbb{S}. \tag{34}$$

Proof: $\Sigma \lhd \Gamma_B$ and $\Sigma \lhd \Gamma_S$ because normality of Σ in subgroups of Γ containing Σ is inherited. Using condition (31) and the normality of Σ,

$$s\Gamma_B s^{-1} = s\left(\Sigma \mathcal{F}_{\frac{\Gamma_B}{\Sigma}}\right)s^{-1} = (s\Sigma s^{-1})\left(s\mathcal{F}_{\frac{\Gamma_B}{\Sigma}} s^{-1}\right)$$
$$= \Sigma \mathcal{F}_{\frac{\Gamma_B}{\Sigma}} = \Gamma_B.$$

But from Lemma 2.1, (30) gives $\Gamma = \Gamma_B S$ which together with Lemma 2.2 implies $\Gamma_B \lhd \Gamma$. Then, since $\Gamma_B \cap S = \{e\}$, it must be that $\Gamma = \Gamma_B \rtimes \mathbb{S}$. Moreover, starting with this result and working backwards, all of the steps are reversible.

Using (27) and recognizing that (31) is equivalent to

$$\frac{\Gamma_B}{\Sigma} \lhd \frac{\Gamma}{\Sigma}$$

(a result that could also be obtained using Theorem 1 and $\Gamma_B \lhd \Gamma$) together with (29) gives (34). Working in reverse and evaluating (27) as a product of fundamental domains mod T takes us back to (30). □

Sample calculations

Consider the nonsymmorphic space group $\Gamma = P2_12_12$ and its maximal lattice translation group $T = P1$. Then, by the COSET function in the Bilbao Crystallographic server, elements $\gamma \in \mathcal{F}_{\frac{\Gamma}{T}}$ can be visualized by their action on $\mathbf{x} = [x, y, z]^t \in \mathbb{R}^3$ as

$$\gamma \cdot \mathbf{x} \in \{(x, y, z);\ (-x, -y, z);\ (-x + 1/2, y + 1/2, -z);$$
$$(x + 1/2, -y + 1/2, -z)\}.$$

The elements $\{(x, y, z); (-x, -y, z)\}$ are a conjugated version of those in the fundamental domain of $P2/P1$, and those in $\{(x, y, z); (-x+1/2, y+1/2, -z)\}$ are a conjugated version of those in $P2_1/P1$. Moreover, each of these subgroups has index 2, and so both are normal. And so we can conclude that

$$\frac{P2_12_12}{P1} = \frac{P2_1}{P1} \times \frac{P2}{P1}$$

and so from Theorem 2,

$$P2_12_12 = P2_1 \rtimes \frac{P2}{P1}$$

where we have used the fact that a direct product is also semi-direct (hence the conditions of the theorem are met); but a direct product in the quotient group does not carry over to the parent group.

As a second example, consider $\Gamma = P4_2$ and $T = P1$. Then elements of $\gamma \in \mathcal{F}_{\frac{\Gamma}{T}}$ are defined by

$$\gamma \cdot \mathbf{x} \in \{(x,y,z);(-x, -y, z);(-y, x, z + 1/2);$$
$$(y, -x, z + 1/2)\}.$$

Here again it is easy to see that a conjugated version of $\mathcal{F}_{P2/P1}$ is present, but the interpretation of the rest is not so clear. However, if we conjugate by α of the form in the section "Isomorphism vs. equality of fundamental domains" with $a=2$, then the fundamental domain $\mathcal{F}_{\frac{\Gamma}{\Sigma}}$ for the resulting sublattice translation group $\Sigma=\alpha T\alpha^{-1}$ is defined as

$$\left\{\begin{array}{l}(x,\,y,\,z);\;(-x,\,-y,\,z);(-y,\,x,\,z+1/4);\\ (y,\,-x,\,z+1/4);\,(x,\,y,\,z+1/2);\\ (-x,\,-y,\,z+1/2);\;(-y,\,x,\,z+3/4);\;(y,\,-x,\,z+3/4)\end{array}\right\}.$$

This result is the same as doubling the basis vector along the c-axis (as is given in the International Tables).

Within this $P2/P1$ is still visible, but now it becomes easier to see that $P4_1/P1$ is also present. And this has an index of 2, indicating normality, and so we can write the external semi-direct product

$$P4_2=P4_1\rtimes\frac{P2}{P1}.$$

Outline of decomposition algorithms for Sohncke groups

We have approached the problem of semi-decomposition of space groups from two different directions. These are called "top-down" and "bottom-up" as described below.

Top-down procedure

Space groups have an infinite number of elements. To reduce to finite computations, in the top-down procedure we perform all calculations in a quotient of the form $\frac{\Gamma}{\Sigma}:=\Gamma/\Sigma=\Sigma\backslash\Gamma$ where $\Sigma\leq T$ and $\Sigma\lhd\Gamma$, and we seek finite subgroups $\mathbb{B}$, $\mathbb{S}<\Gamma/\Sigma$ that respectively have coset representatives with no torsion and with only torsion such that representatives of each coset in Γ/Σ can be written as a product of representatives of cosets in $\mathbb{B}$ and $\mathbb{S}$. Then using the presented theorems, it becomes possible to make statements about the decomposition of Γ itself. Below is our procedure for finding Σ and identifying $\mathbb{B}$ and $\mathbb{S}$. This procedure, which we have done mostly manually, is outlined as an algorithm.

1. Set $n=1$ and read off $[\Gamma:T]=|\mathbb{P}|$ from the International Tables or the Bilbao Server;
2. Compute all subgroup paths from Γ to $P1$ of index $n\cdot[\Gamma:T]$. (For example, this can be done with the Bilbao Server SUBGROUPGRAPH function, which returns the affine transformation α for each path). Retain only those for which $P1\lhd\Gamma^{\alpha}$. If $n>1$ and no subgroup paths exists with $P1\lhd\Gamma^{\alpha}$, skip to 8;
3. Use the information from Step 2 to compute $\mathcal{F}_{\Gamma/\Sigma}$. This is equivalent in terms of affine conjugated fundamental domains to $\mathcal{F}_{\Gamma^{\alpha}/P1}$. This can be computed using the Bilbao Server function COSETS. (It does not matter whether left or right cosets are computed because they are equivalent modulo $P1$, which must be normal from the previous step);
4. Evaluate the elements of $\mathcal{F}_{\Gamma/\Sigma}$ to determine whether they are pure rotations or screw displacements using (20). Screw displacements and pure rotations are held as candidate elements of $\mathbb{B}$ and $\mathbb{S}$, respectively.
5. Construct all possible $\mathbb{B}$ and $\mathbb{S}$ subgroups and retain those pairs for which $|\mathbb{B}|\cdot|\mathbb{S}|=|\Gamma/\Sigma|$;
6. For those that satisfy 5, check if $\mathbb{B}\mathbb{S}=\Gamma/\Sigma$ (or equivalently $\mathcal{F}_{\Gamma_B/\Sigma}S=\mathcal{F}_{\Gamma/\Sigma}\bmod\Sigma$), and keep all of these;
7. Check whether $\mathbb{B}\lhd\Gamma/\Sigma$ or $\mathbb{S}\lhd\Gamma/\Sigma$. If $\mathbb{B}\lhd\Gamma/\Sigma$, then go to Step 9. Otherwise record and continue;
8. If no $(\mathbb{B},\mathbb{S})$ pairs survive and if $[\Gamma:\Sigma]/[\Gamma_B:\Sigma]<[\Gamma:T]$ then increase n by 1 and go to Step 2. Otherwise continue;
9. Having stored all $\mathbb{B}$, $\mathbb{S}$ pairs, find the names of Γ_B and Γ_S that gave rise to them. This can be achieved by comparing the number and nature of these elements (e.g. the value of d and rotation angle θ) against those parameters for the 8 nontrivial Bieberbach Sohncke group types and 23 nontrivial symmorphic Sohncke group types. Alternatively, the information about these groups can be used by the Bilbao Server function IDENTIFY GROUP to find their names. After names are identified in this way, end.

We note that for all P groups except those with names starting $P4_2$ we have found through trial and error that it is possible to take $\Sigma=T=P1$. That is, only a single loop through the above procedure with $n=1$ will suffice. Indeed, this is how our manual search for such decompositions began. Coset representatives with respect to subgroup T computed using the Bilbao Server function COSETS are easily classified as torsion elements or torsion-free by evaluating (20). Those that are torsion free have $d\neq 0$ and are kept as candidates to populate $\mathbb{B}$ and those that have torsion have $d=0$ and are kept as candidates for $\mathbb{S}$. We could visually inspect these candidates to identify different possible $\mathbb{B}$ and $\mathbb{S}$ subgroups. Since these will not necessarily appear as they do in their standard form, we computed screw parameters and rotation angles and axes to identify their type. This can all be done for relatively small $[\Gamma:T]$ by hand.

In cases such as $P4_2$ and several other groups with name "4_2" in it, it was not possible to identify $\mathbb{B}$ using the approach described in the previous paragraph, which led us to use a coarser lattice $\Sigma < T$ and to do the above computations with Γ/Σ instead of Γ/T. Here an affine transformation must be identified that can be used to conjugate $P1$, simultaneously preserving $\mathbb{S}$ and coarsening the translational sublattice. Using this coarser lattice, as in the case of $P4_2$, will unveil $\mathbb{B}$. In particular, we used the affine transformation with linear part diag[1, 1, 2] in conjunction with the Bilbao Server COSET function.

