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RESEARCH ARTICLE

# Self-replicating degrees of crystallographic groups

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Abstract. An integer $d \geq 2$ is called a self-replicating degree of a group $G$ if there exist a subgroup $H \leq G$ of index $d$ and a surjective homomorphism $\phi : H \to G$ with trivial core. These are precisely the alphabet sizes of self-replicating (recurrent) actions of $G$. We investigate self-replicating degrees of crystallographic groups and compare them with self-covering degrees, that is, integers $d$ for which $G$ contains a subgroup of index $d$ isomorphic to $G$. Geometrically, the latter are precisely the degrees of self-coverings of the flat orbifold $\mathbb{R}^n/G$. We establish a method for describing the self-covering and self-replicating degrees of crystallographic groups and obtain explicit polynomial descriptions for all plane and space groups.

## Introduction

Crystallographic groups are discrete, cocompact groups of isometries of Euclidean spaces. They arise naturally in the study of crystals and periodic structures and play an important role in crystallography as well as in several areas of mathematics. The fundamental properties of crystallographic groups were described by Bieberbach (1910–1911). Specifically, every $n$-dimensional crystallographic group contains a maximal, finite-index, free abelian normal subgroup of translations isomorphic to $\mathbb{Z}^n$.

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Furthermore, in each dimension, there are only finitely many crystallographic groups up to isomorphism, thereby answering the first part of Hilbert's 18th problem.

In this paper, we indirectly consider self-similar actions of crystallographic groups. Broadly speaking, an action of a group on a space of words is self-similar if the restriction of the action to any natural subspace resembles the global action of the group. Self-similar actions provide a natural connection between algebra, automata theory, and fractal geometry, and play an important role in geometric group theory and dynamical systems. Self-similar actions have been investigated for a wide variety of group classes, including abelian groups [1–3], nilpotent groups [4–6], polycyclic groups [7], metabelian and solvable groups [8–11], affine groups [12], arithmetic groups [13], and many others. Recently, it was shown [14] that a finitely generated virtually abelian group $G$ admits a self-replicating action if and only if $G$ is crystallographic. In this paper we address a natural follow-up question: which degrees can occur for the self-replicating actions of a given crystallographic group?

For our purposes, we do not need the precise definition of a self-similar action, but rather its connection with virtual endomorphisms. A *virtual endomorphism* of a group $G$ is a homomorphism $\phi : H \to G$, where $H \leq G$ is a subgroup of finite index. A group $G$ admits a self-similar action that is transitive on the alphabet if and only if it admits a virtual endomorphism with trivial core, that is, with no nontrivial $\phi$-invariant normal subgroup in $G$ [15, Proposition 2.7.5]. The *degree* of the action, defined as the size of its alphabet, is equal to the index $[G : H]$. If the virtual endomorphism is surjective, the action is called *self-replicating* (or recurrent). Accordingly, an integer $d \geq 2$ is a *self-replicating degree* of a group $G$ if and only if there exist a subgroup $H \leq G$ of index $d$ and a surjective homomorphism $\phi : H \to G$ with trivial core.

The present paper continues the investigation begun in [16], where we described all virtual endomorphisms of the plane group $pg$ — the fundamental group of the Klein bottle — determined which of them have trivial core, and computed the possible degrees of its self-similar and self-replicating actions. Here we develop a method, based on the point group, the translation lattice, and the defining cocycle, that applies to *every* crystallographic group, and we carry it out explicitly for all plane and space groups.

We study virtual endomorphisms of crystallographic groups in Section 1. In particular, we show that every surjective virtual endomorphism

of a crystallographic group is an isomorphism, and establish a criterion for its core to be trivial. Consequently, if $d$ is a self-replicating degree of a group $G$, then $G$ contains a subgroup of index $d$ isomorphic to $G$. We call an integer $d \geq 1$ a *self-covering degree* of $G$ if it contains a subgroup of index $d$ isomorphic to $G$; geometrically, these are precisely the degrees of self-coverings of the flat orbifold $\mathbb{R}^n/G$. Thus, every self-replicating degree is a self-covering degree, but the converse does not hold in general, as the triviality of the core imposes an additional condition.

In Section 2, we develop a computational method for determining the self-covering and self-replicating degrees of a given crystallographic group. The sets of admissible degrees are described as the values attained by computable polynomials subject to polynomial constraints. In Sections 3 and 4, we treat the two- and three-dimensional cases, providing an algorithm for computing the degrees. The complete results for all 17 plane groups and all 230 space groups are collected in the appendix. The naming conventions are taken from the International Tables for Crystallography, Volume A [17], hereafter abbreviated ITA. The source code used for the computations is available at [18].

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## 1. Crystallographic groups and their virtual endomorphisms

We briefly recall the necessary background on crystallographic groups; a detailed exposition can be found in [19].

Let $\mathrm{Aff}(n)$ denote the group of affine transformations of $\mathbb{R}^n$, and let $\mathrm{E}(n) \leq \mathrm{Aff}(n)$ denote the group of Euclidean isometries. The group $\mathrm{Aff}(n)$ admits the decomposition $\mathrm{Aff}(n) = \mathrm{GL}_n(\mathbb{R}) \ltimes \mathbb{R}^n$, and every element can be written in the form $(A, a)$, where $A \in \mathrm{GL}_n(\mathbb{R})$ and $a \in \mathbb{R}^n$. The group operation is given by

$$(A, a)(B, b) = (AB, Ab + a).$$

**Definition 1.** A *crystallographic group* of dimension $n$ is a discrete cocompact subgroup of $\mathrm{E}(n)$. Crystallographic groups of dimension 2 are called *plane groups*, and those of dimension 3 are called *space groups*.

The algebraic structure of crystallographic groups is described by the following classical theorems of Bieberbach.

**Theorem 1** (Bieberbach)**.** *1. Let $G \leq \mathrm{E}(n)$ be a crystallographic group. Then the subgroup of translations $G \cap (E \times \mathbb{R}^n)$ is a free abelian group of rank $n$, and it is a maximal abelian normal subgroup of finite index in $G$.*

*2. Two crystallographic groups of dimension $n$ are isomorphic if and only if they are conjugate in the affine group $\mathrm{Aff}(n)$.*

*3. For every $n \in \mathbb{N}$, there exist only finitely many isomorphism classes of crystallographic groups of dimension $n$.*

For a crystallographic group $G$, its *translation subgroup* is $T(G) = G \cap (E \times \mathbb{R}^n)$, and the corresponding subgroup $L(G) = \{v \in \mathbb{R}^n : (E, v) \in T(G)\} \cong T(G)$ is called the *translation lattice* of $G$. The *point group* $P(G)$ is the image of $G$ under the natural projection onto $\mathrm{GL}_n(\mathbb{R})$. By the Bieberbach theorems, there is a short exact sequence

$$0 \to L \to G \to P \to 0,$$

where $L = L(G) \cong \mathbb{Z}^n$ and $P = P(G)$ is a finite subgroup of $\mathrm{GL}_n(\mathbb{R})$.

Conversely, given a finite subgroup $P \leq \mathrm{GL}_n(\mathbb{R})$ and a $P$-invariant lattice $L \leq \mathbb{R}^n$, the crystallographic groups fitting this sequence are classified, up to affine conjugacy, by the cohomology group $H^1(P, \mathbb{R}^n/L) \cong H^2(P, L)$. Thus, an arbitrary crystallographic group can be represented as a triple $G = (P, L, \alpha)$, where $[\alpha] \in H^1(P, \mathbb{R}^n/L)$, that is, $\alpha : P \to \mathbb{R}^n/L$ satisfies $\alpha(AB) = \alpha(A) + A\alpha(B)$. Two cocycles $\alpha$ and $\alpha'$ represent the same cohomology class if and only if they differ by a 1-coboundary, meaning $\alpha'(A) = \alpha(A) + Am - m$ for some $m \in \mathbb{R}^n/L$. Choosing representatives of $\alpha(A)$ in $\mathbb{R}^n$ for $A \in P$, we may write:

$$G = \{(A, \alpha(A) + t) \mid A \in P,\, t \in L\}.$$

If the cohomology class of $\alpha$ is trivial, i.e. $\alpha(A) = Am - m$ for some $m \in \mathbb{R}^n/L$ for every $A \in P$, the group $G$ is isomorphic to the semidirect product $P \ltimes L$ and is called *symmorphic*. More details on group cohomology and its applications to crystallographic groups can be found in [19, 20].

The following properties of crystallographic groups will be used below.

**Lemma 1** (cf. [21, Theorem 2])**.** *Every normal subgroup of a crystallographic group is either trivial or infinite.*

**Lemma 2.** *Every finite-index subgroup of a crystallographic group is crystallographic.*

*Proof.* Immediate from the definition: discreteness and cocompactness pass to finite-index subgroups. □

**Lemma 3.** *Let $G$ be a crystallographic group and $H \leq G$ be a subgroup isomorphic to $G$. Then $T(H) = T(G) \cap H$ and $[G : H] = [T(G) : T(H)]$.*

*Proof.* The equality $T(H) = H \cap T(G)$ follows directly from the definition of the translation subgroup. Since $G$ and $H$ are isomorphic, the Bieberbach theorem implies that $P(G) \cong P(H)$. On the other hand, $P(H) \leq P(G)$ and hence $P(H) = P(G)$. Then $[H : T(H)] = |P(H)| = |P(G)| = [G : T(G)]$. The index of $T(H)$ in $G$ can be expressed in two ways as

$$[G : T(H)] = [G : H][H : T(H)] = [G : T(G)][T(G) : T(H)].$$

The equality $[G : H] = [T(G) : T(H)]$ follows. □

**Lemma 4.** *Let $G$ be a crystallographic group, $H \leq G$ a subgroup of finite index, and $\phi : H \to G$ a surjective homomorphism. Then $\phi$ is an isomorphism.*

*Proof.* Let $h(\cdot)$ denote the Hirsch length of a group, and let $K$ be the kernel of $\phi$. Since $\phi$ is surjective, $h(H) = h(G) + h(K)$. As $H \leq G$ has finite index, $h(H) = h(G)$. Hence, $h(K) = 0$, and therefore $K$ is finite. Since $K$ is a normal subgroup of $H$ and $H$ is crystallographic by Lemma 2, Lemma 1 implies $K$ is trivial. Hence $\phi$ is injective, and therefore an isomorphism. □

By the second Bieberbach theorem and Lemma 4, every surjective virtual endomorphism $\phi : H \to G$ of a crystallographic group $G$ is induced by conjugation with an affine element $(A, t) \in \mathrm{Aff}(n)$:

$$\phi(g) = (A, t)^{-1} g (A, t) \quad \text{for} \quad g \in H = (A, t) G (A, t)^{-1}.$$

The action of $\phi$ on the translation subgroup $T(H)$ is determined by the linear part $A$:

$$\phi(E, v) = (A, t)^{-1}(E, v)(A, t) = (E, A^{-1}v) \quad \text{for} \quad (E, v) \in H.$$

It follows that $L(H) = AL(G) \leq L(G)$, and by Lemma 3,

$$[G : H] = [T(G) : T(H)] = [L(G) : L(H)] = [L(G) : AL(G)] = |\det(A)|.$$

Therefore, the set of self-covering degrees coincides with the set of absolute values of determinants of matrices occurring as linear parts of surjective virtual endomorphisms. To determine the self-replicating degrees, it remains to analyze the simplicity condition.

**Theorem 2.** *Let $G \leq \mathrm{E}(n)$ be a crystallographic group, and let $a = (A, t) \in \mathrm{Aff}(n)$ be such that $aGa^{-1} \leq G$. Consider the virtual endomorphism $\phi : H = aGa^{-1} \to G$ defined by $\phi(g) = a^{-1}ga$. Then $\phi$ is simple if and only if no eigenvalue of $A^{-1}$ is an algebraic integer (equivalently, the characteristic polynomial of $A^{-1}$ is not divisible by a nonconstant monic polynomial with integral coefficients).*

*Proof.* We may assume that the translation lattice of $G$ is $\mathbb{Z}^n$. Since $aGa^{-1} \leq G$, we have $A\mathbb{Z}^n \leq \mathbb{Z}^n$, and hence $A$ has integer entries. Consider the virtual endomorphism $\psi : A\mathbb{Z}^n \to \mathbb{Z}^n$, $\psi(v) = A^{-1}v$, of the group $\mathbb{Z}^n$, which is the restriction of $\phi$ to the translation lattice. By Proposition 2.9.1 of [15], the maximal $\psi$-invariant subgroup of $\mathbb{Z}^n$ is given by

$$K(\psi) = \bigcap_{m=1}^{\infty} A^m\mathbb{Z}^n.$$

By Proposition 2.9.2 of [15], $K(\psi) = \{0\}$ if and only if $A^{-1}$ has no eigenvalues that are algebraic integers. It remains to show that $\phi$ is simple if and only if $K(\psi) = \{0\}$.

Assume that $K(\psi) \neq \{0\}$. Since $aGa^{-1} \leq G$, the linear part $A$ normalizes the point group $P$ of $G$, that is, $AP = PA$. Hence each subgroup $A^m\mathbb{Z}^n$ is $P$-invariant, and therefore so is $K(\psi)$. Since $P$-invariant subgroups of the translation lattice give rise to normal subgroups of $G$, the subgroup $E \times K(\psi)$ is a nontrivial normal subgroup of $G$. Moreover, $E \times K(\psi)$ is $\phi$-invariant by construction. Therefore, $\phi$ is not simple.

Conversely, let $K$ be a nontrivial normal $\phi$-invariant subgroup of $G$. By Lemma 1, $K$ is infinite and therefore contains a nontrivial translation. Let $m = \mathrm{lcm}\{\mathrm{ord}(B) : B \in P\}$. Then $g^m \in T(G)$ for every $g \in G$. Consider the subgroup $K_m = \langle g^m, g \in K\rangle \leq T(G)$. Since $K$ is nontrivial, normal in $G$, and $\phi$-invariant, it follows that $K_m$ is also nontrivial, normal in $G$, and $\phi$-invariant. Identifying $K_m$ with the corresponding subgroup of the translation lattice, we obtain a nontrivial $\psi$-invariant subgroup of

$\mathbb{Z}^n$. Hence $K_m \leq K(\psi)$, and therefore $K(\psi) \neq 0$, which completes the proof. □

**Corollary 1.** *An integer $d \geq 2$ is a self-replicating degree of a crystallographic group $G \leq \mathrm{E}(n)$ if and only if there exists $a = (A, t) \in \mathrm{Aff}(n)$ with $|\det(A)| = d$ such that $aGa^{-1} \leq G$ and no eigenvalue of $A^{-1}$ is an algebraic integer.*

We now obtain an upper bound for self-replicating degrees of crystallographic groups.

**Corollary 2.** *Let $G$ be a crystallographic group of dimension $n$ with point group $P$. Then $G$ has a self-replicating degree at most $(|P| + 1)^n$.*

*Proof.* We may assume that the translation lattice of $G$ is $\mathbb{Z}^n$. Let $m$ be any positive integer that annihilates the defining 1-cocycle $[\alpha] \in H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$ of $G$, meaning $mv \in \mathbb{Z}^n$ for all $(B, v) \in G$. Note that $m = |P|$ always satisfies this property by standard group cohomology (see [20, Ch. III, Cor. 10.2]).

Define the scalar matrix $A = (m+1)E$ and the affine transformation $a = (A, 0)$. Conjugating an arbitrary element $(B, v) \in G$ by $a$ gives:

$$a(B, v)a^{-1} = (B, Av) = (B, (m + 1)v) = (E, mv)(B, v).$$

Since $mv \in \mathbb{Z}^n$, the term $(E, mv)$ is a lattice translation, implying $aGa^{-1} \leq G$. The unique eigenvalue of $A^{-1}$ is $\frac{1}{m+1}$, which is not an algebraic integer, making $\det(A) = (m + 1)^n$ a valid self-replicating degree. □

**Corollary 3.**
1. *Every symmorphic crystallographic group of dimension $n$ possesses a self-replicating degree at most $2^n$.*
2. *Every plane group possesses a self-replicating degree at most 9.*
3. *Every space group possesses a self-replicating degree at most 343.*

*Proof.* For a symmorphic crystallographic group, the defining cocycle is trivial. Hence the proof of Corollary 2 applies with $m = 1$, yielding a self-replicating degree at most $2^n$.

For plane groups, the defining cocycle is annihilated by $m = 2$, yielding a degree at most $(2 + 1)^2 = 9$. For space groups, the cocycle is annihilated by a universal scalar $m = \mathrm{lcm}(2, 3, 4, 6)$, yielding a degree at most $(12 + 1)^3 = 2197$. We can improve the bound by observing that

no group contains cocycle denominators divisible by both 4 and 3. As a result, every space group admits annihilation factor $m \leq 6$, which gives a degree at most $(6+1)^3 = 343$. □

## 2. Computing self-replicating degrees of crystallographic groups

In the previous section we characterized the self-covering and self-replicating degrees of crystallographic groups. We now develop a computational method to determine these values for a given group. Hereafter we use $\mathbb{N}$ to denote the set of positive integers excluding 0.

Let $G$ be a crystallographic group given by the tuple $(P, \mathbb{Z}^n, \alpha)$. An integer $d \geq 1$ is a self-covering degree of $G$ if and only if there exists an affine transformation $a = (A, t) \in \mathrm{Aff}(n)$ such that $d = |\det A|$ and $aGa^{-1} \leq G$. This condition splits into three parts:

$(PC)$ Point group compatibility: $APA^{-1} = P$.

$(LC)$ Lattice compatibility: $A\mathbb{Z}^n \leq \mathbb{Z}^n$, which means $A$ must have integer entries.

$(CC)$ Cocycle compatibility: for every $B \in P$,

$$\alpha(ABA^{-1}) \equiv (E - ABA^{-1})t + A\alpha(B) \mod \mathbb{Z}^n.$$

To determine the possible values of $|\det A|$, we first describe the integer matrices $A$ satisfying $(PC)$ and then determine which of them admit a translation $t$ satisfying $(CC)$. Note that for symmorphic groups the condition $(CC)$ is trivial.

The integer matrices $A$ satisfying $(PC)$ can be described as follows. Let $\sigma \in \mathrm{Aut}(P)$. Consider the system of linear equations over $\mathbb{Z}$:

$$XB = \sigma(B)X \quad \text{for all } B \in P,$$

where $X \in M_n(\mathbb{Z})$ is the unknown matrix. The solution set $\mathcal{X}_\sigma$ is a finitely generated $\mathbb{Z}$-module. Hence, one can compute integral matrices $X_1, \ldots, X_m \in \mathcal{X}_\sigma$ such that every $X \in \mathcal{X}_\sigma$ can be written as

$$X = \sum_{i=1}^{m} x_i X_i, \quad x_i \in \mathbb{Z}. \tag{1}$$

The set $\mathcal{X}$ of all matrices $A \in M_n(\mathbb{Z})$ satisfying $(PC)$ is the union of $\mathcal{X}_\sigma$ over all $\sigma \in \mathrm{Aut}(P)$.

Next, we determine which matrices $X \in \mathcal{X}$ admit a translation $t$ satisfying $(CC)$. Let $\sigma \in \mathrm{Aut}(P)$ and write $X \in \mathcal{X}_\sigma$ as the linear combination (1). Then $(CC)$ is equivalent to the following system of congruences in the unknowns $x_1, \dots, x_m \in \mathbb{Z}$ and $t \in \mathbb{Q}^n$:

$$\sum_{i=1}^{m} x_i X_i \alpha(B) - \alpha(\sigma(B)) \equiv (\sigma(B) - E)t \pmod{\mathbb{Z}^n}, \quad B \in P. \tag{2}$$

For each $B \in P$, denote the left-hand side of (2) by $b_B(x_1, \dots, x_m) \in \mathbb{Q}^n$, and let $M_B = \sigma(B) - E \in M_n(\mathbb{Z})$. Collecting these congruences for all $B \in P$ yields the system

$$Mt \equiv b \pmod{\mathbb{Z}^N}, \tag{3}$$

where the matrix $M = (M_B)_{B \in P}$ and the vector $b = (b_B)_{B \in P}$ are obtained by stacking the matrices $M_B$ and the vectors $b_B$, respectively, over all $B \in P$, and $N = n|P|$.

**Proposition 1.** *The congruence system (3) is solvable for $t \in \mathbb{Q}^n$ if and only if $v^\top b \in \mathbb{Z}$ for every vector $v \in \mathbb{Z}^N$ satisfying $v^\top M = 0$.*

*Proof.* Suppose first that (3) is solvable. Then $Mt = b + z$ for some $t \in \mathbb{Q}^n$ and $z \in \mathbb{Z}^N$. Hence, for every $v \in \mathbb{Z}^N$ satisfying $v^\top M = 0$, we have

$$0 = v^\top M t = v^\top b + v^\top z,$$

which implies $v^\top b = -v^\top z \in \mathbb{Z}$.

Conversely, consider the Smith normal form of $M$:

$$UMV = D = \mathrm{diag}(d_1, \dots, d_r, 0, \dots, 0), \quad d_i > 0,$$

where $U \in \mathrm{GL}_N(\mathbb{Z})$ and $V \in \mathrm{GL}_n(\mathbb{Z})$. The condition $Mt - b \in \mathbb{Z}^N$ is equivalent to $Dt' - b' \in \mathbb{Z}^N$, where $t' = V^{-1}t$ and $b' = Ub$. For $1 \le i \le r$, the congruence $d_i t'_i \equiv b'_i \pmod{\mathbb{Z}}$ always has a rational solution $t'_i = b'_i/d_i$. Thus, the system is solvable if and only if $b'_i \in \mathbb{Z}$ for every $i > r$.

Let $u_i$ denote the $i$-th row of $U$. For $i > r$, the corresponding $i$-th row of $D$ is identically zero, implying $u_i M = 0$. By assumption, this gives $b'_i = u_i b \in \mathbb{Z}$ for every $i > r$. Therefore, the transformed system is solvable, and equivalently, so is the original system. □

The preceding proof reduces the solvability of the system (3) to a finite check using the Smith normal form $UMV = D$ of $M$.

**Corollary 4.** *Let $u_i(M)$ denote the $i$-th row of $U$. The system $Mt \equiv b \pmod{\mathbb{Z}^N}$ has a rational solution if and only if $u_i(M)b \in \mathbb{Z}$ for all $i > \operatorname{rank}(M)$.*

This gives us a constructive way to eliminate the rational vector $t$ from the system (2), reducing it to a finite system of linear congruences in the integer variables $x_i$. Let $b(x_1, \ldots, x_m)$ be the stacked column vector

$$b_B(x_1, \ldots, x_m) = \sum_{i=1}^{m} x_i X_i \alpha(B) - \alpha(\sigma(B)).$$

By the corollary, (2) is solvable for $t$ if and only if

$$u_j(M)b(x_1, \ldots, x_m) \equiv 0 \pmod{\mathbb{Z}} \quad \text{for all } j > \operatorname{rank}(M). \tag{4}$$

Solving this system and substituting the general integer solution back into $X = \sum_{i=1}^{m} x_i X_i$ yields a finite, computable set of integral basis matrices $Y_0, Y_1, \ldots, Y_k$. The subset $\mathcal{Y}_\sigma \subseteq \mathcal{X}_\sigma$ consisting of all matrices satisfying conditions $(PC)$–$(CC)$ is then parameterized by

$$Y = Y_0 + \sum_{i=1}^{k} y_i Y_i, \quad y_i \in \mathbb{Z}. \tag{5}$$

The determinant of $Y$ can be expressed as a polynomial with integral coefficients $f_\sigma(y_1, \ldots, y_k)$. Ranging over all $\sigma \in \operatorname{Aut}(P)$, this gives a finite collection of computable polynomials associated to the group $G$. Finally, let $\mathcal{Y} = \bigcup_{\sigma \in \operatorname{Aut}(P)} \mathcal{Y}_\sigma$ denote the union of these solution spaces.

We obtain the following description for the sets of self-covering and self-replicating degrees:

$$\begin{aligned} SCD(G) &= \{|\det A| : A \in \mathcal{Y} \text{ and } \det A \neq 0\} = \\ &= \{|f_\sigma(y_1, \ldots, y_k)| : y_i \in \mathbb{Z}, \sigma \in Aut(P), f_\sigma(y_1, \ldots, y_k) \neq 0\}, \\ SRD(G) &= \{|\det A| : A \in \mathcal{Y}, \det A \neq 0, \text{and no eigenvalue of } A^{-1} \text{ is an} \\ &\qquad \text{algebraic integer}\}. \end{aligned}$$

The set of integer values of a multivariate integer polynomial generally admits no simple or computable arithmetic description. Determining

whether a given integer $d$ belongs to $SCD(G)$ amounts to deciding the solvability of the Diophantine equation $|f_\sigma(y_1, \ldots, y_k)| = d$ for some $\sigma \in Aut(P)$. By Matiyasevich's theorem on Hilbert's Tenth Problem, such questions are undecidable for arbitrary polynomials. It remains open whether this problem is decidable in our specific geometric setting:

**Problem 1.** Let $G$ be a crystallographic group.

(1) Given an integer $d \geq 1$, is it decidable whether there exists a subgroup $H < G$ of index $d$ such that $H \cong G$? Equivalently, does the orbifold $\mathbb{R}^n/G$ admit a self-covering of degree $d$?

(2) Given an integer $d \geq 1$, is it decidable whether $G$ admits a self-replicating action over an alphabet of size $d$?

Despite the potential undecidability of this problem in arbitrary dimensions, the algebraic complexity of the polynomials $f_\sigma$ remains low in dimensions 2 and 3. In the final sections, we restrict our attention to the two- and three-dimensional cases, where explicit computation of these parameterizations completely resolves the problem.

## 3. Plane groups

There are 17 plane groups (also known as wallpaper groups). We computed the set of matrices $\mathcal{Y}$ satisfying conditions $(PC)$–$(CC)$ for each group. For the groups $p1$ and $p2$, we have $\mathcal{Y} = M_2(\mathbb{Z})$, and thus every positive integer occurs as a self-covering degree. For all the other plane groups, the polynomials $f_\sigma$ depend on at most 2 variables and the equation $|f_\sigma| = d$ can be solved explicitly. Table 1 presents the computed matrices $\mathcal{Y}$, the polynomials $f_\sigma$ together with explicit excluded values that describe $SRD(G)$ for every plane group, and finally the minimal possible values of $SRD(G)$.