A similar approach is pursued for C, I, and F type groups. In some cases such as $C222_1$, it is possible to take $\Sigma = T$. But in most cases we have found that valid $\mathbb{B}$ and $\mathbb{S}$ subgroups can be identified when using $\Sigma = P1 < T$. We call this approach "top down" because we start with the finest translation lattice shared by both Γ_B and Γ_S. When the search successfully concludes with $\Sigma = T$, then $\mathbb{S}$ and the $\mathbb{B}$ obtained in this way are both the largest ones possible in their respective categories in the sense of having the minimal indices in Γ/Σ.

The "bottom up" procedure described below is an alternative that seems to lend itself more easily to automation, and hence is useful for more difficult cases where $[\Gamma{:}\Sigma]$ is large.

Bottom-up procedure

When the top-down procedure described above becomes too laborious, an entirely different approach can be taken. If $\Gamma_B, \Gamma_S < \Gamma$ share the same normal lattice translation subgroup, i.e. $\Sigma = T \cap \Gamma_B = T \cap \Gamma_S$, then

$$\Gamma = \Sigma \mathcal{F}_{\Gamma_B/\Sigma} S = \Gamma_B S = \Gamma_S \mathcal{F}_{\Gamma_B/\Sigma}$$

and

$$[\Gamma{:}\Gamma_B] = |S| \text{ and } [\Gamma{:}\Gamma_S] = [\Gamma_B{:}\Sigma] = |\mathbb{B}|.$$

And if $[\Gamma, \Sigma] = |\mathbb{B}| \cdot |\mathbb{S}|$ we will have that

$$|\mathbb{B}| \cdot |\mathbb{S}| = [\Gamma{:}\Gamma_S] \cdot [\Gamma{:}\Gamma_B]. \tag{35}$$

These statements hold regardless of whether or not $\Gamma_B \lhd \Gamma$, and can be used to assess potential compatibility of Γ_B and S in the sense of (3), as outlined below.

1. Search for all subgroup paths from Γ to Γ_B and from Γ to Γ_S until $[\Gamma{:}\Gamma_B] \leq |\mathbb{S}_{\max}|$ and $[\Gamma{:}\Gamma_S] \leq 6$. Here $|\mathbb{S}_{\max}|$ is the order of the point group of the maximal symmorphic subgroup of Γ. If none exists use $[\Gamma{:}T]$ in place of $|\mathbb{S}_{\max}|$, since there is no way for a proper subgroup of the point group to have order greater than this. The number 6 is used for limiting the search for Γ_S because this is the largest possible value for $|\mathbb{B}|$. (We use the SUBGROUPGRAPH function in the Bilbao server to identify candidate Bieberbach and symmorphic subgroups);
2. Whereas in the "top down" approach, T (or Σ) are guaranteed a priori to be common to both Γ_S and Γ_B, there is no guarantee that this will be the case here. That is, it is possible for

$$\Sigma_B := T \cap \Gamma_B \neq \Sigma_S := T \cap \Gamma_S,$$

in which case (35) will not hold. If $\Gamma_S = \Sigma_S \rtimes \mathbb{S}$ and $\Sigma_B < \Gamma_B$ and $\Sigma_S, \Sigma_B < T$ with $\Sigma_B < \Sigma_S$, then they are not compatible for use in a semi-decomposition because then $\Gamma_B \cap \Gamma_S \neq \Sigma_S$. But if $\Sigma_S = \Sigma_B := \Sigma$, then we check all pairs for which $|\mathbb{B}| \cdot |\mathbb{S}| = [\Gamma{:}\Sigma]$ and keep these as candidates.
3. The coset representatives for the remaining compatible candidate pairs obtained in the previous step are then multiplied. If they reproduce $\mathcal{F}_{\Gamma/\Sigma}$, then they represent a valid decomposition, and the procedure terminates here once all such decompositions are found.

Note that if a $\mathbb{B}$ or $\mathbb{S}$ group appears in the top node of the maximal subgroup graph then it will naturally have minimal index within its type. That is, this copy will have smaller index in the parent group than a copy found further down in the maximal subgroup tree. If in addition it is normal (which we determine in the usual way by conjugating elements of the subgroup by all elements of the group and determining if the conjugates reside in the subgroup), then this is a good candidate for a semi-decomposition. If not, then working down the tree will yield all minimal-index groups of a particular Bieberbach or symmorphic type.

When decompositions cannot be found using the above algorithms

In very few cases, the above procedures do not return results because there is no $\Sigma \lhd \Gamma$ common to both Γ_B and Γ_S. In these rare cases (208, 214) we apply specialized methods as described in the Appendix. Assessing whether or not Σ is normal in Γ is easy. Given $\sigma = (I, t_\sigma) \in \Sigma$, then define the lattice $\Lambda := \{t_\sigma | \sigma \in \Sigma\}$. Then $\Sigma \lhd \Gamma$ if and only if $R_\gamma \cdot \Lambda = \Lambda$ for all $R_\gamma \in \mathbb{P}$.

Table of semi-decomposable non-symmorphic Sohncke space groups

Of the 230 space group types that are inequivalent under conjugation by $Aff^+(3)$, 13 types are Bieberbach groups. Included in this 13 is the group of pure lattice translations of the primitive lattice, $T = (P1)^\alpha$. Since this translation group is both Bieberbach and symmorphic and contains no rotations, reflections, screws, or glides, we refer to it as both a “trivially Bieberbach” and “trivially symmorphic” space group.

Nontrivial Sohncke and non-Sohncke Bieberbach types

The table below excludes T and indicates which of the remaining Bieberbach groups are also Sohncke.

Intl.	Γ	Sohncke?	$[\Gamma_B:T]$
4	$P2_1$	Y	2
7	Pc	N	2
9	Cc	N	2
19	$P2_12_12_1$	Y	4
29	$Pca2_1$	N	4
33	$Pna2_1$	N	4
76	$P4_1$	Y	4
78	$P4_3$	Y	4
144	$P3_1$	Y	3
145	$P3_2$	Y	3
169	$P6_1$	Y	6
170	$P6_5$	Y	6

The quotient groups $P2_12_12_1/P1$, $Pca2_1/P1$, and $Pna2_1/P1$ can, respectively, be written as direct products of the form $(P2_1)^\alpha/P1\times(P2_1)^\beta/P1$, $(Pc)^\alpha/P1\times(P2_1)^\beta/P1$, and $(Pc)^\alpha/P1\times(P2_1)^\beta/P1$ for different conjugations α and β.

Note that in mathematics books, 10 space group types are given including the trivial one consisting of only lattice translations. This is because they do not distinguish between the enantiomorphic pairs $(P3_1, P3_2)$, $(P4_1, P4_3)$, $(P6_1, P6_5)$.

As there are 230 isomorphism classes of space groups, showing all of the explicit calculations to decompose them would require hundreds of pages of text. Instead here we only summarize the results for the Sohncke groups, giving enough information to retrace our calculations using routines in the Bilbao Crystallographic Server [45–47].

Most Sohncke groups are semi-decomposable

Of the 230 space group types, 65 are Sohncke. Of these 65, 24 are symmorphic (including T) and eight are nontrivial Bieberbach. Of the remaining 33 nonsymmorphic non-Bieberbach Sohncke space groups, 29 are semi-decomposable, which corresponds to a ‘Y’ in the $\mathbb{B}\lhd\Gamma/\Sigma$ column below and no $|\Xi|>1$.[6] Groups that we are not able to semi-decompose are 90, 208, 210, 214, and these are explained in greater detail in the Appendix. In the case of 90 and 210 it is possible to write $\Gamma=\Gamma_B S$ with Γ_B not normal in Γ. In all cases it is possible to write $\Gamma=\Gamma_{B'}\Gamma_S$ where multiple choices exist for $\Gamma_{B'}$. In such cases, it is possible to find a $\Sigma<\Gamma$ such that[7]

$$\mathcal{F}_{\Sigma\backslash\Gamma}=B'\Xi S \text{ and } \Sigma\backslash\Gamma=\mathbb{B}'\mathbb{X}\mathbb{S} \tag{36}$$

where B' is a fundamental domain of $\dfrac{\Gamma_{B'}}{\Gamma_{B'}\cap T}$ in Γ, Ξ is a set of translations such that $\Sigma\Xi\le T$, and S is as before. $\mathbb{X}$ is the group with elements that are cosets of the form $\xi\Sigma=\Sigma\xi$ with $\xi\in\Xi$. When $|\Xi|=1$, Γ is decomposed into a product (semi-direct or otherwise) of Γ_B and S.

Decompositions of the form in (36) are generally not unique, and unlike the case when $|\Xi|=1$, there is no clear criteria for stopping the search. Therefore, when $|\Xi|\neq1$ we list examples to show that (36) is possible rather than to attempt an exhaustive enumeration.

Using the frequencies of occurrence tabulated in [3], altogether these groups that are not semi-decomposable are only represented in the PDB less than one percent of the time.

In constructing the table below, we seek $\Gamma_B\lhd\Gamma$ and $\Gamma_S<\Gamma$ that enable the sorts of decompositions described earlier. We start our search with small values of the product of indices

$$\Pi:=[\Gamma:\Gamma_B]\cdot[\Gamma:\Gamma_S].$$

When two combinations of Γ_B and Γ_S have the same minimal value of Π we list both next to each other in the table to the left of the | symbol, and those with larger values of Π are listed to the right of the | symbol. In all but one case, the complementing S is the same for decompositions corresponding to minimal-value of Π (which we call an “efficient” decomposition) and for those with larger value of Π. In the one case when this happens, $C222_1$, another $\Gamma_{S'}$ is listed such that S' is the complement of the less efficient $\Gamma_{B'}$. When the answer to the normality question about S is different for the efficient and inefficient decompositions, it is listed to the right of | in the normality column. This only happens for one Sohncke group, $P6_322$.