To describe the set of self-replicating degrees, we reduce the eigenvalue condition to a simpler arithmetic criterion.

**Proposition 2.** *Let $A \in M_2(\mathbb{Z})$ and $\det(A) \neq 0$. No eigenvalue of $A^{-1}$ is an algebraic integer if and only if $\det(A) \neq \pm 1$ and $\det(A) \pm \mathrm{tr}(A) \neq -1$.*

*Proof.* The characteristic polynomials of $A$ and $A^{-1}$ are

$$\chi_A(x) = x^2 - \mathrm{tr}(A)x + \det(A) \in \mathbb{Z}[x],$$
$$\chi_{A^{-1}}(x) = x^2 - \frac{\mathrm{tr}(A)}{\det(A)}x + \frac{1}{\det(A)} \in \mathbb{Q}[x].$$

If $\det(A) = \pm 1$, then $\chi_{A^{-1}}(x) \in \mathbb{Z}[x]$ and its roots are algebraic integers. If $\det(A) \pm \operatorname{tr}(A) = -1$, then $A^{-1}$ has an eigenvalue 1 or $-1$.

Conversely, assume $\chi_{A^{-1}}(x)$ is divisible by a monic polynomial $p(x) \in \mathbb{Z}[x]$. If $\deg p(x) = 2$, then $p(x) = \chi_{A^{-1}}(x)$ and $\det(A) = \pm 1$. If $\deg p(x) = 1$ and $p(x) = x - a$, then $a$ is an integer eigenvalue of $A^{-1}$. Now $a^{-1}$ is a root of a monic integer polynomial $\chi_A(x)$. Since $a$ and $a^{-1}$ are both algebraic integer, we have $a = \pm 1$ and

$$\chi_A(\pm 1) = 1 \mp \operatorname{tr}(A) + \det(A) = 0 \quad \Rightarrow \quad \det(A) \mp \operatorname{tr}(A) = -1.$$

□

We define the affine linear form $g_\sigma(y_1, \ldots, y_k)$ as the trace of a matrix $Y \in \mathcal{Y}_\sigma$ written in the form (5). Then $SRD(G)$ admits the following characterization:

$$SRD(G) = \{|f_\sigma(y_1, \ldots, y_k)| \,:\, \sigma \in Aut(P) \text{ and } y_i \in \mathbb{Z} \text{ such that } f_\sigma(y_1, \ldots, y_k) \notin \{0, 1, -1\} \text{ and } (f_\sigma \pm g_\sigma)(y_1, \ldots, y_k) \neq -1\}.$$

For the groups $p1$ and $p2$, every integer $d \geq 2$ occurs as a self-replicating degree. For all other plane groups, the polynomials $f_\sigma$ and $g_\sigma$ depend on at most 2 variables; thus the excluded values $f_\sigma \notin \{0, 1, -1\}$ and $f_\sigma \pm g_\sigma \neq -1$ can be computed explicitly. Table 1 presents the computed polynomials $f_\sigma$, the excluded set of integer solutions that violate these inequalities, and the smallest self-replicating degree for each group.

**Example 1.** The plane group $p2mg$ (ITA No. 7) is generated by

$$G_7 = \left\langle \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 1/2 \\ 0 & 1 & 0 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \end{array}\right) \right\rangle.$$

The matrices $\mathcal{X}$ satisfying condition $(PC)$ have one of two forms:

$$A_1 = \begin{pmatrix} 0 & x_1 \\ x_0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} x_0 & 0 \\ 0 & x_1 \end{pmatrix}, \quad x_0, x_1 \in \mathbb{Z}.$$

Solving the system of congruences arising from $(CC)$, we find that there are no solutions for matrices of the form $A_1$. For matrices of the form $A_2$, we obtain $x_0 = 2y_0 + 1$ and $x_1 = y_1$ for $y_0, y_1 \in \mathbb{Z}$. Therefore, the set of matrices satisfying both $(PC)$ and $(CC)$ is given by:

$$\mathcal{Y} = \left\{ \begin{pmatrix} 2y_0 + 1 & 0 \\ 0 & y_1 \end{pmatrix} \,:\, y_0, y_1 \in \mathbb{Z} \right\},$$

and the set of self-covering degrees is

$$SCD(G_7) = \{|(2y_0+1)y_1| : y_0, y_1 \in \mathbb{Z} \text{ and } (2y_0+1)y_1 \neq 0\} = \mathbb{N}.$$

By Proposition 2, the condition that no eigenvalue of $A_2^{-1}$ which is an algebraic integer is equivalent to the system

$$\begin{aligned} (2y_0+1)y_1 &\neq 0, \pm 1, \\ (2y_0+1)y_1 \pm (2y_0+1+y_1) &\neq -1. \end{aligned}$$

The solution set is given by:

$$y_0 \notin \{-1, 0\} \quad \text{and} \quad y_1 \notin \{-1, 0, 1\}.$$

Consequently, the set of self-replicating degrees is given by:

$$SRD(G_7) = \{(2y_0+1)(y_1+1) \,|\, y_0, y_1 \in \mathbb{N}\} = \{6, 9, 10, 12, 14, 15, 18, \dots\},$$

which consists of all composite positive integers that are not powers of 2. In particular, the smallest self-replicating degree of $G_7$ is equal to 6.

**Example 2.** The plane group $p3$ (ITA No. 13) is generated by

$$G_{13} = \left\langle \left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & -1 & 0 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \end{array}\right) \right\rangle.$$

The matrices $\mathcal{X}$ satisfying $(PC)$ have one of the following two forms:

$$A_1 = \begin{pmatrix} -x_0 & x_0+x_1 \\ x_1 & x_0 \end{pmatrix}, \; A_2 = \begin{pmatrix} x_0+x_1 & -x_0 \\ x_0 & x_1 \end{pmatrix}, \quad x_0, x_1 \in \mathbb{Z}.$$

The group $G_{13}$ is symmorphic, i.e. $G_{13} = P \ltimes \mathbb{Z}^2$, and the condition $(CC)$ is vacuous. Observe that $|\det(A_1)| = |\det(A_2)| = |x_0^2 + x_0x_1 + x_1^2|$. Therefore, the set of self-covering degrees is given by:

$$\begin{aligned} SCD(G_{13}) &= \{|x_0^2 + x_0x_1 + x_1^2| : x_0, x_1 \in \mathbb{Z} \text{ and } x_0^2 + x_0x_1 + x_1^2 \neq 0\} = \\ &= \{1, 3, 4, 7, 9, 12, 13, 16, 19, 21, 25 \dots\}. \end{aligned}$$

These are precisely the positive Löschian numbers (OEIS A003136): the integers $d$ such that, in the prime factorization of $d$, every prime factor $p \equiv 2 \pmod 3$ has an even exponent.

By Proposition 2, the condition that no eigen value of $A_1^{-1}$ is an algebraic integer is equivalent to the system

$$\begin{aligned} x_0^2 + x_0x_1 + x_1^2 &\neq 0, \pm 1, \\ -(x_0^2 + x_0x_1 + x_1^2) &\neq -1. \end{aligned}$$

The excluded set of solutions is:

$$(x_0, x_1) \notin \{(0,0), (0,1), (-1,1), (1,-1), (-1,0), (1,0), (0,-1)\}.$$

The analogous conditions for $A_2$ give the system

$$\begin{aligned} x_0^2 + x_0x_1 + x_1^2 &\neq 0, \pm 1, \\ x_0^2 + x_0x_1 + x_1^2 \pm (x_0 + 2x_1) &\neq -1, \end{aligned}$$

having the same solution set. The values of $|x_0^2 + x_0x_1 + x_1^2|$ evaluated at all integer pairs $(x_0, x_1) \in \mathbb{Z}^2$ outside of the 7 excluded pairs are all Löschian numbers greater than 1. Consequently, the set of self-replicating degrees is given by:

$$SRD(G_{13}) = \{|x_0^2 + x_0x_1 + x_1^2| : x_0, x_1 \in \mathbb{Z} \text{ and } |x_0^2 + x_0x_1 + x_1^2| \neq 0, 1\}.$$

In particular, the smallest self-replicating degree of $G_{13}$ is equal to 3.

## 4. Space groups

Space groups can be classified in two main ways: algebraically into 219 abstract isomorphism classes, or geometrically into 230 classes, defined by orientation-preserving affine conjugation. Note that we use the ITA naming convention [17], which is based on the geometric classification.

We computed the set of matrices $\mathcal{Y}$ satisfying conditions $(PC)$–$(CC)$ together with the corresponding multivariable polynomials $f_\sigma$ for each group. Although every polynomial $f_\sigma$ is cubic and cannot be solved explicitly in general, we show how to reduce the problem to the two-dimensional case and apply Proposition 2.

Consider an arbitrary integral $3 \times 3$ matrix

$$A = \begin{pmatrix} x_0 & x_1 & x_2 \\ x_3 & x_4 & x_5 \\ x_6 & x_7 & x_8 \end{pmatrix}.$$

Its characteristic polynomial is

$$\chi_A(x) = x^3 - \operatorname{tr}(A)x^2 + \tau(A)x - \det(A), \quad \text{where}$$
$$\tau(A) = x_0x_4 - x_1x_3 + x_0x_8 - x_2x_6 + x_4x_8 - x_5x_7$$

is a sum of determinants of the three principal $2 \times 2$ minors of $A$. Consequently,

$$\chi_{A^{-1}}(x) = x^3 - \frac{\tau(A)}{\det(A)}x^2 + \frac{\operatorname{tr}(A)}{\det(A)}x - \frac{1}{\det(A)}.$$

Let $G$ be a space group with translation lattice $\mathbb{Z}^3$ and point group $P < \mathrm{GL}_3(\mathbb{Z})$. Let $Y(y_1, \ldots, y_r) \in \mathcal{Y}_\sigma$ be a family of matrices satisfying conditions $(PC)$–$(CC)$, written in the form (5) for a fixed automorphism $\sigma \in Aut(P)$. Our computations show that, for every space group $G$ and every $\sigma \in \mathrm{Aut}(P)$, one of the following holds:

(1) $\operatorname{tr}(Y) = \tau(Y) = 0$;

(2) $Y$ is block triangular.

The only exceptions are, similarly to the two-dimensional case, the groups $P1$ and $P-1$ (Nos. 1 and 2 in ITA) that have point groups consisting of scalar matrices. Likewise plane groups $p1$ and $p2$, these space groups admit every positive integer $\geq 1$ as a self-covering degree and every positive integer $\geq 2$ as a self-replicating degree. The complete list of the families $Y \in \mathcal{Y}_\sigma$ is omitted due to their large variety.[1]

Consider the first case. Since $\tau(Y) = \operatorname{tr}(Y) = 0$, the characteristic polynomial of $Y^{-1}$ reduces to

$$\chi_{Y^{-1}}(x) = x^3 - \frac{1}{\det(Y)}.$$

Hence, if $|\det(Y)| > 1$, then $\chi_{Y^{-1}}(x)$ is not divisible by any nonconstant monic polynomial with integral coefficients. It follows that every value of $f_\sigma = \det(Y)$ with $|f_\sigma| > 1$ is a self-replicating degree. The complete list of $f_\sigma$ falling into this case are provided in Table 9 in the appendix.

Consider the second case. Without loss of generality, assume that $Y$ has the following form:

$$Y = \begin{pmatrix} C & c \\ 0 & p \end{pmatrix}, \quad Y^{-1} = \begin{pmatrix} C^{-1} & d \\ 0 & \frac{1}{p} \end{pmatrix},$$

[1]The source code used to generate the complete list of $\mathcal{Y}_\sigma$ is provided in [18].

where $C \in M_2(\mathbb{Z})$. Then $f_\sigma = \det(Y) = p_\sigma\, q_\sigma$, where $p_\sigma(y_1, \dots, y_k)$ is an affine linear form and $q_\sigma(y_1, \dots, y_k) = \det(C)$ is a quadratic polynomial. Moreover,

$$\chi_{Y^{-1}}(x) = \chi_{C^{-1}}(x)\left(x - \frac{1}{p}\right) = \left(x^2 - \frac{\operatorname{tr}(C)}{\det(C)}x + \frac{1}{\det(C)}\right)\left(x - \frac{1}{p}\right).$$

We now apply Proposition 2. Put $g_\sigma(y_1, \dots, y_k) = \operatorname{tr}(C)$. Then the subset of $SRD(G)$ corresponding to the fixed automorphism $\sigma$ is

$$\begin{aligned}\big\{\, |(p_\sigma q_\sigma)(y_1, \dots y_k)| \;&: y_i \in \mathbb{Z} \text{ such that} \\ &p_\sigma(y_1, \dots y_k), q_\sigma(y_1, \dots y_k) \notin \{0, 1, -1\} \\ &\text{and} \quad (q_\sigma \pm g_\sigma)(y_1, \dots y_k) \neq -1 \,\big\}.\end{aligned} \tag{6}$$

Therefore, the contribution of $\sigma$ to $SRD(G)$ is completely determined by the triple $(p_\sigma, q_\sigma, g_\sigma)$, whereas the product $f_\sigma = p_\sigma q_\sigma$ determines the corresponding self-covering degrees. The complete list of triples $(p_\sigma, q_\sigma, g_\sigma)$ for all space groups is given in Tables 2–8 in the appendix.

In summary, to determine the self-covering and self-replicating degrees of a given crystallographic group $G$, locate the corresponding group number in Tables 2–9. Since a group may appear in several rows, corresponding to different automorphisms $\sigma \in \operatorname{Aut}(P)$, each row contributes a subset of both $SCD(G)$ and $SRD(G)$. For each row of Table 9, the polynomial $f_\sigma$ determines the corresponding contributions to both $SCD(G)$ and $SRD(G)$. For each row of Tables 2–8, the product $f_\sigma = p_\sigma q_\sigma$ determines the contribution to $SCD(G)$, whereas the corresponding triple $(p_\sigma, q_\sigma, g_\sigma)$ determines the contribution to $SRD(G)$ via (6). The resulting $SCD(G)$ and $SRD(G)$ are obtained by taking the union of the contributions over all rows corresponding to $G$.

Finally, the Diophantine equations arising in the conditions of (6) admit explicit solutions. In most cases, they reduce to quadratic Diophantine equations in two variables, which already appear in Table 1 together with their solution sets. However, there are four exceptional kinds of matrices that require a separate analysis. The first two are

$$X_1 = \begin{pmatrix} z_0 & 0 & z_1 \\ 0 & z_2 & 0 \\ z_3 & 0 & z_4 \end{pmatrix}, \quad X_2 = \begin{pmatrix} z_0 & 0 & 2\,z_1 \\ z_2 & z_0 + 2\,z_2 & -z_1 \\ z_3 & 0 & z_4 \end{pmatrix}.$$

The matrix $X_1$ occurs in the symmorphic groups Nos. 3, 6, and 10, and in modified form in Nos. 4, 7, 11, 13, and 14, after substituting the

solutions of the cocycle compatibility condition. Likewise, $X_2$ occurs in the symmorphic groups Nos. 5, 8, and 12, while the modified versions occur in Nos. 9 and 15.

The remaining two matrices contain minors that do not appear in the plane case:

$$X_3 = \begin{pmatrix} z_0 & 0 & 0 \\ z_0 + 2\,z_1 & z_0 + 2\,z_1 & 2\,z_0 + 4\,z_1 \\ -z_0 - z_1 & z_2 & -z_0 - 2\,z_1 \end{pmatrix},$$

$$X_4 = \begin{pmatrix} z_0 & 0 & 0 \\ z_1 & 0 & z_0 + 2\,z_1 \\ z_2 & z_0 + 2\,z_2 & 0 \end{pmatrix}.$$

The matrix $X_3$ has $q_\sigma = -(z_0 + 2\,z_1)^2 - 2\,(z_0 + 2\,z_1)z_2$. It occurs in the symmorphic groups Nos. 22 and 69, and, with some variations, in the group No. 70. The matrix $X_4$ has $q_\sigma = -(z_0 + 2\,z_1)(z_0 + 2\,z_2)$. It occurs in the symmorphic groups Nos. 23 and 71, and, with some variations, in the groups Nos. 24, 72, 73, and 74. In both cases, $q_\sigma$ is a quadratic polynomial in three variables.

**Example 3.** The space group $P\,1\,2_1/m\,1$ (ITA No. 11) is generated by:

$$G_{11} = \left\langle \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 0 \end{array}\right), \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{array}\right), e_1, e_2, e_3 \right\rangle.$$

From Table 2 we obtain a single triple $p_\sigma, q_\sigma$ and $g_\sigma$ that describes $SRD$ via the equation (6):

$$p_\sigma(y_0 \dots y_4) = 2y_2 + 1, \quad q_\sigma(y_0 \dots y_4) = -y_1y_3 + y_0y_4,$$

$$g_\sigma(y_0 \dots y_4) = y_0 + y_4.$$

It is clear that the pair $(q_\sigma, g_\sigma)$ falls into the special case for the plane groups Nos. 1 and 2, and every integer $d \geq 2$ occurs in the set

$$\{|q_\sigma(y_0 \dots y_4)| \,:\, q_\sigma(y_0 \dots y_4) \notin \{0, 1, -1\}, (q_\sigma \pm g_\sigma)(y_0 \dots y_4) \neq -1\}.$$

Combining with the condition $p_\sigma(y_0 \dots y_4) \notin \{0, 1, -1\}$ we get the following description of $SRD$:

$$SRD = \{(2k + 1)(m + 1) \,:\, k, m \in \mathbb{N}\} = \{6, 9, 10, 12, 14, 15, 18, \dots\},$$

which is, similarly to the plane group $p2mg$ from the previous section, the set of all composite positive integers that are not powers of 2. In particular, the minimal self-replicating degree is 6.

**Example 4.** The space group $I\,2_1\,2_1\,2_1$ (ITA No. 24) is generated by:

$$G_{24} = \left\langle \left(\begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & -\frac{1}{2} \\ 1 & 0 & 1 & 0 \end{array}\right), \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & -1 & \frac{1}{2} \end{array}\right), e_1, e_2, e_3 \right\rangle.$$

For the sake of succinctness, we consider only two families of matrices from $\mathcal{Y}$ for $G_{24}$. The first family falls into the case $\operatorname{tr}(Y) = \tau(Y) = 0$; its determinant is the cubic polynomial No. 7 in Table 9:

$$\begin{aligned} f_\sigma(y_0, y_1, y_2) = {} & 4\,(2\,y_0 - 1)y_2^2 + 4\,y_0^2 + 2\,(2\,y_0 - 1)y_1 \\ & + 4\,\big(2\,y_0^2 + (2\,y_0 - 1)y_1 + y_0 - 1\big)y_2 - 1. \end{aligned}$$

It factorizes as

$$f_\sigma(y_0, y_1, y_2) = (2y_0 - 1)(2y_2 + 1)(2y_0 + 2y_1 + 2y_2 + 1),$$

so all its values are odd. Conversely, every odd integer $n$ is attained: taking $y_0 = \frac{n+1}{2}$, $y_1 = -\frac{n+1}{2}$, $y_2 = 0$ gives $f_\sigma = n \cdot 1 \cdot 1 = n$. Since $\operatorname{tr}(Y) = \tau(Y) = 0$, every value with $|f_\sigma| > 1$ is a self-replicating degree, and hence

$$SCD_1 = \{1, 3, 5, \dots\}, \qquad SRD_1 = \{3, 5, 7, \dots\}.$$

The second family is block-triangular, with the triple $(p_\sigma, q_\sigma, g_\sigma)$ from Table 2:

$$\begin{aligned} p_\sigma(y_0, y_1, y_2) &= -2y_1 - 1, \\ q_\sigma(y_0, y_1, y_2) = 4y_0^2 - 2(2y_0 + 1)y_1 - 2(2y_0 + 1)y_2 - 1, &\qquad g_\sigma = 0. \end{aligned}$$

The polynomial $q_\sigma$ factorizes as

$$q_\sigma = (2y_0 + 1)(2y_0 - 2y_1 - 2y_2 - 1),$$

so both $p_\sigma$ and $q_\sigma$ take only odd values. Since $g_\sigma = 0$, the eigenvalue condition (6) reduces to $p_\sigma, q_\sigma \notin \{0, 1, -1\}$, that is, $|p_\sigma|, |q_\sigma| \geq 3$.

For the self-covering degrees no such restriction exists: taking $y_0 = 0$, $y_1 = -\frac{n+1}{2}$, $y_2 = \frac{n-1}{2}$ gives $q_\sigma = 1$ and $p_\sigma q_\sigma = n$, so every odd integer occurs, and

$$SCD_2 = \{1, 3, 5, \dots\}.$$

For the self-replicating degrees, write an odd composite number as $d = ab$ with $a, b \geq 3$ odd, and take $y_0 = 0$, $y_1 = -\frac{a+1}{2}$, $y_2 = \frac{a-b}{2}$; then $p_\sigma = a$ and $q_\sigma = b$, so $d$ is attained. Hence

$$SRD_2 = \{9, 15, 21, 25, 27, \dots\}$$

is the set of odd composite numbers.

Observe that the substitution $y_0 \mapsto -y_1$, $y_1 \mapsto -y_2 - 1$, $y_2 \mapsto y_0$ is a bijection of $\mathbb{Z}^3$ that transforms $f_\sigma$ into $p_\sigma \cdot q_\sigma$; in particular, the two determinant polynomials have the same set of values, and $SCD_1 = SCD_2$. Nevertheless, the two families contribute differently to $SRD$: $SRD_2 \subsetneq SRD_1$, since, for example, $5 \in SRD_1$ but $5 \notin SRD_2$. This shows that the eigenvalue condition has to be verified for each family separately and cannot be read off from the determinant polynomial alone.

Note that these two families do not exhaust the sets $SCD(G_{24})$ and $SRD(G_{24})$. To compute them completely, one must repeat the procedure for every row of Tables 2–8 and 9 corresponding to the group No. 24.

**Example 5.** The space group $I\,-4\,3\,d$ (ITA No. 220) is generated by:

$$G_{220} = \left\langle \left(\begin{array}{ccc|c} -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & -\frac{1}{2} \\ 1 & 0 & 1 & 0 \end{array}\right), \left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 1 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & -1 & \frac{1}{2} \end{array}\right), \right.$$
$$\left. \left(\begin{array}{ccc|c} 1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \end{array}\right), \left(\begin{array}{ccc|c} 1 & 2 & 0 & \frac{1}{2} \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \end{array}\right), e_1, e_2, e_3 \right\rangle.$$

The matrices $\mathcal{X}$ satisfying the condition $PC$ have one of 24 possible forms. Consider one of them:

$$A = \begin{pmatrix} -x_0 & 0 & -2\,x_0 \\ 0 & -x_0 & x_0 \\ 0 & 0 & x_0 \end{pmatrix}.$$

The point group of $G_{220}$ has 24 elements, so both congruence systems (2) and (4) are too big to include. Nevertheless, there are some comments that should be given regarding congruences appearing in the $(CC)$ condition. After conjugating the element $\left(\begin{array}{ccc|c} 1 & 0 & 0 & -\frac{1}{2} \\ -1 & 0 & -1 & \frac{1}{2} \\ -1 & -1 & 0 & 1 \end{array}\right)$ we get the following sub-system of congruences:

$$\begin{pmatrix} 2\,a_0 + 2\,a_1 - \frac{3}{2}\,x_0 \\ \frac{1}{2}\,x_0 \\ -a_0 - a_1 + x_0 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} \mod \mathbb{Z}^3.$$

It is a rare case when we cannot simply fix a trivial translation $a = 0 \in \mathbb{Z}^3$, as it leads to a contradiction: the row $\frac{1}{2}x_0 \equiv -\frac{1}{2}$ forces $x_0$ to be odd integer, while simultaneously $x_0 \equiv -\frac{1}{2}$ forces $x_0$ to be fractional.

The resulting matrix $A'$ that satisfies $(CC)$ condition has the following form:

$$A' = \begin{pmatrix} -2\,y_0 + 3 & 0 & -4\,y_0 + 6 \\ 0 & -2\,y_0 + 3 & 2\,y_0 - 3 \\ 0 & 0 & 2\,y_0 - 3 \end{pmatrix}.$$

$A'$ is a block-triangular matrix and the respective triple of polynomials are (can be found in Table 8):

$$p = 2y_0 - 3, \quad q = 4y_0^2 - 12y_0 + 9, \quad g = -4y_0 + 6.$$

The solution to the condition on eigenvalues $(q \pm g) \neq -1$ is a finite set of roots $y_0 \notin \{1, 2\}$, which combining with $|p| \neq \pm 1$ gives us set of cubes of odd integers:

$$\begin{aligned} SRD &= \left\{(2y_0 - 3)(4y_0^2 - 12y_0 + 9) \,:\, y_0 \notin \{1, 2\}\right\} \\ &= \left\{(2k - 3)^3 \,:\, k \in \mathbb{N}, k \notin \{1, 2\}\right\}. \end{aligned}$$

Again, to compute the full sets $SCD$ and $SRD$, one must repeat this process for every entry of the Tables 2–9 that contains the group No. 220.

## 5. Algorithm specification

In this section we describe the implementation details used to compute the sets $SCD(G)$ and $SRD(G)$ for plane and space groups, following the mathematical scheme of Section 2. The implementation is written in Python on top of SageMath [22] and uses the GAP package Cryst [23] as the source of crystallographic data. The full source code is at the author's GitHub [18].

### Normalization of the group

For a given ITA number $n$ and dimension $\dim \in \{2, 3\}$, the group $G =$ `SpaceGroupOnLeftIT`$(\dim, n)$ is constructed via the GAP Cryst package. Since the translation lattice $L(G)$ is in general not the standard lattice, we conjugate the generators by the translation basis matrix returned by `TranslationBasis`. After this change of basis we may assume $L(G) = \mathbb{Z}^n$, so that the group is represented as a triple $G = (P, \mathbb{Z}^n, \alpha)$.

The point group $P$ is finite, and its elements are enumerated by a breadth-first search over the generating set with inverses, storing for

every element a word in the generators that produces it. The cocycle is stored as a lookup table $\alpha : P \to \mathbb{Q}^n$, and membership of an element $(B, v)$ in $G$ is decided by the two conditions $B \in P$ and $v - \alpha(B) \in \mathbb{Z}^n$.

### Finding the normalizer (*PC*)

The first stage computes all matrices $A \in \mathrm{GL}_n(\mathbb{Q})$ satisfying $APA^{-1} = P$, i.e. the normalizer of the point group in $\mathrm{GL}_n(\mathbb{Q})$, in the form of parametric symbolic matrices.