6 Here Ξ consists of all pure translation elements of $\mathcal{F}_{\Sigma\backslash\Gamma}$ and when $\Sigma\lhd\Gamma$, $\dfrac{\Gamma}{\Sigma}=\mathbb{B}\mathbb{X}\mathbb{S}$, where $\mathbb{X}=\dfrac{\Sigma\Xi}{\Sigma}<\dfrac{\Gamma}{\Sigma}$.

7 Note that even if Σ is not normal in Γ, if $\Sigma\lhd\Gamma_{B'}$ and $\Sigma\Xi S=\Gamma_S$ then multiplying (36) on the left by Σ and using (22) gives $\Gamma=\Gamma_{B'}\Gamma_S$.

If we cannot find a $\Gamma_B \lhd \Gamma$ such that $[\Gamma{:}\Gamma_B] \le |\mathbb{S}|$, where $\mathbb{S}$ is the point group of the the symmorphic subgroup $\Gamma_S < \Gamma$ with minimal $[\Gamma{:}\Gamma_S]$, then we terminate the search. This strategy ensures that the calculation is finite.

In the table that follows, we identify elements of a Bieberbach or symmorphic subgroup with the name given if we can find Γ', Γ'' and affine transformations α, β such that

$$\mathcal{F}_{\frac{\Gamma_B}{\Sigma_B}} = \alpha \mathcal{F}_{\frac{\Gamma'}{T'}} \alpha^{-1}$$

and

$$\mathcal{F}_{\frac{\Gamma_S}{\Sigma_S}} = \beta \mathcal{F}_{\frac{\Gamma''}{T''}} \beta^{-1}.$$

In this case Γ_B inherits the name of Γ' and Γ_S inherits the name of Γ''.

Intl.	Γ	Γ_B	Γ_S	$\lvert\Xi\rvert$	$\mathbb{B}, \mathbb{S} \lhd \Sigma\backslash\Gamma$?	$\Sigma = T$?
17	$P222_1$	$P2_1$	$P2$	1	Y, Y	Y
18	$P2_12_12$	$P2_1\vert P2_12_12_1$	$P2$	1	Y, Y	Y
20	$C222_1$	$P2_1\vert P2_12_12_1$	$C2\vert P2$	1	Y, Y	Y
24	$I2_12_12_1$	$P2_12_12_1$	$P2$	1	Y, N	N
77	$P4_2$	$P4_1$, $P4_3$	$P2$	1	Y, N	N
80	$I4_1$	$P4_1$, $P4_3$	$P2$	1	Y, N	N
90	$P42_12$	$P2_1$	$C222$, $P4$	1	N, Y	Y
91	$P4_122$	$P4_1$	$P2$	1	Y, N	Y
92	$P4_12_12$	$P2_12_12_1$, $P4_1$	$C2$	1	Y, N	Y
93	$P4_222$	$P4_1$, $P4_3$	$P222$	1	Y, N	N
94	$P4_22_12$	$P2_12_12_1$, $P4_1$, $P4_3$	$C222$	1	Y, N	N
95	$P4_322$	$P4_3$	$P2$	1	Y, N	Y
96	$P4_32_12$	$P2_12_12_1$, $P4_3$	$C2$	1	Y, N	Y
98	$I4_122$	$P2_12_12_1$, $P4_1$, $P4_3$	$C222$	1	Y, N	N
151	$P3_112$	$P3_1$	$C2$	1	Y, Y	Y
152	$P3_121$	$P3_1$	$C2$	1	Y, Y	Y
153	$P3_212$	$P3_2$	$C2$	1	Y, N	Y
154	$P3_221$	$P3_2$	$C2$	1	Y, N	Y
171	$P6_2$	$P3_2\vert P6_1$	$P2$	1	Y, Y	Y
172	$P6_4$	$P3_1\vert P6_5$	$P2$	1	Y, Y	Y
173	$P6_3$	$P2_1\vert P6_1$, $P6_5$	$P3$	1	Y, Y	Y
178	$P6_122$	$P6_1$	$C2$	1	Y, N	Y
179	$P6_522$	$P6_5$	$C2$	1	Y, N	Y
180	$P6_222$	$P3_2\vert P6_1$	$C222$	1	Y, N	Y
181	$P6_422$	$P3_1\vert P6_5$	$C222$	1	Y, N	Y
182	$P6_322$	$P2_1\vert P6_1$, $P6_5$	$P321$, $P312$	1	Y, Y |N	Y
198	$P2_13$	$P2_12_12_1$	$R3$	1	Y, N	Y
199	$I2_13$	$P2_12_12_1$	$R3$	1	Y, N	N
208	$P4_232$	$P2_1$	$P23$	4	N/A, N/A	N
210	$F4_132$	$P2_12_12_1$, $P4_1$, $P4_3$	$F23$	1	N, Y	N
212	$P4_332$	$P2_12_12_1$	$R32$	1	Y, N	Y
213	$P4_132$	$P2_12_12_1$	$R32$	1	Y, N	Y
214	$I4_132$	$P2_12_12_1$	$R32$	2	Y, N	N

In the instance where $|\Xi| > 1$ and N appears in this table in the $\mathbb{S}$ column, the largest normal Bieberbach group (i.e. the one with smallest possible index $[\Gamma{:}\Gamma_B]$) has a $\mathcal{F}_{\Gamma/\Gamma_B}$ that consists of not only point transformations, but pure fractional translations. This happens when the largest lattice translation subgroup of Γ_B is smaller than that for Γ_S, i.e. $\Sigma_B < \Sigma_S$. And similarly, when there exists $\Gamma_S \lhd \Gamma$ and $\mathcal{F}_{\Gamma/\Gamma_S}$ contains Bieberbach group elements for a coarser lattice than Σ_S we write $|\Xi| > 1$ and N in the $\mathbb{B}$ column. In cases when $\Sigma = T \cap \Gamma_B$ is not normal in Γ, then $\Sigma\backslash\Gamma$ is not a group and it does not make sense to evaluate normality of $\mathbb{B}$ and $\mathbb{S}$, and so 'N/A' is listed in the table. Since these cases do not fit the semi-decomposition paradigm, this leads us to state and prove the following theorem so as to include these cases in a decomposition that is more general than $\Gamma = \Gamma_B S$ (but not as useful for our application).

Theorem 3: Every Sohncke space group can be written as a product of the form

$$\Gamma = \Gamma_B \Gamma_S.$$

Proof: There are several cases in the above table:
(1), $\Sigma \lhd \Gamma$ and $\mathbb{B} \lhd \Gamma/\Sigma$ with $\mathbb{S} < \Gamma/\Sigma$;
(2), $\Sigma \lhd \Gamma$ and $\mathbb{S} \lhd \Gamma/\Sigma$ with $\mathbb{B} \lhd \Gamma/\Sigma$;
(3), $\Sigma \lhd \Gamma$ and $\mathbb{B}, \mathbb{S} \lhd \Gamma/\Sigma$;
(4), $\Sigma \lhd \Gamma$ and $\mathbb{B} \lhd \Gamma/\Sigma$ with $S \ne \mathcal{F}_{\Gamma/\Gamma_B}$.
(5), $\Sigma \lhd \Gamma$ and $\mathbb{S} \lhd \Gamma/\Sigma$ with $\mathcal{F}_{\Gamma_B/\Sigma_B} \ne \mathcal{F}_{\Gamma/\Gamma_S}$.
(6), Σ is not normal in Γ and $\Sigma\backslash\Gamma = \mathbb{B}\mathbb{X}\mathbb{S}$ with $\Sigma \lhd \Gamma_B$ and $\Gamma_S = \Sigma\Xi S$.

In Cases 1, 2, and 3, $\Gamma = \Sigma \mathcal{F}_{\frac{\Gamma}{\Sigma}} S$. But since $\Sigma = \Sigma\Sigma$, and $\Sigma \lhd \Gamma$, in all of these cases we can write

$$\begin{aligned}\Gamma &= \Sigma\Sigma\mathcal{F}_{\Gamma_B/\Sigma} S \\ &= (\Sigma\mathcal{F}_{\Gamma_B/\Sigma})(\Sigma S) = \Gamma_B \Gamma_S.\end{aligned}$$

The only difference between the cases is which of the subgroups Γ_B or Γ_S are normal. In fact, as per Lemma 2.1 these calculations do not require either of them to be normal. But when it does exist, normality will be inherited from the quotient groups according to the fifth column in the table.

Case 4 is slightly different. In this case $\Gamma_B \lhd \Gamma$ but $\Sigma_B < \Sigma_S$. And so

$$\Gamma = \Sigma_B \mathcal{F}_{\Gamma_B/\Sigma_B} \mathcal{F}_{\Gamma_S/\Sigma_B}.$$

But again using the fact that $\Sigma_B = \Sigma_B\Sigma_B$ and $\Sigma_B \lhd \Gamma$, we get

$$\Gamma = (\Sigma_B \mathcal{F}_{\Gamma_B/\Sigma_B})(\Sigma_B \mathcal{F}_{\Gamma_S/\Sigma_B}) = \Gamma_B \Gamma_S,$$

which follows from Lemma 2.1. Case 5 follows in the same way with the roles of B and S reversed.

Case 6 follows because

$$\begin{aligned}\Gamma &= \Sigma\mathcal{F}_{\Sigma\backslash\Gamma} = \Sigma B \Xi S \\ &= \Sigma\Sigma B \Xi S = (\Sigma B)(\Sigma \Xi S) = \Gamma_B \Gamma_S.\end{aligned} \qquad \square$$

Discussion

From the table, we see that 29 of the 33 nonsymmorphic Sohncke space groups can be decomposed into semi-direct products of Bieberbach subgroups and point subgroups. We also mention that in several cases in addition to being able to write $\Gamma/\Sigma = \mathbb{B} \rtimes \mathbb{S}$ it is also the case that $\Gamma/\Sigma = \mathbb{B} \ltimes \mathbb{S}$, and so $\Gamma/\Sigma = \mathbb{B} \times \mathbb{S}$. This is true for groups with the following international numbers: 17, 18, 20, 151, 152, 171, 172, 173, 182.

We note also that amongst the space groups that cannot be semi-decomposed, there is at least some product structure in the quotient group. For example space group 90 only has a normal copy of Bieberbach group $P2_1$ with index 8, and so $[\Gamma:\Gamma_B] \neq |\mathbb{S}|$ where $|\mathbb{S}| = 4$ for the largest subgroup of the point group, $\mathbb{S}$, which has an associated symmorphic subgroup of Γ.

The reason why the quotient in the case of 214 does not decompose into two factors is that the only normal Bieberbach group with $[\Gamma:\Gamma_B] < [\Gamma:T]$ is $\Gamma_B = P2_12_12_1$ with $[\Gamma:\Gamma_B] = 12$. But the largest symmorphic subgroup of 214 is $R32$ which has $|\mathbb{S}| = [R32:T_R] = 6$. And so there is no way to make $[\Gamma:\Gamma_B] = |\mathbb{S}|$. And it is not reverse semi-decomposable because $R32$ is not a normal subgroup. Nevertheless, Theorem 3 applies and provides a simple tool to write $I4_132$ as a product of affine-conjugated versions of $P2_12_12_1$ and $R32$ even in this case.

It should be noted that these four cases of 90, 208, 210, and 214 that do not semi-decompose, respectively, represent 0.43, 0.03, 0.08, and 0.10 percent of all protein crystal structures in the PDB [3]. In other words, more than 99 percent of protein crystals occur in space groups that are either Bieberbach, symmorphic, or a semidirect product of a Bieberbach subgroup and a point subgroup.

Conclusions

In this paper we introduced the idea that space groups lie along a spectrum with Bieberbach groups at one extreme and symmorphic groups at the other. Moreover, we observe that 29 of the 33 nonsymmorphic Sohncke space groups can be decomposed into semi-direct products of Bieberbach subgroups and point subgroups, and all Sohncke space groups can be written as products of Bieberbach and symmorphic subgroups.

We focus on the Sohncke case because that is what arises in the application that motivated us to study this subject. Moreover, the frequency of occurrence of Sohncke space groups populated by macromolecular crystals are predominantly those that admit such decompositions. The approach outlined for obtaining these decompositions can be applied to a number of non-Sohncke space groups as well, and we will pursue this in future work.

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A Additional examples of the decomposition procedure

Here additional examples of decompositions are provided. First, we show an example where decomposing Γ/T does not work, but Γ/Σ does. Next we show a case when no semi-decomposition is possible. Finally, we show a case where an additional (less efficient) semi-decomposition is possible.

A.1 24, $I2_12_12_1$

As another example, consider $\Gamma = I2_12_12_1$. To determine T, we use the Bilbao function HERMANN which gives

$$\alpha = \begin{pmatrix} -1/2 & -1/2 & 0 & 0 \\ -1/2 & -1/2 & 1 & 1/4 \\ -1/2 & 1/2 & 0 & 0 \end{pmatrix}$$

(where the perfunctory bottom row in the affine transformation as a 4×4 matrix has been removed to save space.)

The coset representatives in the decomposition of Γ with respect to T (in the basis of T) are given below:

$$\begin{aligned}\mathcal{F}_{\Gamma/T} = \{&(x, y, z);\ (-y, -x, -z);\\ &(-x+1/2, -y+1/2, -x-y+z+1/2);\\ &(y+1/2, x+1/2, x+y-z+1/2)\}.\end{aligned}$$

Here $S = \{(x, y, z); (-y, -x, -z)\}$ is identical with $\mathcal{F}_{C2/T_C}$, which is consistent with the fact that MAXSUB gives $[I2_12_12_1:C2] = 2$. If $\mathcal{F}_{\Gamma/T}$ can be semi-decomposed, then it should be possible to find a Bieberbach subgroup with

$[\Gamma_B{:}P1]=2$. But the only Bieberbach group that could satisfy this is $P2_1$, and MAXSUB does not list $P2_1$ as a maximal subgroup. Therefore, there is no need to investigate the case when $[I2_12_12_1{:}T_I]=4$ further, and so we investigate $[I2_12_12_1{:}\Sigma]=8$, which is the next smallest candidate.

When $\Sigma=P1<T$ the Bilbao COSET function (left and right are the same so $\Sigma \lhd \Gamma$) gives

$$\mathcal{F}_{I2_12_12_1/P1}=\{(x,y,z);\ (-x+1/2,\ -y,\ z+1/2);\ (-x,\ y+1/2,\ -z+1/2);\ (x+1/2,\ -y+1/2,\ -z);\ (x+1/2,\ y+1/2,\ z+1/2);\ (-x,\ -y+1/2,\ z);\ (-x+1/2,\ y,\ -z);\ (x,\ -y,\ -z+1/2)\}$$

Here $(x+1/2, y+1/2, z+1/2)$ is a pure translation. Such will only occur when $\Sigma<T$. In contrast, $(-x+1/2, -y, z+1/2)$; $(-x, y+1/2, -z+1/2)$; $(x+1/2, -y+1/2, -z)$ are all screw motions with $d=1/2$, and all of the rotation axes are mutually orthogonal with an angle of rotation of π. So this is a clue that it may be related to $P2_12_12_1/P1$. We verify this by using the Bilbao COSET function to give

$$\mathcal{F}_{P2_12_12_1/P1}=\{(x,y,z);\ (-x+1/2,\ -y,\ z+1/2);\ (-x,\ y+1/2,\ -z+1/2);\ (x+1/2,\ -y+1/2,\ -z)\}$$

This matches with four entries in $\mathcal{F}_{I2_12_12_1/P1}$. In more complicated cases we might need to search for an affine transformation to relate a subgroup of $\mathcal{F}_{\Gamma/\Sigma}$ with a candidate Bieberbach group quotient by an appropriate translation group.

In contrast, looking at the elements $(-x, -y+1/2, z)$; $(-x+1/2, y, -z)$; $(x, -y, -z+1/2)$, we observe that they are all rotations because $d=0$. But if we seek $\mathbb{B}$ and $\mathbb{S}$ such that their product reproduces $\mathcal{F}_{I2_12_12_1/P1}$, then both cannot have order 4. And because $\mathbb{B}=2_12_12_1/P1$ is of order 2 in $\mathcal{F}_{I2_12_12_1/P1}$ when evaluated modulo $P1$, it is normal, and so we do not need to check that the conjugation action of $\mathbb{S}_i$ on $\mathcal{F}_{I2_12_12_1/P1}$.

We see that we can define a two-element point group (which fixes a point other than the origin) from the identity and any one of $(-x, -y+1/2, z)$; $(-x+1/2, y, -z)$; $(x, -y, -z+1/2)$. For example,

$$\mathbb{S}_1:=\{(x,y,z);\ (-x,\ -y+1/2,\ z)\},$$
$$\mathbb{S}_2:=\{(x,y,z);\ (-x+1/2,\ y,\ -z)\},$$
$$\mathbb{S}_3:=\{(x,y,z);\ (x,\ -y,\ -z+1/2)\}.$$

Abstractly, every two-element group is isomorphic, and so candidates for these are $P2/P1$ or $C2/T_C$. But concretely, we can only find affine transformations such that $\alpha_i\mathcal{F}_{P2/P1}\alpha_i^{-1}=\mathbb{S}_i$. Again examining left and right COSETS using Bilbao (or doing finite calculations in the factor group) we find that

$$I2_12_12_1/P1=(P2_12_12_1/P1)\rtimes(P2/P1).$$

There is no guarantee that this decomposition is unique.

Using the bottom-up approach employing the Bilbao MAXSUB function, we see that $[I2_12_12_1{:}P2_12_12_1]=2$. and as $[P2_12_12_1{:}P1]=4$ and $[P2{:}P1]=2$ we conclude that it is not possible to find a decomposition with smaller values than this, and so our search terminates.

A.2 90, $P42_12$

Consider group no. 90, and use $\Gamma=P42_12$ and $T=P1$. When using the identity transformation, the Bilbao COSET function gives

$$\mathcal{F}_{P42_12/P1}=\{(x,y,z);\ (-x,\ -y,\ z);\ (-y+1/2,\ x+1/2,\ z);\ (y+1/2,\ -x+1/2,\ z);\ (-x+1/2,\ y+1/2,\ -z);\ (x+1/2,\ -y+1/2,\ -z);\ (y,\ x,\ -z);\ (-y,\ -x,\ -z)\}$$

This is convenient because we can immediately identify

$$\mathbb{S}_1:=\{(x,y,z);\ (-x,\ -y,\ z);\ (y,\ x,\ -z);\ (-y,\ -x,\ -z)\}$$

with a point group of order 4 (and index 2 in Γ). Therefore it is normal. Searching for every symmorphic space group with point group of order 4, we find that this corresponds to $C222/T_C$. The complementing subgroup can be chosen as

$$\mathbb{B}:=\{(x,y,z);\ (-x+1/2,\ y+1/2,\ -z)\}.$$

(In fact, there are four possible choices, but they all act in the same way as described below.) It is easy to check that this is a group.