Let $P = \langle g_1, \ldots, g_k \rangle$. Brute-force enumeration of all maps $P \to P$ is impractical. Every automorphism $\sigma \in \mathrm{Aut}(P)$ is determined by the images of the generators, and the image $\sigma(g_i)$ must have the same order as $g_i$. We therefore group the elements of $P$ by their order, enumerate all tuples of candidate images $(h_1, \ldots, h_k)$ with $\mathrm{ord}(h_i) = \mathrm{ord}(g_i)$ (discarding tuples with repeated elements), and keep a tuple only if the map $g_i \mapsto h_i$ extends to a homomorphism with trivial kernel, i.e. an automorphism.

For every automorphism $\sigma$ obtained in this way, we introduce a symbolic $n \times n$ matrix $X = (x_{ij})$ of indeterminates and solve the homogeneous linear system over $\mathbb{Q}$:

$$XB = \sigma(B)X \quad \text{for all } B \in P.$$

The solution space is a vector subspace of $\mathbb{Q}^{n^2}$, returned in parametric form; if the determinant is zero on the solution space, the family is discarded. Renaming the free parameters canonically, we obtain a finite list of symbolic matrices

$$X_\sigma(x_0, \ldots, x_{m-1}) = \sum_{i=0}^{m-1} x_i X_i, \qquad X_i \in M_n(\mathbb{Q}).$$

To match the description (1) of the set $\mathcal{X}_\sigma$ we also need to address the restriction $X_i \in M_n(\mathbb{Z})$, which will be done later.

### (*LC*), (*CC*) and solving over $\mathbb{Q}/\mathbb{Z}$

Condition $(LC)$ requires the entries of $A$ to be integers. Substituting the parametric matrix $X_\sigma(x_0, \ldots, x_{m-1})$, every entry is a rational linear form in the $x_i$, and we must determine for which integer values of the parameters all entries are integral. This is a homogeneous system of

linear congruences

$$X_\sigma(x) \equiv 0 \mod M_n(\mathbb{Z}),$$

that is, a system of linear equations over the quotient module $\mathbb{Q}/\mathbb{Z}$. Solving it, we get the admissible parameters as a sublattice of $\mathbb{Z}^m$, $x = \sum_j z_j v_j$. Substituting these expressions back into $X_\sigma$ gives the lattice-compatible family

$$A(z_0, \dots, z_{s-1}) = \sum_j z_j A_j, \qquad A_j \in M_n(\mathbb{Z}),$$

with free integral parameters $z_j$ (renamed canonically as $z_0, z_1, \dots$).

For symmorphic groups the cocycle is trivial and $(CC)$ imposes no restrictions. Otherwise, for a lattice-compatible parametric matrix $A(z)$ we determine the restrictions on the parameters $z_j$ given by the cocycle compatibility (2). The implementation forms the finite system of linear congruences (4):

$$u_j(M)\, b(z_0, \dots, z_{s-1}) \equiv 0 \pmod 1, \qquad j > r,$$

in the integral indeterminates $z_j$ only. Note that this is an inhomogeneous linear system of equations over $\mathbb{Q}/\mathbb{Z}$.

The same auxiliary problem arises in the algorithmic classification of crystallographic groups up to affine equivalence, where the first cohomology group $H^1(P, \mathbb{R}^n/L)$ parameterizing the space-group types with fixed point group $P$ and lattice $L$ is computed by solving such congruences. It is treated in the CARAT interface [24] and in the algorithm of Plesken and Schulz [25] through Hermite/Smith normal form.

We solve these systems by lifting them to the integers with extra free variables. Given $Mx \equiv b \mod \mathbb{Z}^N$ with $M \in M_N(\mathbb{Q})$ and $b \in \mathbb{Q}^N$, let $m$ be the least common multiple of the denominators of $M$ and $b$. Introducing an auxiliary integral vector $y \in \mathbb{Z}^N$, the congruence is equivalent to the integral linear system

$$-m\, y + (mM)\, x = mb.$$

The general solution of the homogeneous system (i.e. $b = 0$) is the right kernel of the augmented matrix $M_{aug} = (-mE | mM)$. The kernel basis is returned in echelon form and the auxiliary variables $y$ are placed first. As a result, the free variables of the solution are exactly the auxiliary variables together with the genuinely free parameters, and each dependent

parameter is an integral linear combination of them. The inhomogeneous system also requires a particular solution, which we compute using SageMath's `solve_right` over $\mathbb{Z}$.

### Simplicity test and quadratic Diophantine equations

Some notes should also be added regarding solvers of the Diophantine equations that appear in the simplicity test. For the computed families $Y(y)$ for plane groups these are quadratic Diophantine equations in at most two variables (the only exceptions being the groups p1 and p2, for which $f_\sigma$ is a quadratic form in four variables). Such equations are decidable and can be solved automatically; we use the algorithm of Grunewald and Segal [26] (see also its algorithmic implementation by Alpern [27]), as provided by SageMath's `solve_diophantine`. The implementation solves $f_\sigma(y) = \pm 1$ and $(f_\sigma \pm g_\sigma)(y) = -1$ over $\mathbb{Z}$ and collects the (finite) sets of excluded parameter values.

### Recovering the virtual endomorphism: the translation part $t$

The stages in Section 2 produce only the linear part $A$ of the conjugating affine element, which is all that is needed to determine the degree sets $SCD(G)$ and $SRD(G)$. To actually recover the self-replicating action one must also produce a translation part $t \in \mathbb{Q}^n$ and build the virtual endomorphism by conjugation by an element $(A, t)$. For a fixed integral matrix $A \in \mathcal{Y}_\sigma$ the cocycle condition (3) becomes a system over $\mathbb{Q}/\mathbb{Z}$:

$$Mt \equiv b \pmod{\mathbb{Z}^N}, \qquad b = A\alpha(B) - \alpha(\sigma(B)),$$

in the unknown rational $t$ only.

The method follows the `cong_solve` function of the aforementioned CARAT [24, 25], which solves a homogeneous system of linear congruences $Ax \equiv 0 \pmod{\mathbb{Z}^n}$ for $x \in \mathbb{Q}^n$. The system is similarly lifted to the (mod $m$) congruences for the least common multiple of denominators. It is then simplified using Smith normal form decomposition $(UMV)V^{-1}t \equiv Ub$. For a one-dimensional equation $d_i x_i \equiv b_i \mod m$ the general solution is $x_i \equiv \frac{b_i}{d_i} + \frac{nm}{d_i}$, where $n$ is an arbitrary integer. Transforming back by $V$ yields $t = t_0 + VR + VN$, where $R$ is the basis of the lattice of solutions and $N$ is the basis of the nullspace. Note that the lattice is isomorphic to $\mathbb{Z}^r$, while the nullspace is isomorphic to $\mathbb{Q}^{n-r}$, where $r$ is the rank of $M$.

# 1. Appendix

| No. [1] | $A \in \mathcal{Y}$ | $f_\sigma$ | $MinSRD$ | Excluded values |
|---|---|---|---|---|
| 1 | $\begin{pmatrix} y_0 & y_1 \\ y_2 & y_3 \end{pmatrix}$ | $\lvert y_0y_3 - y_1y_2\rvert$ | 2 | |
| 2 | $\begin{pmatrix} y_0 & y_1 \\ y_2 & y_3 \end{pmatrix}$ | $\lvert y_0y_3 - y_1y_2\rvert$ | 2 | |
| 3 | $\begin{pmatrix} y_0 & 0 \\ 0 & y_1 \end{pmatrix}$ | $\lvert y_0y_1\rvert$ | 4 | $(y_0,y_1) \notin \left\{ \begin{array}{lll} (-1,-1), & (-1,1), & (-1,n) \\ (1,n), & (1,1), & (n,-1) \\ (1,-1), & (n,1) & : n \in \mathbb{Z} \end{array} \right\}$ |
| 4 | $\begin{pmatrix} y_0 & 0 \\ 0 & -2\,y_1+1 \end{pmatrix}$ | $\lvert y_0(2\,y_1-1)\rvert$ | 6 | $(y_0,y_1) \notin \left\{ \begin{array}{lll} (-1,0), & (-1,1), & (-1,n) \\ (1,n), & (1,0), & (1,1) \\ (n,0), & (n,1) & : n \in \mathbb{Z} \end{array} \right\}$ |
| 5 | $\begin{pmatrix} y_0 & 0 \\ y_1 & y_0+2\,y_1 \end{pmatrix}$ | $\lvert(y_0+2\,y_1)y_0\rvert$ | 4 | $(y_0,y_1) \notin \left\{ \begin{array}{lll} (-1,1), & (1,n), & (-2\,m-1,m) \\ (-1,0), & (1,-1), & (-2\,m+1,m) \\ (-1,n), & (1,0) & : n,m \in \mathbb{Z} \end{array} \right\}$ |
| 6 | $\begin{pmatrix} y_0 & 0 \\ 0 & y_1 \end{pmatrix}$ | $\lvert y_0y_1\rvert$ | 2 | $(y_0,y_1) \notin \left\{ \begin{array}{lll} (-1,-1), & (-1,1), & (-1,n) \\ (1,n), & (1,1), & (n,-1) \\ (1,-1), & (n,1) & : n \in \mathbb{Z} \end{array} \right\}$ |
| 7 | $\begin{pmatrix} -2\,y_0+1 & 0 \\ 0 & y_1 \end{pmatrix}$ | $\lvert(2\,y_0-1)y_1\rvert$ | 6 | $(y_0,y_1) \notin \left\{ \begin{array}{lll} (0,1), & (1,n), & (1,1) \\ (n,-1), & (1,-1), & (n,1) \\ (0,n), & (0,-1) & : n \in \mathbb{Z} \end{array} \right\}$ |
| 8 | $\begin{pmatrix} 0 & 2\,y_0-1 \\ -2\,y_1-1 & 0 \end{pmatrix}$ | $\lvert(2\,y_0-1)(2\,y_1+1)\rvert$ | 3 | $(y_0,y_1) \notin \{(0,-1),(0,0),(1,-1),(1,0)\}$ |
| 9 | $\begin{pmatrix} y_0 & 2\,y_0 \\ y_1 & -y_0 \end{pmatrix}$<br>$\begin{pmatrix} y_0 & 0 \\ y_1 & y_0+2\,y_1 \end{pmatrix}$ | $\lvert -y_0^2-2\,y_0y_1\rvert$<br>$\lvert(y_0+2\,y_1)y_0\rvert$ | 3 | $(y_0,y_1) \notin \{(-1,0),(-1,1),(1,-1),(1,0)\}$<br>$(y_0,y_1) \notin \left\{ \begin{array}{lll} (-1,1), & (1,n), & (-2\,m-1,m) \\ (-1,0), & (1,-1), & (-2\,m+1,m) \\ (-1,n), & (1,0) & : n,m \in \mathbb{Z} \end{array} \right\}$ |
| 10 | $\begin{pmatrix} y_0 & y_1 \\ -y_1 & y_0 \end{pmatrix}$ | $\lvert y_0^2+y_1^2\rvert$ | 2 | $(y_0,y_1) \notin \{(-1,0),(0,-1),(0,1),(1,0)\}$ |
| 11 | $\begin{pmatrix} y_0 & y_0 \\ -y_0 & y_0 \end{pmatrix}$<br>$\begin{pmatrix} 0 & y_0 \\ -y_0 & 0 \end{pmatrix}$ | $2\lvert y_0^2\rvert$<br>$\lvert y_0\rvert^2$ | 2 | $y_0 \notin \{-1,1\}$ |
| 12 | $\begin{pmatrix} 0 & -2\,y_0-1 \\ 2\,y_0+1 & 0 \end{pmatrix}$ | $\lvert 2\,y_0+1\rvert^2$ | 9 | $y_0 \notin \{-1,0\}$ |
| 13 | $\begin{pmatrix} y_0 & y_1 \\ y_0+y_1 & -y_0 \end{pmatrix}$<br>$\begin{pmatrix} y_0 & y_1 \\ -y_1 & y_0+y_1 \end{pmatrix}$ | $\lvert -y_0^2-(y_0+y_1)y_1\rvert$<br>$\lvert(y_0+y_1)y_0+y_1^2\rvert$ | 3 | $(y_0,y_1) \notin \{(-1,0),(-1,1),(0,-1),(0,1),(1,-1),(1,0)\}$<br>$(y_0,y_1) \notin \{(-1,0),(-1,1),(0,-1),(0,1),(1,-1),(1,0)\}$ |
| 14 | $\begin{pmatrix} y_0 & -y_0 \\ y_0 & 0 \end{pmatrix}$ | $\lvert y_0\rvert^2$ | 4 | $y_0 \notin \{-1,1\}$ |
| 15 | $\begin{pmatrix} y_0 & -y_0 \\ y_0 & 0 \end{pmatrix}$ | $\lvert y_0\rvert^2$ | 4 | $y_0 \notin \{-1,1\}$ |
| 16 | $\begin{pmatrix} y_0 & y_1 \\ -y_1 & y_0+y_1 \end{pmatrix}$<br>$\begin{pmatrix} y_0 & y_1 \\ y_0+y_1 & -y_0 \end{pmatrix}$ | $\lvert(y_0+y_1)y_0+y_1^2\rvert$<br>$\lvert -y_0^2-(y_0+y_1)y_1\rvert$ | 3 | $(y_0,y_1) \notin \{(-1,0),(-1,1),(0,-1),(0,1),(1,-1),(1,0)\}$<br>$(y_0,y_1) \notin \{(-1,0),(-1,1),(0,-1),(0,1),(1,-1),(1,0)\}$ |
| 17 | $\begin{pmatrix} y_0 & -y_0 \\ y_0 & 0 \end{pmatrix}$<br>$\begin{pmatrix} y_0 & y_0 \\ 2\,y_0 & -y_0 \end{pmatrix}$ | $\lvert y_0\rvert^2$<br>$3\lvert y_0^2\rvert$ | 3 | $y_0 \notin \{-1,1\}$ |

Table 1: Self-replicating and self-covering degrees for the 17 plane groups. For each group, the table gives the group number, the corresponding matrices in $Y$, the polynomials $f_\sigma$, the excluded integer values arising from the conditions $f_\sigma \neq 0, \pm 1$ and $f_\sigma \pm g_\sigma \neq -1$, and the smallest self-replicating degree.

[1] A positional number of the plane group in the International Tables for Crystallography, Volume A (ITA).

| Groups No.[1] [2] | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 3,6,10 | $y_2$ | $-y_1y_3 + y_0y_4$ | $y_0 + y_4$ |
| 4 | $-2\,y_2 + 1$ | $-y_1y_3 + y_0y_4$ | $y_0 + y_4$ |
| 5,8,12 | $y_0 + 2\,y_2$ | $-2\,y_1y_3 + y_0y_4$ | $y_0 + y_4$ |
| 7 | $y_2$ | $2\,y_1y_3 - 2\,y_0y_4 + y_0$ | $y_0 - 2\,y_4 + 1$ |
| 9 | $y_0 + 2\,y_2$ | $2\,y_1y_3 - 2\,y_0y_4 + y_0$ | $y_0 - 2\,y_4 + 1$ |
| 11 | $2\,y_2 + 1$ | $-y_1y_3 + y_0y_4$ | $y_0 + y_4$ |
| 13 | $y_2$ | $-2\,y_1y_3 + 2\,y_0y_4 + y_0$ | $y_0 + 2\,y_4 + 1$ |
| 14 | $2\,y_2 + 1$ | $-2\,y_1y_3 + 2\,y_0y_4 + y_0$ | $y_0 + 2\,y_4 + 1$ |
| 15 | $y_0 + 2\,y_2$ | $-2\,y_1y_3 + 2\,y_0y_4 + y_0$ | $y_0 + 2\,y_4 + 1$ |
| 16,47 | $y_0$ | $-y_1y_2$ | $0$ |
| 16,25,47 | $y_0$ | $y_1y_2$ | $y_1 + y_2$ |
| 16,25,47 | $y_2$ | $-y_0y_1$ | $0$ |
| 16,47 | $y_1$ | $-y_0y_2$ | $0$ |
| 17,27,49 | $y_0$ | $2\,y_1y_2 + y_1$ | $y_1 + 2\,y_2 + 1$ |
| 17,27 | $2\,y_2 - 1$ | $-y_0y_1$ | $0$ |
| 18,50 | $-2\,y_0 + 1$ | $(2\,y_1 + 1)y_2$ | $2\,y_1 + y_2 + 1$ |
| 18 | $y_2$ | $2\,(2\,y_0 - 1)y_1 + 2\,y_0 - 1$ | $0$ |
| 19,48 | $2\,y_0 - 1$ | $-2\,(2\,y_1 + 1)y_2 - 2\,y_1 - 1$ | $0$ |
| 19,56,60,64 | $2\,y_0 + 1$ | $2\,(2\,y_1 + 1)y_2 + 2\,y_1 + 1$ | $2\,y_1 + 2\,y_2 + 2$ |
| 19 | $2\,y_2 - 1$ | $-2\,(2\,y_0 + 1)y_1 - 2\,y_0 - 1$ | $0$ |
| 19 | $2\,y_1 - 1$ | $-2\,(2\,y_0 - 1)y_2 + 2\,y_0 - 1$ | $0$ |
| 20,37,63,66 | $y_0$ | $2\,(y_0 + 2\,y_1)y_2 + y_0 + 2\,y_1$ | $y_0 + 2\,y_1 + 2\,y_2 + 1$ |
| 20,37 | $2\,y_2 - 1$ | $-y_0^2 - 2\,y_0y_1$ | $0$ |
| 21,65 | $2\,y_0$ | $-2\,y_1y_2$ | $0$ |
| 21,35,65 | $y_0$ | $(y_0 + 2\,y_1)y_2$ | $y_0 + 2\,y_1 + y_2$ |
| 21,65 | $2\,y_1$ | $-2\,y_0y_2$ | $0$ |
| 21,35,65 | $y_2$ | $-y_0^2 - 2\,y_0y_1$ | $0$ |
| 22,23,42,44 69,71 | $y_0$ | $y_0^2 + 2\,y_0y_1 + 2\,(y_0 + 2\,y_1)y_2$ | $2\,y_0 + 2\,y_1 + 2\,y_2$ |
| 22,42,69 | $y_0 + 2\,y_1 + 2\,y_2$ | $-y_0^2 - 2\,y_0y_1$ | $0$ |
| 22,69 | $y_0$ | $-y_0^2 - 4\,y_0y_1 - 4\,y_1^2 - 2\,(y_0 + 2\,y_1)y_2$ | $0$ |
| 22,23,69,71 | $y_0 + 2\,y_1$ | $-y_0^2 - 2\,y_0y_2$ | $0$ |
| 23,71 | $y_0$ | $-y_0^2 - 2\,y_0y_1 - 2\,(y_0 + 2\,y_1)y_2$ | $0$ |
| 23,44,71 | $y_0 + 2\,y_2$ | $-y_0^2 - 2\,y_0y_1$ | $0$ |
| 24 | $-2\,y_1 - 1$ | $4\,y_0^2 - 2\,(2\,y_0 + 1)y_1 - 2\,(2\,y_0 + 1)y_2 - 1$ | $0$ |
| 24 | $2\,y_0 - 3$ | $-4\,y_0y_1 - 4\,y_1^2 + 2\,(2\,y_1 - 3)y_2 + 6\,y_0 + 9$ | $-2\,y_0 + 2\,y_2 - 6$ |
| 24 | $2\,y_0 - 3$ | $4\,y_0y_1 + 4\,y_1^2 - 2\,(2\,y_1 - 3)y_2 - 6\,y_0 - 9$ | $0$ |
| 24 | $-2\,y_1 + 2\,y_2 + 3$ | $4\,y_0^2 - 2\,(2\,y_0 + 3)y_1 - 9$ | $0$ |
| 26 | $y_0$ | $-2\,y_1y_2 + y_1$ | $y_1 - 2\,y_2 + 1$ |
| 28,51 | $2\,y_0 + 1$ | $y_1y_2$ | $y_1 + y_2$ |
| 29,31 | $2\,y_0 + 1$ | $-2\,y_1y_2 + y_1$ | $y_1 - 2\,y_2 + 1$ |
| 30,57 | $y_0$ | $-2\,(2\,y_1 - 1)y_2 - 2\,y_1 + 1$ | $-2\,y_1 + 2\,y_2 + 2$ |
| 32 | $2\,y_0 + 1$ | $-(2\,y_1 - 1)y_2$ | $-2\,y_1 + y_2 + 1$ |
| 32,50 | $y_2$ | $2\,(2\,y_0 + 1)y_1 - 2\,y_0 - 1$ | $0$ |
| 33,62 | $2\,y_0 + 1$ | $2\,(2\,y_1 - 1)y_2 - 2\,y_1 + 1$ | $-2\,y_1 - 2\,y_2 + 2$ |
| 34,61 | $2\,y_0 + 1$ | $-2\,(2\,y_1 - 1)y_2 - 2\,y_1 + 1$ | $-2\,y_1 + 2\,y_2 + 2$ |
| 34 | $2\,y_2 - 1$ | $2\,(2\,y_0 + 1)y_1 - 2\,y_0 - 1$ | $0$ |
| 36 | $y_0$ | $-2\,(y_0 + 2\,y_1)y_2 + y_0 + 2\,y_1$ | $y_0 + 2\,y_1 - 2\,y_2 + 1$ |
| 38 | $2\,y_2$ | $-2\,y_0y_1$ | $0$ |
| 38 | $y_0$ | $y_1^2 + 2\,y_1y_2$ | $2\,y_1 + 2\,y_2$ |
| 39 | $y_0$ | $4\,y_1^2 + 2\,(2\,y_1 + 1)y_2 + 4\,y_1 + 1$ | $4\,y_1 + 2\,y_2 + 2$ |
| 40 | $2\,y_0 + 1$ | $y_1^2 + 2\,y_1y_2$ | $2\,y_1 + 2\,y_2$ |
| 41 | $2\,y_0 + 1$ | $4\,y_1^2 + 2\,(2\,y_1 + 1)y_2 + 4\,y_1 + 1$ | $4\,y_1 + 2\,y_2 + 2$ |
| 43 | $2\,y_0 - 2\,y_1 + 2\,y_2 + 1$ | $2\,(2\,y_0 - 1)y_1 + 2\,y_0 - 1$ | $0$ |
| 43 | $-2\,y_0 - 2\,y_1 + 1$ | $4\,y_0y_2 - 4\,y_2^2 - 2\,y_0 + 1$ | $-2\,y_0 + 2$ |

Table 2: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 3–43

[1] A positional number of the space group in the International Tables for Crystallography, Volume A (ITA).

[2] Groups Nos. 1 and 2 are not included since they fall into a separate reduced case: every matrix belongs to the point group normalizer.

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 45 | $-2y_0-2y_1+1$ | $4y_0^2+2(2y_0-1)y_1-2(2y_0-1)y_2-4y_0+1$ | $-4y_0-2y_1+2y_2+2$ |
| 45 | $-2y_0+2y_1+2y_2+1$ | $4y_0^2-2(2y_0+1)y_1-1$ | $0$ |
| 46 | $-2y_0+1$ | $4y_0^2-2(2y_0-1)y_1-2(2y_0-2y_1-1)y_2-4y_0+1$ | $-4y_0+2y_1+2y_2+2$ |
| 48 | $-2y_0+1$ | $2(2y_1+1)y_2+2y_1+1$ | $2y_1+2y_2+2$ |
| 48 | $2y_2+1$ | $2(2y_0+1)y_1-2y_0-1$ | $0$ |
| 48 | $2y_1+1$ | $2(2y_0+1)y_2-2y_0-1$ | $0$ |
| 49 | $2y_2+1$ | $-y_0y_1$ | $0$ |
| 52,58 | $-2y_0+1$ | $-2(2y_1-1)y_2-2y_1+1$ | $-2y_1+2y_2+2$ |
| 53 | $-2y_0+1$ | $2y_1y_2+y_1$ | $y_1+2y_2+1$ |
| 54 | $2y_0+1$ | $2y_1y_2+y_1$ | $y_1+2y_2+1$ |
| 55 | $-2y_0+1$ | $-(2y_1-1)y_2$ | $-2y_1+y_2+1$ |
| 55,59 | $y_2$ | $-2(2y_0+1)y_1-2y_0-1$ | $0$ |
| 56,58 | $2y_2+1$ | $-2(2y_0+1)y_1-2y_0-1$ | $0$ |
| 59,67 | $2y_0+1$ | $(2y_1+1)y_2$ | $2y_1+y_2+1$ |
| 66 | $2y_2+1$ | $-y_0^2-2y_0y_1$ | $0$ |
| 67 | $y_2$ | $-4y_0^2+2(2y_0+1)y_1-4y_0-1$ | $0$ |
| 68 | $-2y_0+1$ | $-2(2y_0-2y_1-1)y_2-2y_0+2y_1+1$ | $-2y_0+2y_1+2y_2+2$ |
| 68 | $2y_2+1$ | $-2(2y_0-1)y_1+2y_0-1$ | $0$ |
| 70 | $2y_0-3$ | $-2(2y_0+3)y_1-2(2y_1-3)y_2+6y_0+9$ | $-2y_0+2y_1-2y_2-6$ |
| 70 | $-2y_1-2y_2-3$ | $-2(2y_0-3)y_1+6y_0-9$ | $0$ |
| 70 | $2y_0-3$ | $4y_0^2-8y_0y_1+4y_1^2+2(2y_0-2y_1+3)y_2-9$ | $0$ |
| 70 | $2y_0-3$ | $2(2y_0+2y_1-3)y_2+6y_0+6y_1-9$ | $0$ |
| 72 | $-2y_0+1$ | $-4y_0^2-2(2y_0-1)y_1+2(2y_0+2y_1+1)y_2+1$ | $2y_1+2y_2+2$ |
| 72 | $2y_0+2y_1+2y_2-1$ | $4y_0^2+2(6y_0-1)y_1+8y_1^2-1$ | $0$ |
| 73 | $-2y_0+1$ | $-4(y_0-1)y_1+4y_1^2+2(2y_1+1)y_2-2y_0+1$ | $-2y_0+4y_1+2y_2+2$ |
| 73 | $2y_1-2y_2+1$ | $4y_0^2-2(2y_0-1)y_1-1$ | $0$ |
| 73 | $-2y_0-1$ | $4(y_0+1)y_1-4y_1^2-2(2y_1-1)y_2-2y_0-1$ | $0$ |
| 73 | $-2y_0-4y_1+5$ | $-2(2y_0+2y_1+5)y_2-10y_0-10y_1-25$ | $0$ |
| 74 | $2y_0+1$ | $2(2y_0+1)y_1+2(2y_1+1)y_2+2y_0+1$ | $2y_0+2y_1+2y_2+2$ |
| 74 | $-2y_0+2y_2-1$ | $-4y_0^2+2(2y_0+1)y_1-4y_0-1$ | $0$ |
| 75,81,83 | $y_2$ | $y_0^2+y_1^2$ | $2y_0$ |
| 75,81,83 | $y_2$ | $-y_0^2-y_1^2$ | $0$ |
| 76 | $-4y_2+1$ | $y_0^2+y_1^2$ | $2y_0$ |
| 76 | $-4y_2-1$ | $-y_0^2-y_1^2$ | $0$ |
| 77 | $-2y_2+1$ | $y_0^2+y_1^2$ | $2y_0$ |
| 77,84 | $-2y_2-1$ | $-y_0^2-y_1^2$ | $0$ |
| 78 | $-4y_2+9$ | $y_0^2+y_1^2$ | $2y_0$ |
| 78 | $-4y_2-9$ | $-y_0^2-y_1^2$ | $0$ |
| 79,82,87 | $y_0+2y_2$ | $-y_0^2+2y_0y_1-2y_1^2$ | $0$ |
| 79,82,87 | $y_0+2y_2$ | $y_0^2-2y_0y_1+2y_1^2$ | $2y_0-2y_1$ |
| 80 | $4y_0-2y_2+1$ | $-4y_0^2-2(2y_0-1)y_1-2y_1^2+2(2y_0+2y_1-1)y_2-2y_2^2-1$ | $0$ |
| 80 | $-2y_1+4y_2-3$ | $2y_0^2-2(2y_0+3)y_1+2y_1^2+4(y_0-y_1+3)y_2+4y_2^2+6y_0+9$ | $-2y_0+2y_1-4y_2-6$ |
| 84 | $2y_2+1$ | $y_0^2+y_1^2$ | $2y_0$ |
| 85 | $y_2$ | $2y_0^2+2y_1^2-2y_0-2y_1+1$ | $-2y_0-2y_1+2$ |
| 85 | $y_2$ | $-2y_0^2-2y_1^2+2y_0-2y_1-1$ | $0$ |
| 86 | $2y_2+1$ | $2y_0^2-4(y_0-1)y_1+4y_1^2-2y_0+1$ | $-2y_0+4y_1+2$ |
| 86 | $2y_2+1$ | $-2y_0^2+4(y_0-1)y_1-4y_1^2+2y_0-1$ | $0$ |