For the nontrivial transformation in this group, R is a rotation around $\mathbf{n}=\mathbf{e}_2$ by π. And $\mathbf{v}(R)=[1/2, 1/2, 0]^t$. And so $\mathbf{v}\cdot\mathbf{n}=1/2$. We conclude that $\mathbb{B}$ is isomorphic with $P2_1/P1$. To find affine transformations that will make the relationship between $\mathbb{B}$ and $P2_1/P1$, we solve the equation $\alpha g=g'\alpha$ where g and g' are respectively representatives taken from $\mathbb{B}$ and $P2_1/P1$.

Clearly $\mathcal{F}_{P42_12/P1}=\mathbb{S}_1\mathbb{B}$. Next we ask if $\mathbb{B}$ is normal. To do this, we use the Bilbao COSET function with the information about α that has been computed. We find that left and right cosets do not match modulo $P1$, and $\mathbb{B}$ is not normal, and

$$\mathcal{F}_{P42_12/P1}=\mathbb{S}_1\rtimes\mathbb{B}.$$

The benefit of this top-down approach is that we need not worry about whether the two components correspond to space subgroups with a common lattice, since that is guaranteed a priori. But this does not provide a complete list of all possible decompositions. We therefore go to the Bilbao MAXSUB function, and look for other low-index symmorphic and Bieberbach subgroups. We find that $[P42_12{:}P4]=2$. Hence $P4 \lhd P42_12$. The same subroutine provides a transformation, and we find (after moding out extraneous 1's returned by Bilbao) that

$$\mathcal{F}_{(\alpha P42_12\alpha^{-1})/P1}=\{(x,y,z);\,(-x,-y,z);\,(-y,x,z);\,(y,-x,z);\,(-x+1/2,\,y+1/2,\,-z);\,(x+1/2,\,-y-1/2,\,-z);\,(y+1/2,\,x-1/2,\,-z);\,(-y-1/2,\,-x-1/2,\,-z)\}.$$

Here we see that the first four elements correspond to $\mathbb{S}_2 := P4/P1$, and with $(-x+1/2,\, y+1/2,\, -z)$ clearly visible, we can define the complement $\mathbb{B}$ as before. And it is not normal here either. Therefore, we conclude that

$$\mathcal{F}_{(\alpha P42_12\alpha^{-1})/P1}=\mathbb{S}_2 \rtimes \mathbb{B}.$$

Though the quotient is "reverse-semi-decomposable" the Bieberbach subgroup is <u>not</u> normal (and no other Bieberbach subgroup with $[\Gamma{:}\Gamma_B]<[\Gamma{:}T]$ is normal either.

There is a copy of $P2_12_12_1$ that has index 4, which we can identify using the HERMANN subroutine in the Bilbao server, and gradually increasing the index of candidate Bieberbach subgroups. But left and right cosets do not match, and hence it is not normal.

Another route to index-4 $P2_12_12_1$ is by observing that none of the coset representatives in $\mathcal{F}_{(\alpha P42_12\alpha^{-1})/P1}$ given above have translations in the z component. Then, using the affine transformation α with linear part diag[1, 1, 2] and zero translation in the COSET function in Bilbao can double the size of the quotient group, giving enough room to fit both a copy of a conjugated $\mathcal{F}_{P2_12_12_1/P1}$ and the same $\mathbb{S}$ as before, which is left unaffected by this affine conjugation. Moreover, $\mathbb{S}$ is normal in the resulting 16-element quotient group as well. And so we can write $\Gamma/\Sigma=(C222/T_C)\rtimes(P2_12_12_1/P1)$. But $P2_12_12_1$ is not normal in $P42_12$, and because this quotient group has 16 elements as opposed to the 8 of the original, we do not include this in the table.

There is an affine-conjugated copy of $P2_1$ with $\alpha=\mathrm{diag}[1,1,2]$ that is normal in $P42_12$ with index 8, but this index does not match the order of the largest point subgroup, and so the compatibility conditions fail, and so it cannot be used in a semi-decomposition.

We therefore conclude that 90 cannot be efficiently semi-decomposed, but the quotient group can be "reverse-semi-decomposed" in multiple ways, each with the pure rotation part being normal rather than the Bieberbach part. As a consequence of this, and of Theorem 3, it is possible to write

$$P42_12=P2_1P4=P2_1C222$$

where it is understood that in the above different copies of $P2_1$ are used. Moroever, from Lemma 2.1, this is a case where even though Γ_B is not normal, it is nevertheless possible to perform decompositions of the form $\Gamma=\Gamma_B S$.

A.3 93, $P4_222$

Using the Bilbao COSET function, and taking the top-down approach, $[P4_222{:}P1]=8$ and

$$\mathcal{F}_{P4_222/P1}=\{(x,y,z);\,(-x,-y,z);\,(-y,x,z+1/2);\,(y,-x,z+1/2);\,(-x,y,-z);\,(x,-y,-z);\,(y,x,-z+1/2);\,(-y,-x,-z+1/2)\}.$$

Of these,

$$\mathbb{S}=\{(x,y,z);\,(-x,-y,z);\,(-x,y,-z);\,(x,-y,-z)\}=\mathcal{F}_{P222/P1}$$

is a subgroup with $[P4_222{:}P222]=2$ and hence it is normal. But there is no way to construct a two-element subgroup from the remaining elements, which appear to be $P4_1$ or $P4_3$ transformations. And so we look for ways to conjugate so that all elements of these subgroups are present as representatives in the coset decomposition.

Using HERMANN routine in Bilbao with $G=93$ and $H=76$ with index 4, we find that with

$$\alpha=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&2&1/2\end{pmatrix}$$

$$\mathcal{F}_{(\alpha P4_222\alpha^{-1})/P1}=\{(x,y,z);\,(-x,-y,z);\,(-y,x,z+1/4);\,(y,-x,z+1/4);\,(-x,y,-z-1/2);\,(x,-y,-z-1/2);\,(y,x,-z-1/4);\,(-y,-x,-z-1/4);\,(x,y,z+1/2);\,(-x,-y,z+1/2);\,(-y,x,z+3/4);\,(y,-x,z+3/4);\,(-x,y,-z);\,(x,-y,-z);\,(y,x,-z-3/4);\,(-y,-x,-z-3/4)\}.$$

Several subgroups can be visually identified:

$$\mathbb{S}=\{(x,y,z);\ (-x,-y,z);$$
$$(-x,y,-z);\ (x,-y,-z)\}=\mathcal{F}_{P222/P1},$$
$$\mathbb{B}_1=\{(x,y,z);\ (y,-x,z+1/4);$$
$$(-x,-y,z+1/2);\ (-y,x,z+3/4)\}=\mathcal{F}_{P4_1/P1},$$
$$\mathbb{B}_2=\{(x,y,z);\ (-y,x,z+1/4);$$
$$(-x,-y,z+1/2);\ (y,-x,z+3/4)\}=\mathcal{F}_{P4_1/P1}.$$

We find that $\mathbb{B}_1\mathbb{S}=\mathbb{B}_2\mathbb{S}=\mathcal{F}_{P222/P1}$ mod P1. And by conjugating each element of $\mathbb{B}_1$ by all elements of $\mathbb{S}$ and evaluating mod P1, we see that $\mathbb{B}_1$ is closed under conjugation. The same is true for $\mathbb{B}_2$. Hence, we find that $\mathbb{B}_1$ and $\mathbb{B}_2$ are normal in $\mathcal{F}_{P4_222/P1}$, and so

$$P4_222=P4_1\rtimes(P222/P1)$$

and

$$P4_222=P4_3\rtimes(P222/P1)$$

A.4 94, $P4_22_12$

$[P4_22_12,\ P1]=8$. When computing $\mathcal{F}_{P4_22_12/P1}$ using the Bilbao COSET function, we find four coset reps that are pure rotations.

But also present are elements such as $(-x+1/2, y+1/2, -z+1/2)$ and $(x+1/2, -y+1/2, -z+1/2)$, each of which are conjugated versions of elements of $P2_1$. But, computing all right coset reps for $P4_22_12/P2_1$ in HERMANN, and computing the corresponding left cosets in COSET, we see that the $P2_1$ elements corresponding to this are not normal.

In contrast, $(-y+1/2,\ x+1/2,\ z+1/2)$ and $(y+1/2, -x+1/2,\ z+1/2)$ which are in $P4_1$, and neither of which forms a 2-element group mod $P1$ with the identity. But when using

$$\alpha=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&2&0\end{pmatrix}$$

in Bilbao, $[(P4_22_12)^\alpha, P1]=16$.

$P4_1\lhd(P4_22_12)^\alpha$; $[(P4_22_12)^\alpha,\ P4_1]=4$ and $[(P4_22_12)^\alpha,\ C222]=4$.