Table 3: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 45–86

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 88 | $4\,y_0+2\,y_1-3$ | $20\,y_0^2+6\,(2\,y_0+1)y_1+2\,y_1^2+2\,(6\,y_0+2\,y_1+3)y_2+2\,y_2^2+24\,y_0+9$ | $-8\,y_0-2\,y_1-2\,y_2-6$ |
| 88 | $2\,y_1+5$ | $-4\,y_0^2+2\,(2\,y_0+5)y_1-2\,y_1^2+2\,(2\,y_0-2\,y_1+5)y_2-2\,y_2^2-25$ | $0$ |
| 89,99,123 | $y_1$ | $2\,y_0^2$ | $2\,y_0$ |
| 89,99,111,115 123,149,150,156 157,162,164,177 183,187,189,191 | $y_1$ | $-y_0^2$ | $0$ |
| 89,99,111,115 123 | $y_1$ | $y_0^2$ | $0$ |
| 89,99,123 | $y_1$ | $-2\,y_0^2$ | $0$ |
| 89,99,111,115 123,149,150,156 157,162,164,177 183,187,189,191 | $y_0$ | $-y_0y_1$ | $-y_0+y_1$ |
| 89,99,111,115 123,149,150,156 157,162,164,177 183,187,189,191 | $y_0$ | $y_0y_1$ | $y_0+y_1$ |
| 90 | $y_1$ | $-4\,y_0^2+12\,y_0-9$ | $0$ |
| 90 | $y_1$ | $4\,y_0^2+12\,y_0+9$ | $0$ |
| 90,125,129 | $2\,y_0-1$ | $-(2\,y_0-1)y_1$ | $-2\,y_0+y_1+1$ |
| 90,100,113,117 127,129 | $2\,y_0+1$ | $(2\,y_0+1)y_1$ | $2\,y_0+y_1+1$ |
| 91 | $4\,y_1+1$ | $2\,y_0^2$ | $2\,y_0$ |
| 91 | $4\,y_1-1$ | $-y_0^2$ | $0$ |
| 91 | $4\,y_1+1$ | $y_0^2$ | $0$ |
| 91,95 | $4\,y_1-1$ | $-2\,y_0^2$ | $0$ |
| 91 | $y_0$ | $-4\,y_0y_1-3\,y_0$ | $-y_0+4\,y_1+3$ |
| 91,95 | $4\,y_1-3$ | $2\,y_0^2$ | $2\,y_0$ |
| 91,95 | $y_0$ | $4\,y_0y_1+y_0$ | $y_0+4\,y_1+1$ |
| 92 | $4\,y_1-1$ | $-4\,y_0^2+12\,y_0-9$ | $0$ |
| 92 | $4\,y_1+1$ | $4\,y_0^2+12\,y_0+9$ | $0$ |
| 92 | $2\,y_0-1$ | $-4\,(2\,y_0-1)y_1-6\,y_0+3$ | $-2\,y_0+4\,y_1+4$ |
| 92,96 | $2\,y_0+1$ | $4\,(2\,y_0+1)y_1+2\,y_0+1$ | $2\,y_0+4\,y_1+2$ |
| 93,103,124 | $-2\,y_1-1$ | $2\,y_0^2$ | $2\,y_0$ |
| 93,101,112,131 185,188 | $-2\,y_1+1$ | $-y_0^2$ | $0$ |
| 93,103,105,124 131,132 | $-2\,y_1-1$ | $y_0^2$ | $0$ |
| 93,103,124 | $-2\,y_1-1$ | $-2\,y_0^2$ | $0$ |
| 93,101,103,105 116,124,131,132 158,159,163,165 184,185,186,188 190,192,193 | $y_0$ | $2\,y_0y_1+y_0$ | $-y_0-2\,y_1-1$ |
| 93,103 | $-2\,y_1+1$ | $2\,y_0^2$ | $2\,y_0$ |
| 93,103 | $-2\,y_1+1$ | $-2\,y_0^2$ | $0$ |
| 93,112,116,131 158,159,182,185 186,188,194 | $y_0$ | $-2\,y_0y_1+y_0$ | $y_0-2\,y_1+1$ |
| 94 | $-2\,y_1+1$ | $-4\,y_0^2+12\,y_0-9$ | $0$ |
| 94 | $-2\,y_1-1$ | $4\,y_0^2+12\,y_0+9$ | $0$ |
| 94 | $2\,y_0-1$ | $2\,(2\,y_0-1)y_1+2\,y_0-1$ | $-2\,y_0-2\,y_1$ |
| 94,114,135 | $2\,y_0+1$ | $-2\,(2\,y_0+1)y_1+2\,y_0+1$ | $2\,y_0-2\,y_1+2$ |
| 95 | $4\,y_1+3$ | $-y_0^2$ | $0$ |
| 95 | $4\,y_1-3$ | $y_0^2$ | $0$ |
| 95 | $y_0$ | $-4\,y_0y_1+5\,y_0$ | $-y_0+4\,y_1-5$ |
| 95 | $4\,y_1+5$ | $2\,y_0^2$ | $2\,y_0$ |
| 95 | $4\,y_1+3$ | $-2\,y_0^2$ | $0$ |
| 96 | $4\,y_1+3$ | $-4\,y_0^2+12\,y_0-9$ | $0$ |
| 96 | $4\,y_1-3$ | $4\,y_0^2+12\,y_0+9$ | $0$ |
| 96 | $2\,y_0-1$ | $-4\,(2\,y_0-1)y_1+10\,y_0-5$ | $-2\,y_0+4\,y_1-4$ |
| 97,107,119,121 139 | $y_0+2\,y_1$ | $y_0^2$ | $0$ |
| 97,107,139 | $2\,y_0+2\,y_1$ | $2\,y_0^2$ | $2\,y_0$ |
| 97,107,119,121 139 | $-y_0$ | $y_0^2+2\,y_0y_1$ | $2\,y_0+2\,y_1$ |
| 97,107,139 | $2\,y_1$ | $-2\,y_0^2$ | $0$ |
| 97,107,139 | $2\,y_0+2\,y_1$ | $-2\,y_0^2$ | $0$ |
| 97,107,139 | $2\,y_1$ | $2\,y_0^2$ | $-2\,y_0$ |