In particular,

$$\mathcal{F}_{(P4_22_12)^\alpha/P1}=\{(x,y,z);(-x,-y,z);(y,x,-z);(-y,-x,-z);$$
$$(-y+1/2,x+1/2,z+1/4);(y+1/2,-x+1/2,z+1/4);$$
$$(-x+1/2,y+1/2,-z+1/4);(x+1/2,-y+1/2,-z+1/4);$$
$$(x,y,z+1/2);(-x,-y,z+1/2);$$
$$(-y+1/2,x+1/2,z+3/4);(y+1/2,-x+1/2,z+3/4);$$
$$(-x+1/2,y+1/2,-z-1/4);(x+1/2,-y+1/2,-z-1/4);$$
$$(y,x,-z-1/2);(-y,-x,-z-1/2)\}$$

And

$$\mathbb{S}=\{(x,y,z);\ (-x,-y,z);\ (y,x,-z);\ (-y,-x,-z)\}$$

looks like $\mathcal{F}_{C222/T_C}$

Of the remainder of elements, we can construct

$$\mathbb{B}:=\{(x,y,z);\ (-y+1/2,x+1/2,z+1/4);$$
$$(-x,-y,z+1/2);\ (y+1/2,-x+1/2,z+3/4)\}.$$

$\mathbb{B}$ is normal in $\mathcal{F}_{(P4_22_12)^\alpha/P1}$, and so

$$P4_22_12=P4_1\rtimes(C222/T_C)$$

And the same is true for $P4_3$:

$$P4_22_12=P4_3\rtimes(C222/T_C)$$

We note also that there are normal affine-conjugated copies of $P222$ and $P2_12_12_1$ inside of $P4_22_12$ with $[(P4_22_12)^\alpha{:}P222]=[(P4_22_12)^\beta{:}P2_12_12_1]=4$. The difficulty with $P222$ is that it has a different lattice than the Bieberbach subgroups with compatible orders, and so it cannot be used to semi-decompose. $P2_12_12_1$ does have a complement that is $C222/T_C$ (about a point that is not the origin when expressed in the basis of $P2_12_12_1$ in the standard setting) giving

$$P4_22_12=P2_12_12_1\rtimes(C222/T_C).$$

A.5 98, $I4_122$

$P4_1$ with index 4 is normal. $[I4_122{:}P1]=16$ in standard setting. Subgroup of pure rotations is order 4. So should be decomposable.

$$\mathcal{F}_{I4_122/P1}=$$
$$\{(x,y,z);\ (-x+1/2,-y+1/2,z+1/2);$$
$$(-y,x+1/2,z+1/4);\ (y+1/2,-x,z+3/4);$$
$$(-x+1/2,y,-z+3/4);\ (x,-y+1/2,-z+1/4);$$
$$(y+1/2,x+1/2,-z+1/2);\ (-y,-x,-z);$$
$$(x+1/2,y+1/2,z+1/2);\ (-x,-y,z);$$
$$(-y+1/2,x,z+3/4);\ (y,-x+1/2,z+1/4);$$
$$(-x,y+1/2,-z+1/4);\ (x+1/2,-y,-z+3/4);$$
$$(y,x,-z);\ (-y+1/2,-x+1/2,-z+1/2)\}$$

Of these,

$$\mathbb{S}=\{(x, y, z); (-y, -x, -z); (-x, -y, z); (y, x, -z);$$

This is a conjugated version of $\mathcal{F}_{C222/T_C}$.

$$\mathbb{B}=\{(x, y, z); (y, -x+1/2, z+1/4);$$
$$(-x+1/2, -y+1/2, z+1/2); (-y+1/2, x, z+3/4)\}$$

This is of the form $\alpha\mathcal{F}_{P4_1/P1}\alpha^{-1}$ where $\alpha\in SE(3)$, and $\mathbb{B}$ is normal in $\mathcal{F}_{I4_122/P1}$, and so

$$I4_122=P4_1\rtimes(C222/T_C).$$

Similarly, by choosing different coset representatives to define $\mathbb{B}$ we find

$$I4_122=P4_3\rtimes(C222/T_C).$$

It is also possible to identify elements of $P2_12_12_1$ in $\mathcal{F}_{I4_122/P1}$ and to write

$$I4_122=P2_12_12_1\rtimes(C222/T_C).$$

A.6 171 *P*6$_2$ – A case that can be alternatively decomposed with larger [Γ:Σ]

It is obvious from examining $\mathcal{F}_{\frac{P6_2}{P1}}$ that it is possible to write $P6_2=P3_2\rtimes(P2/P1)$, and in this case $[\Gamma:\Gamma_B]=[P6_2:P3_2]=2$ and $[\Gamma_B:T]=[P3_2:P_1]=3$.

Here we show that it is possible to find other decompositions where $[\Gamma:\Gamma_{B'}]$ is the same but $[\Gamma_{B'}:\Sigma]$ is larger. In particular, $[P6_2:P6_1]=2$ and $[P6_1:P1]=6$ with

$$\alpha=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&2&0\end{pmatrix}.$$

The coset representatives from the two cosets are

$$\{(x, y, z); (-y, x-y, z+1/3);$$
$$(-x+y, -x, z+2/3); (-x, -y, z+1/2);$$
$$(y, -x+y, z+5/6); (x-y, x, z+1/6)\}$$

and

$$\{(-x+y, -x, z+1/6); (x, y, z+1/2);$$
$$(-y, x-y, z+5/6); (x-y, x, z+2/3);$$
$$(-x, -y, z); (y, -x+y, z+1/3)\}.$$

From these we can construct

$$\mathcal{F}_{P6_2/P6_1}=\{(x, y, z); (-x, -y, z)\},$$

which is a pure rotation group.

This is a case where we could decompose Γ/Σ (which has 12 elements)

$$\Gamma/\Sigma=\mathbb{B}\rtimes\mathbb{S}$$

where $\mathbb{B}=P6_1/\Sigma$ and

$$\mathbb{S}:=\{(x, y, z); (-x, -y, z)\}=P2/P1.$$

Similar less-efficient decompositions are possible for $P222_1$, $C222_1$, $P6_3$, $P6_4$, $P6_222$, $P6_422$, $P6_322$. These are listed in the table after the | symbol. In most cases they have the same type of complementing S as the Γ_B in the more efficient decomposition of the same group, and the answer to the question of whether $\mathbb{S}$ is normal in $\Sigma\backslash\Gamma$ is the same as well. When the answers differ, the answer for the less efficient decomposition is written to the right of the | symbol.

A.7 208 and 210

These two groups each have large symmorphic subgroups of index 2, indicating normality of Γ_S. Since in a semi-decomposition all of the torsion must reside in $\mathbb{S}$, if a compatible Bieberbach subgroup exists it must be the case that $[\Gamma:\Gamma_B]=|\mathbb{S}|$. Each of the groups 208 and 210 have a symmorphic subgroup with point group of order 12 (195 in 208, and 196 in 210). Moreover, in each of these two groups are Bieberbach groups of index 12 (76 and 78 in 208, and 76, 78 and 19 in 210). Checking these (e.g. by conjugating generators of each candidate Γ_B by all generators of Γ) none of these Bieberbach subgroups are normal. In some cases there is a faster way to rule out Γ_B's that are not normal, based on the discussion at the end of Section 6, which leads to the following theorem.

Theorem 4: If $\Sigma=\Gamma_B\cap T\lhd\Gamma_B<\Gamma$ and Σ is <u>not</u> normal in Γ, then Γ_B is not normal in Γ.

Proof: Every element of Γ_B can be written as $\gamma_B=\sigma b$ for some $\sigma\in\Sigma$ and $b\in\mathcal{F}_{\frac{\Gamma_B}{\Sigma}}$. By construction, $\mathcal{F}_{\frac{\Gamma_B}{\Sigma}}\cap T=\{e\}$ where T is the minimal-index translation subgroup of Γ. Conjugating by an arbitrary $\gamma\in\Gamma$ gives

$$\gamma\gamma_B\gamma^{-1}=\gamma\sigma b\gamma^{-1}=(\gamma\sigma\gamma^{-1})(\gamma b\gamma^{-1}).$$

Conjugation does not change the nature of a rigid-body displacement, i.e. pure translations remain pure translations, pure rotations remain pure rotations, and screw displacements remain screw displacements with the same θ and d. Therefore, $\gamma\sigma\gamma^{-1}$ must be a translation, but since Σ is not normal in Γ it must be that $\gamma\sigma\gamma^{-1}\notin\Sigma$ for at least one $\gamma \in \Gamma$. Therefore, $\gamma\gamma_B\gamma^{-1}$ cannot be decomposed as $\sigma' b'$. But since every element of Γ_B can be decomposed in this way, it must be that $\gamma\gamma_B\gamma^{-1} \notin \Gamma_B$ and therefore Γ_B cannot be normal in Γ. □

Note that whereas the proof of this theorem is specific to space groups, it can be viewed as an example of the contrapositive of the statement

$$\Sigma, \Gamma_B \triangleleft \Gamma \Rightarrow \Sigma \cap \Gamma_B \triangleleft \Gamma$$

which is true in more general (abstract) settings. That is, the intersection of normal subgroups is also normal.

As a consequence of this theorem, if $\Sigma = \Gamma_B \cap T$ is the primitive translation group for Γ_B, and $\Gamma_B < \Gamma$, then if Σ is not normal in Γ we need not even check if Γ_B is normal, because it is guaranteed not to be. Therefore, in such cases it cannot be the case that $\Gamma = \Gamma_B \rtimes \mathbb{S}$.

Moreover, even if there were normal Bieberbach subgroups further down the subgroup tree, these would be irrelevant for such decompositions because there would be no way to match $[\Gamma:\Gamma_B]$ and $|\mathbb{S}|$. In searching for Γ_B and S such that $\Gamma = \Gamma_B S$, the indices and orders of coset spaces must match even if Γ_B is not normal in Γ because $\Gamma_B \cap S = e$. The above mentioned groups have compatible indices and orders for this, and these are explored in the subsections that follow.

A.7.1 Details of 208

There are no normal Bieberbach subgroups in this group of an index compatible with the condition $[\Gamma:\Gamma_B] = |\mathbb{S}|$. The largest symmorphic subgroup has

$$\begin{aligned} S = \{&(x, y, z); (-x, -y, z); (-x, y, -z);\\ &(x, -y, -z); (z, x, y); (z, -x, -y);\\ &(-z, -x, y); (-z, x, -y); (y, z, x);\\ &(-y, z, -x); (y, -z, -x); (-y, -z, x)\} = \mathcal{F}_{\frac{P23}{P1}} \end{aligned}$$

It has index 2, and hence it is normal and the quotient is a group of order 2. The only Bieberbach group with $|\mathbb{B}| = 2$ is $\Gamma_B = P2_1$. But none of the elements of $P4_232$ are elements of $P2_1$ with the same lattice. For example, $\{(x, y, z); (y+1/2, x+1/2, -z+1/2)\}$ is a 2-element subgroup of $\mathcal{F}_{P4_232/P1}$ that is not in S. Though it is isomorphic with $P2_1/P1$, it is not equal to $\mathcal{F}_{P2_1/P1}$. Rather, it is an element of $C2$ sharing the same lattice as $P4_232$ and so we can write

$$P4_232 = P23 \rtimes \left(\frac{C2}{T_C}\right) = P23C2.$$

But our goal was not to decompose space groups into products of symmorphic subgroups, and so we look further down the tree. To do this, we double the unit cell as before by choosing $\alpha = \text{diag}[1, 1, 2]$. This results in 48-element coset spaces

$$(P4_232)^\alpha / P1 \neq P1 \backslash (P4_232)^\alpha.$$

In other words, this is a case where Σ is not normal in Γ. Nevertheless, within $\mathcal{F}_{P1\backslash(P4_232)^\alpha}$ we can identify groups

$$\begin{aligned} B_1 = \{&(x, y, z); (-y+1/2, x+1/2, z+1/4);\\ &(-x, -y, z+1/2); (y+1/2, -x+1/2, z+3/4)\} = \mathcal{F}_{\frac{(P4_1)^\alpha}{P1}}\\ B_2 = \{&(x, y, z); (y+1/2, -x+1/2, z+1/4);\\ &(-x, -y, z+1/2); (-y+1/2, x+1/2, z+3/4)\} = \mathcal{F}_{\frac{(P4_3)^\alpha}{P1}} \end{aligned}$$

and

$$\begin{aligned} &S = \alpha \mathcal{F}_{\frac{P23}{P1}} \alpha^{-1} =\\ &\{(x, y, z); (-x, y, -z); (x, -y, -z);\\ &(-x, -y, z); (2z, x, 1/2y); (-2z, -x, 1/2y);\\ &(-2z, x, -1/2y); (2z, -x, -1/2y); (y, 2z, 1/2x);\\ &(y, -2z, -1/2x); (-y, -2z, 1/2x); (-y, 2z, -1/2x)\} \end{aligned}$$

Unfortunately,

$$\Gamma \neq \Sigma B_i S = \Gamma_{B_i} S.$$

And no other α was found that would enable such a decomposition. Searching further down the subgroup graph cannot result in a $\Gamma_B S$ decomposition. We therefore search for products of the form $\Gamma_B \Gamma_S$.

Choosing $\alpha = \text{diag}[1, 2, 1]$ we can identify inside of $\mathcal{F}_{P1\backslash(P4_232)^\alpha}$ (which is not a group) three groups B, Ξ, S:

$$\begin{aligned} &S = \alpha \mathcal{F}_{\frac{P23}{P1}} \alpha^{-1} =\\ &\{(x, y, z); (-x, y, -z); (x, -y, -z);\\ &(-x, -y, z); (z, 1/2x, 2y); (z, -1/2x, -2y);\\ &(-z, -1/2x, 2y); (-z, 1/2x, -2y); (2y, 1/2z, x);\\ &(-2y, 1/2z, -x); (2y, -1/2z, -x); (-2y, -1/2z, x)\}\\ &\Xi = \{(x, y, z); (x, y+1/2, z)\} = \mathcal{F}_{\frac{(P1)^\alpha}{P1}} \end{aligned}$$

and

$$B = \{(x, y, z); (-x, y+1/2, -z)\} = \mathcal{F}_{\frac{P2_1}{P1}}.$$

But the product of these three does not reproduce $\mathcal{F}_{P1\backslash(P4_232)^\alpha}$ because even though $B \cap \Xi = \Xi \cap S = B \cap S = \{e\}$ we find that $(\Xi S) \cap B \neq \{e\}$.

Therefore we search deeper down the subgroup graph (i.e. for larger $[\Gamma:\Sigma]$) and find that there are multiple affine transformations with linear part

$$A=\begin{pmatrix}1 & 1 & 0\\ -1 & 1 & 0\\ 0 & 0 & 2\end{pmatrix}$$

or a similarity-transformed version of this corresponding to permutations of coordinate axis names. We therefore express Γ^{α} in the basis of $\Sigma=P1$ with $\alpha=(A, \mathbf{0})$ (since translations are irrelevant to identifying Bieberbach subgroups in the top-down procedure, and making the translation zero retains the origin allows us to easily identify point rotations.) This makes it easy to identify the largest S (corresponding to $P23$) as

$$\begin{aligned}
&S=\{(x, y, z)(-x, -y, z)(-y, -x, -z)(y, x, -z);\\
&(-1/2x-1/2y+z,\ 1/2x+1/2y+z,\ -1/2x+1/2y);\\
&(1/2x+1/2y+z,\ -1/2x-1/2y+z,\ 1/2x-1/2y);\\
&(1/2x+1/2y-z,\ -1/2x-1/2y-z,\ -1/2x+1/2y);\\
&(-1/2x-1/2y-z,\ 1/2x+1/2y-z,\ 1/2x-1/2y);\\
&(-1/2x+1/2y-z,\ -1/2x+1/2y+z,\ 1/2x+1/2y);\\
&(1/2x-1/2y-z,\ 1/2x-1/2y+z,\ -1/2x-1/2y);\\
&(-1/2x+1/2y+z,\ -1/2x+1/2y-z,\ -1/2x-1/2y);\\
&(1/2x-1/2y+z,\ 1/2x-1/2y-z,\ 1/2x+1/2y)\}.
\end{aligned}$$

We also identify

$$B_1=\{(x, y, z);\ (x+1/2, -y, -z+1/4)\}$$

(which is a conjugated version of $\mathcal{F}_{P2_1/P1}$),

$$\begin{aligned}\Xi_1=\{&(x, y, z);\ (x+1/2, y+1/2, z);\\ &(x, y, z+1/2);\ (x+1/2, y+1/2, z+1/2)\}\end{aligned}$$

and

$$\begin{aligned}B_2=\{&(x, y, z);\ (-x+1/2, -y+1/2, z+1/2);\\ &(-x, y+1/2, -z+3/4);\ (x+1/2, -y, -z+1/4)\}\end{aligned}$$

(which is a conjugated version of $\mathcal{F}_{P2_12_12_1/P1}$)

$$\Xi_2=\{(x, y, z);\ (x, y, z+1/2)\}.$$

In this case[8]

$$\mathcal{F}_{\Sigma\backslash\Gamma^{\alpha}}=B_i\Xi_i S$$

for $i=1, 2$. Whereas $\Gamma_S=\Sigma\Xi_1 S$, we find that $\Gamma_S=\Sigma\Xi_1 S$ and so it cannot be used. But changing the order we find $\Xi_1 S B_1=\mathcal{F}_{\Sigma\backslash\Gamma^{\alpha}}$, since a necessary condition for the product of subgroups to be a group is permutability. This results in $\Gamma=\Gamma_{B_1}\Gamma_S=\Gamma_S\Gamma_{B_1}$.

8 Even though $\mathcal{F}_{\Sigma\backslash\Gamma^{\alpha}}$ is not a group, equality is still assessed by evaluating the translational part modulo $\mathbb{Z}^3$ since multiplication on the left by $(I, \mathbf{z})\in\Sigma=P1$ only has the effect of changing the coset representatives used to define $\mathcal{F}_{\Sigma\backslash\Gamma^{\alpha}}$ by adding an arbitrary translation.

A.7.2 Details of 210

Using SUBGROUPGRAPH provides a number of transformations to generate $\mathcal{F}_{\Sigma\backslash\Gamma}$ of order 48. We choose this order because that is what is required to match $|B|\cdot|S|$. The linear parts of all of the transformations are all equivalent under relabeling of axes, and the translational part is set to zero so that it is easier to identify point transformations. Therefore, we choose

$$\alpha=\begin{pmatrix}1/2 & 1/2 & 0 & 0\\ -1/2 & 1/2 & 0 & 0\\ 0 & 0 & 1 & 0\end{pmatrix}.$$

Then the resulting

$$\mathcal{F}_{\Sigma\backslash\Gamma}=\mathcal{F}_{P1\backslash(F4_132)^{\alpha}}$$

has the following subsets

$$\begin{aligned}
B_1=\{&(x, y, z);\ (-x+1/2, -y+1/2, z+1/2);\\
&(-x, y+1/2, -z+1/4);\ (x+1/2, -y, -z+3/4)\}\\
B_2=\{&(x, y, z);\ (-y, x+1/2, z+1/4);\\
&(-x+1/2, -y+1/2, z+1/2);\ (y+1/2, -x, z+3/4)\}\\
B_3=\{&(x, y, z);\ (y, -x+1/2, z+1/4);\\
&(-x+1/2, -y+1/2, z+1/2);\ (-y+1/2, x, z+3/4)\}
\end{aligned}$$

and

$$\begin{aligned}
&S=\{(x, y, z);\ (-x, -y, z);\ (y, x, -z);\ (-y, -x, -z);\\
&(-1/2x-1/2y+z,\ 1/2x+1/2y+z,\ -1/2x+1/2y);\\
&(-1/2x-1/2y-z,\ 1/2x+1/2y-z,\ 1/2x-1/2y);\\
&(-1/2x+1/2y-z,\ -1/2x+1/2y+z,\ 1/2x+1/2y);\\
&(1/2x-1/2y-z,\ 1/2x-1/2y+z,\ -1/2x-1/2y);\\
&(1/2x+1/2y+z,\ -1/2x-1/2y+z,\ 1/2x-1/2y);\\
&(1/2x+1/2y-z,\ -1/2x-1/2y-z,\ -1/2x+1/2y);\\
&(-1/2x+1/2y+z,\ -1/2x+1/2y-z,\ -1/2x-1/2y);\\
&(1/2x-1/2y+z,\ 1/2x-1/2y-z,\ 1/2x+1/2y);
\end{aligned}$$

These respectively correspond to $P2_12_12_1$, $P4_1$, $P4_3$, and $F23$. It can be shown that

$$\mathcal{F}_{\Sigma\backslash\Gamma}=B_i S$$

for $i=1, 2, 3$ and so we could write

$$\Gamma = \Sigma B_i S = \Gamma_{B_i} S$$

even though none of the Γ_{B_i}'s are normal with index 12.

A.8 213, $P4_132$ and 212, $P4_332$

Taking the top-down approach, we use COSET to compute representatives of the cosets in $P4_132/P1$. The result is $[P4_132{:}P1] = 24$. Of these, we identify four elements to construct $\mathcal{F}_{P2_12_12_1/P1}$, and we find that this is normal in $\mathcal{F}_{P4_132/P1}$.

We also find three representatives (x, y, z); (z, x, y); (y, z, x) that are clearly rotations that preserve the origin. However, these rotations all have the axis of rotation $\mathbf{n}^t = [1, 1, 1]/\sqrt{3}$, and so any point on the line passing through the origin with this direction will be preserved by them. Since the goal is to clearly separate point and Bieberbach transformations, we seek the translation to the point along this line that maximizes the number of entries that have $\mathbf{v} = 0$. In particular, we find that when using

$$\alpha = \begin{pmatrix} 1 & 0 & 0 & 3/8 \\ 0 & 1 & 0 & 3/8 \\ 0 & 0 & 1 & 3/8 \end{pmatrix}$$

in the Bilbao COSET function, $\mathcal{F}_{(\alpha P4_132\alpha^{-1})/P1} = BS$ where

$$S = \{(x, y, z);\ (z, x, y);\ (y, z, x);\ (-y, -x, -z);\ (-x, -z, -y);\ (-z, -y, -x)\}$$

and

$$B = \{(x, y, z);\ (-x-1/4,\ -y-3/4,\ z+1/2);\ (-x-3/4,\ y+1/2,\ -z-1/4);\ (x+1/2,\ -y-1/4,\ -z-3/4)\} = \alpha\mathcal{F}_{P2_12_12_1/P1}\alpha^{-1}.$$

We note also that $\mathcal{F}_{(\alpha P4_132\alpha^{-1})/P1} = B'S$ where

$$B' = \{(x, y, z);\ (-y-1/2,\ x+3/4,\ z+1/4);\ (-x-1/4,\ -y-3/4,\ z+1/2);\ (y+1/4,\ -x-1/2,\ z+3/4)\}$$

and $\Gamma_{B'}$ can be identified with $P4_1$. Using the Bilbao Server function IDENTIFY GROUP finds that $\Gamma_S = R32$.

Alternatively, using the bottom-up approach we search for Bieberbach and symmorphic subgrouos respectively of order 4 and 6 (index 6 and 4) with SUBGROUPGRAPH. This shows that $R32$ is the only symmorphic subgroup of $P4_132$ with these properties, and so we identify it with

$$\mathbb{S} = \beta\mathcal{F}_{R32/T_R}\beta^{-1}.$$

SUBGROUPGRAPH can also be used to identify $P4_1$ and $P2_12_12_1$ as subgroups of $P4_132$ with the correct index with fundamental domains $\mathcal{F}_{\Gamma_B/T}$ of the correct order. Of these only $P2_12_12_1$ is normal.

We note that using any α given by SUBGROUPGRAPH for $P4_132$ and $P4_1$ with index 6 gives

$$\mathcal{F}_{\Gamma/T} = \mathcal{F}_{\Gamma_{B'}/T}\,\mathcal{F}_{\Gamma/\Gamma_{B'}}.$$

For example, when α is a translation by $[1/4, 0, 1/2]^t$,

$$\mathcal{F}_{\Gamma_{B'}/T} = \{(x, y, z);\ (-x, -y, z+1/2);\ (-y, x, z+1/4);\ (y, -x, z+3/4)\}$$

and we choose

$$\mathcal{F}_{\Gamma/\Gamma_{B'}} = \{(x, y, z);\ (-z+3/4,\ -x+3/4,\ y);\ (-y+3/4,\ z,\ -x+3/4);\ (-x+1/4,\ -z+1/4,\ -y+1/4);\ (z+1/2,\ -y+1/4,\ x+1/2);\ (y+1/2,\ x+1/2,\ -z+1/4)\}$$

which IDENTIFY GROUP identifies with $R32/T_R$. And so, even though this $\Gamma_{B'}$ is not normal, we can write $\Gamma = \Gamma_{B'}S$ by conjugating $\mathcal{F}_{\Gamma/\Gamma_{B'}}$ to make it a set of rotations around the origin, and calling this S. Even so, we do not list $P4_1$ in the table because it is not normal, and is $P2_12_12_1$ is normal, and hence the most useful for our application.

From the above it is clear that the top-down and bottom-up approaches provide the same results. And the final result is

$$P4_132 = P2_12_12_1 \rtimes \left(\frac{R32}{T_R}\right) = P4_1R32.$$

Group 212, $P4_332$ follows in a similar way, but with $\alpha \to \alpha^{-1}$ (corresponding to a translation by $-[3/8, 3/8, 3/8]^t$ instead of $[3/8, 3/8, 3/8]^t$). $P4_3$ and $P2_12_12_1$ as subgroups of $P4_332$ with the correct index with fundamental domains to decompose, but again only $P2_12_12_1$ is normal, leading to

$$P4_332 = P2_12_12_1 \rtimes \left(\frac{R32}{T_R}\right) = P4_3R32.$$

A.9 214, $I4_132$

$[\Gamma{:}T] = 24$ with minimal index symmorphic subgroup 155 (which has index 4 and point group of order 6). Bieberbach subgroups with the compatible value of $|\mathbb{B}| = 4$ are groups 19, 76, 78. However, these all have index 12 in group 214.

Therefore, Γ/T cannot be decomposed into the form $\mathbb{BS}$ because $[\Gamma:\Gamma_B] > |\mathbb{S}|$ and no $\mathcal{F}_{\Gamma_B/T}$ for these Γ_B's exists in $\mathcal{F}_{\Gamma/T}$.

The next finest lattice Σ is the lattice in the conventional setting, with $[\Gamma:\Sigma] = 48$. Σ is normal in Γ. As with 213, translating the origin by $[3/8, 3/8, 3/8]^t$ relative to that in the standard centering allows us to write

$$\mathcal{F}_{\frac{\Gamma}{\Sigma}} = \mathcal{F}_{\frac{\Gamma_B}{\Sigma}} \mathcal{F}_{\frac{\Gamma_S}{\Sigma}} = B\Xi S$$

where in the case of 214,

$$\mathcal{F}_{\frac{\Gamma_B}{\Sigma}} = B = \{(x, y, z);\ (-x-1/4, -y-3/4, z+1/2);\ (-x-3/4, y+1/2, -z-1/4);\ (x+1/2, -y-1/4, -z-3/4)\}$$

and

$$S = \{(x, y, z);\ (z, x, y);\ (y, z, x);\ (-y, -x, -z);\ (-x, -z, -y);\ (-z, -y, -x)\}$$

and

$$\Xi = \{(x, y, z);\ (x+1/2, y+1/2, z+1/2)\}$$

where $\Gamma_B = P2_12_12_1$ and $\Gamma_S = R32$.

As can be seen by the translation subgroup $\{(x, y, z); (x+1/2, y+1/2, z+1/2)\}$, the fundamental domain $\mathcal{F}_{\frac{\Gamma_S}{\Sigma}}$ is not a valid S. As mentioned earlier, attempting to use a finer lattice to remove this translation also prevents any normal Bieberbach groups from existing. And seeking a coarser Σ will only worsen the problem by resulting in more translational elements in $\mathcal{F}_{\frac{\Gamma_S}{\Sigma}}$. Therefore, a semi-decomposition is not possible for group 214. Nevertheless by the reasoning in Theorem 3, it is the case from the above that

$$I4_132 = P2_12_12_1 R32.$$

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