Table 4: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 88–139

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 97,107,119,121 139 | $y_0$ | $-y_0^2 - 2\,y_0y_1$ | $2\,y_1$ |
| 98,130,136,137 138 | $2\,y_1 + 1$ | $4\,y_0^2 - 4\,y_0 + 1$ | $0$ |
| 98,122 | $2\,y_0 - 1$ | $-8\,y_0^2 - 2\,(2\,y_0 - 1)y_1 + 2\,y_0 + 1$ | $2\,y_0 + 2\,y_1 + 2$ |
| 98,108,126,134 135,137,140 | $2\,y_0 + 1$ | $-2\,(2\,y_0 + 1)y_1 - 2\,y_0 - 1$ | $-2\,y_0 + 2\,y_1$ |
| 98 | $-2\,y_0 - 2\,y_1 + 1$ | $4\,y_0^2 + 6\,(2\,y_0 - 1)y_1 + 8\,y_1^2 - 4\,y_0 + 1$ | $-4\,y_0 - 6\,y_1 + 2$ |
| 100,113,117,127 | $y_1$ | $-4\,y_0^2 - 4\,y_0 - 1$ | $0$ |
| 100,125,127 | $y_1$ | $4\,y_0^2 + 4\,y_0 + 1$ | $0$ |
| 101,112,116 | $2\,y_1 - 1$ | $y_0^2$ | $0$ |
| 101,103,105,124 132,163,165,184 190,192,193 | $y_0$ | $-2\,y_0y_1 - y_0$ | $-y_0 + 2\,y_1 + 1$ |
| 102,114,135 | $2\,y_1 - 1$ | $-4\,y_0^2 - 4\,y_0 - 1$ | $0$ |
| 102 | $2\,y_1 - 1$ | $4\,y_0^2 + 4\,y_0 + 1$ | $0$ |
| 102 | $2\,y_0 - 3$ | $-2\,(2\,y_0 - 3)y_1 - 2\,y_0 + 3$ | $-2\,y_0 + 2\,y_1 + 4$ |
| 102,104,106,108 118,120,128,130 133,138,140 | $2\,y_0 + 1$ | $2\,(2\,y_0 + 1)y_1 + 2\,y_0 + 1$ | $2\,y_0 + 2\,y_1 + 2$ |
| 103,105,116,124 132,158,159,163 165,182,184,186 190,192,193,194 | $2\,y_1 + 1$ | $-y_0^2$ | $0$ |
| 104,106,118,128 136 | $2\,y_1 + 1$ | $-4\,y_0^2 - 4\,y_0 - 1$ | $0$ |
| 104,106,108,126 128,133,134,135 140 | $2\,y_1 + 1$ | $4\,y_0^2 + 4\,y_0 + 1$ | $0$ |
| 109 | $-2\,y_0 + 3$ | $4\,y_0^2 + 4\,(2\,y_0 + 3)y_1 + 4\,y_1^2 + 12\,y_0 + 9$ | $0$ |
| 109,110 | $2\,y_0 + 1$ | $2\,(2\,y_0 + 1)y_1 - 2\,y_0 - 1$ | $-2\,y_0 - 2\,y_1$ |
| 109,110 | $2\,y_0 + 1$ | $-8\,y_0^2 + 2\,(2\,y_0 + 1)y_1 - 2\,y_0 + 1$ | $2\,y_0 - 2\,y_1 - 2$ |
| 109 | $-2\,y_0 - 3$ | $-8\,y_0^2 + 2\,(2\,y_0 + 3)y_1 - 6\,y_0 + 9$ | $2\,y_0 - 2\,y_1 - 6$ |
| 110 | $-2\,y_0 + 3$ | $16\,y_0^2 + 4\,(4\,y_0 + 3)y_1 + 4\,y_1^2 + 24\,y_0 + 9$ | $0$ |
| 110 | $-2\,y_0 - 2\,y_1 - 3$ | $-4\,y_0^2 - 6\,(2\,y_0 + 1)y_1 - 8\,y_1^2 + 9$ | $2\,y_1 - 6$ |
| 112,182,185,194 | $y_0$ | $2\,y_0y_1 - y_0$ | $-y_0 - 2\,y_1 + 1$ |
| 113,117 | $-2\,y_0 + 1$ | $(2\,y_0 - 1)y_1$ | $2\,y_0 + y_1 - 1$ |
| 113,117,129 | $y_1$ | $4\,y_0^2 - 4\,y_0 + 1$ | $0$ |
| 114,120 | $-2\,y_0 + 1$ | $-2\,(2\,y_0 - 1)y_1 + 2\,y_0 - 1$ | $2\,y_0 - 2\,y_1$ |
| 114,118,120 | $-2\,y_1 + 1$ | $4\,y_0^2 - 4\,y_0 + 1$ | $0$ |
| 118,122,133,137 | $-2\,y_0 + 1$ | $2\,(2\,y_0 - 1)y_1 - 2\,y_0 + 1$ | $2\,y_0 + 2\,y_1 - 2$ |
| 122 | $2\,y_0 + 1$ | $36\,y_0^2 - 4\,(6\,y_0 + 1)y_1 + 4\,y_1^2 + 12\,y_0 + 1$ | $0$ |
| 122 | $-2\,y_0 - 5$ | $4\,y_0^2 - 2\,(2\,y_0 + 5)y_1 - 25$ | $4\,y_0 - 2\,y_1$ |
| 125,129 | $y_1$ | $-4\,y_0^2 + 4\,y_0 - 1$ | $0$ |
| 125 | $2\,y_0 + 1$ | $-(2\,y_0 + 1)y_1$ | $-2\,y_0 + y_1 - 1$ |
| 126,130,134,138 | $2\,y_1 + 1$ | $-4\,y_0^2 + 4\,y_0 - 1$ | $0$ |
| 126,130,134,138 | $-2\,y_0 + 1$ | $-2\,(2\,y_0 - 1)y_1 - 2\,y_0 + 1$ | $-2\,y_0 + 2\,y_1 + 2$ |
| 133,137 | $-2\,y_1 + 1$ | $-4\,y_0^2 + 4\,y_0 - 1$ | $0$ |
| 136 | $2\,y_0 + 3$ | $-2\,(2\,y_0 + 3)y_1 - 2\,y_0 - 3$ | $-2\,y_0 + 2\,y_1 - 2$ |
| 136 | $2\,y_0 - 3$ | $2\,(2\,y_0 - 3)y_1 + 2\,y_0 - 3$ | $2\,y_0 + 2\,y_1 - 2$ |
| 141 | $2\,y_0 - 3$ | $-8\,y_0^2 - 2\,(2\,y_0 - 3)y_1 + 6\,y_0 + 9$ | $2\,y_0 + 2\,y_1 + 6$ |
| 141 | $-2\,y_0 - 2\,y_1 - 3$ | $4\,(y_0 + 3)y_1 + 4\,y_1^2 + 6\,y_0 + 9$ | $-2\,y_0 - 4\,y_1 - 6$ |
| 141 | $-2\,y_0 - 2\,y_1 + 1$ | $-4\,(y_0 - 1)y_1 - 4\,y_1^2 + 2\,y_0 - 1$ | $2\,y_0$ |
| 141 | $-2\,y_0 + 4\,y_1 - 1$ | $4\,y_0^2 - 4\,(2\,y_0 + 1)y_1 + 4\,y_1^2 + 4\,y_0 + 1$ | $0$ |
| 142 | $-2\,y_0 - 1$ | $-8\,y_0^2 - 2\,(2\,y_0 + 1)y_1 - 2\,y_0 + 1$ | $-2\,y_0 - 2\,y_1 + 2$ |
| 142 | $-2\,y_0 + 1$ | $-8\,y_0^2 + 2\,(2\,y_0 - 1)y_1 + 2\,y_0 + 1$ | $2\,y_0 - 2\,y_1 + 2$ |
| 142 | $-2\,y_0 + 1$ | $8\,y_0^2 - 2\,(2\,y_0 - 1)y_1 - 2\,y_0 - 1$ | $6\,y_0 - 2\,y_1$ |
| 142 | $-4\,y_0 - 2\,y_1 - 3$ | $4\,y_0^2 + 12\,y_0 + 9$ | $0$ |
| 143,147,168,174 175 | $y_2$ | $-y_0^2 - y_0y_1 - y_1^2$ | $0$ |
| 143,147,168,174 175 | $y_2$ | $y_0^2 + y_0y_1 + y_1^2$ | $2\,y_0 + y_1$ |
| 144,172 | $-3\,y_2 - 1$ | $-y_0^2 - y_0y_1 - y_1^2$ | $0$ |
| 144,172 | $-3\,y_2 + 1$ | $y_0^2 + y_0y_1 + y_1^2$ | $2\,y_0 + y_1$ |
| 145,171 | $-3\,y_2 - 4$ | $-y_0^2 - y_0y_1 - y_1^2$ | $0$ |
| 145,171 | $-3\,y_2 + 4$ | $y_0^2 + y_0y_1 + y_1^2$ | $2\,y_0 + y_1$ |
| 146,148 | $y_0 + 3\,y_2$ | $-y_0^2 + 3\,y_0y_1 - 3\,y_1^2$ | $0$ |
| 146,148 | $y_0 + 3\,y_2$ | $y_0^2 - 3\,y_0y_1 + 3\,y_1^2$ | $2\,y_0 - 3\,y_1$ |
| 149,150,156,157 162,164,177,183 187,189,191 | $y_1$ | $y_0^2$ | $y_0$ |

Table 5: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 97–191

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 151,152,181 | $-3\,y_1-2$ | $y_0^2$ | $y_0$ |
| 151,152,181 | $-3\,y_1+1$ | $y_0^2$ | $y_0$ |
| 151,152,181 | $-y_0$ | $-3\,y_0y_1-y_0$ | $y_0-3\,y_1-1$ |
| 151,152,181 | $y_0$ | $3\,y_0y_1-2\,y_0$ | $-y_0-3\,y_1+2$ |
| 151,152,181 | $-3\,y_1-1$ | $-y_0^2$ | $0$ |
| 151,152,181 | $y_0$ | $-3\,y_0y_1+y_0$ | $y_0-3\,y_1+1$ |
| 153,154,180 | $-3\,y_1-8$ | $y_0^2$ | $y_0$ |
| 153,154,180 | $-3\,y_1+4$ | $y_0^2$ | $y_0$ |
| 153,154,180 | $-y_0$ | $-3\,y_0y_1-4\,y_0$ | $y_0-3\,y_1-4$ |
| 153,154,180 | $y_0$ | $3\,y_0y_1-8\,y_0$ | $-y_0-3\,y_1+8$ |
| 153,154,180 | $-3\,y_1-4$ | $-y_0^2$ | $0$ |
| 153,154,180 | $y_0$ | $-3\,y_0y_1+4\,y_0$ | $y_0-3\,y_1+4$ |
| 155,160,166 | $-y_0$ | $y_0^2+3\,y_0y_1$ | $2\,y_0+3\,y_1$ |
| 155,160,166 | $2\,y_0+3\,y_1$ | $-y_0^2$ | $0$ |
| 155,160,166 | $y_0+3\,y_1$ | $y_0^2$ | $-y_0$ |
| 155,160,166 | $2\,y_0+3\,y_1$ | $y_0^2$ | $y_0$ |
| 155,160,166 | $y_0$ | $-y_0^2-3\,y_0y_1$ | $3\,y_1$ |
| 158,159,182,186 188,194 | $2\,y_1-1$ | $y_0^2$ | $y_0$ |
| 158,159,163,165 182,184,185,186 190,192,193,194 | $2\,y_1+1$ | $y_0^2$ | $y_0$ |
| 161,167 | $2\,y_0-3$ | $-y_0^2-6\,y_0y_1-9\,y_1^2$ | $0$ |
| 161,167 | $-2\,y_0-3\,y_1-1$ | $4\,y_0^2+3\,(2\,y_0+1)y_1+4\,y_0+1$ | $4\,y_0+3\,y_1+2$ |
| 161 | $2\,y_0-1$ | $4\,y_0^2+6\,(2\,y_0-1)y_1+9\,y_1^2-4\,y_0+1$ | $-2\,y_0-3\,y_1+1$ |
| 161,167 | $2\,y_0-3$ | $y_0^2+6\,y_0y_1+9\,y_1^2$ | $y_0+3\,y_1$ |
| 161 | $2\,y_0+3\,y_1-1$ | $-4\,y_0^2-3\,(2\,y_0-1)y_1+4\,y_0-1$ | $-3\,y_1$ |
| 167 | $2\,y_0+1$ | $4\,y_0^2+6\,(2\,y_0+1)y_1+9\,y_1^2+4\,y_0+1$ | $-2\,y_0-3\,y_1-1$ |
| 167 | $2\,y_0+3\,y_1+1$ | $-4\,y_0^2-3\,(2\,y_0+1)y_1-4\,y_0-1$ | $-3\,y_1$ |
| 169 | $-6\,y_2+25$ | $y_0^2+y_0y_1+y_1^2$ | $2\,y_0+y_1$ |
| 169 | $-6\,y_2-25$ | $-y_0^2-y_0y_1-y_1^2$ | $0$ |
| 170 | $-6\,y_2-35$ | $y_0^2+y_0y_1+y_1^2$ | $2\,y_0+y_1$ |
| 170 | $-6\,y_2+35$ | $-y_0^2-y_0y_1-y_1^2$ | $0$ |
| 173,176 | $-2\,y_2+1$ | $y_0^2+y_0y_1+y_1^2$ | $2\,y_0+y_1$ |
| 173,176 | $-2\,y_2-1$ | $-y_0^2-y_0y_1-y_1^2$ | $0$ |
| 177,183,191 | $y_1$ | $3\,y_0^2$ | $3\,y_0$ |
| 177,183,191 | $y_1$ | $-3\,y_0^2$ | $0$ |
| 177,183,191 | $y_1$ | $3\,y_0^2$ | $0$ |
| 178 | $-y_0$ | $-6\,y_0y_1-61\,y_0$ | $y_0-6\,y_1-61$ |
| 178 | $-6\,y_1+61$ | $3\,y_0^2$ | $3\,y_0$ |
| 178 | $-6\,y_1-1$ | $-y_0^2$ | $0$ |
| 178 | $-6\,y_1+61$ | $y_0^2$ | $y_0$ |
| 178 | $y_0$ | $6\,y_0y_1-47\,y_0$ | $-y_0-6\,y_1+47$ |
| 178 | $-6\,y_1-139$ | $-3\,y_0^2$ | $0$ |
| 178 | $-6\,y_1-1$ | $-3\,y_0^2$ | $0$ |
| 178 | $-6\,y_1+155$ | $-3\,y_0^2$ | $0$ |
| 178 | $-6\,y_1+109$ | $3\,y_0^2$ | $0$ |
| 178 | $-6\,y_1-155$ | $3\,y_0^2$ | $3\,y_0$ |
| 178 | $-6\,y_1-77$ | $y_0^2$ | $y_0$ |
| 178 | $y_0$ | $-6\,y_0y_1+y_0$ | $y_0-6\,y_1+1$ |
| 179 | $-y_0$ | $-6\,y_0y_1-595\,y_0$ | $y_0-6\,y_1-595$ |
| 179 | $-6\,y_1+595$ | $3\,y_0^2$ | $3\,y_0$ |
| 179 | $-6\,y_1-505$ | $-y_0^2$ | $0$ |
| 179 | $-6\,y_1+595$ | $y_0^2$ | $y_0$ |
| 179 | $y_0$ | $6\,y_0y_1-1085\,y_0$ | $-y_0-6\,y_1+1085$ |
| 179 | $-6\,y_1-1405$ | $-3\,y_0^2$ | $0$ |
| 179 | $-6\,y_1-505$ | $-3\,y_0^2$ | $0$ |
| 179 | $-6\,y_1+1925$ | $-3\,y_0^2$ | $0$ |
| 179 | $-6\,y_1+1345$ | $3\,y_0^2$ | $0$ |
| 179 | $-6\,y_1-1925$ | $3\,y_0^2$ | $3\,y_0$ |
| 179 | $-6\,y_1-1115$ | $y_0^2$ | $y_0$ |
| 179 | $y_0$ | $-6\,y_0y_1+505\,y_0$ | $y_0-6\,y_1+505$ |
| 180 | $-3\,y_1+4$ | $3\,y_0^2$ | $3\,y_0$ |
| 180 | $-3\,y_1-4$ | $-3\,y_0^2$ | $0$ |
| 180 | $-3\,y_1+8$ | $-3\,y_0^2$ | $0$ |
| 180 | $-3\,y_1+4$ | $3\,y_0^2$ | $0$ |
| 180 | $-3\,y_1-8$ | $3\,y_0^2$ | $3\,y_0$ |
| 181 | $-3\,y_1+1$ | $3\,y_0^2$ | $3\,y_0$ |
| 181 | $-3\,y_1-1$ | $-3\,y_0^2$ | $0$ |
| 181 | $-3\,y_1+2$ | $-3\,y_0^2$ | $0$ |

Table 6: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 151–181

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 181 | $-3\,y_1+1$ | $3\,y_0^2$ | $0$ |
| 181 | $-3\,y_1-2$ | $3\,y_0^2$ | $3\,y_0$ |
| 182,184,192 | $-2\,y_1-1$ | $3\,y_0^2$ | $3\,y_0$ |
| 182,184,192 | $-2\,y_1-1$ | $-3\,y_0^2$ | $0$ |
| 182,184 | $-2\,y_1+1$ | $-3\,y_0^2$ | $0$ |
| 182 | $-2\,y_1+1$ | $3\,y_0^2$ | $0$ |
| 184,192 | $2\,y_1+1$ | $3\,y_0^2$ | $0$ |
| 184 | $2\,y_1-1$ | $3\,y_0^2$ | $3\,y_0$ |
| 195,196,197,200<br>202,204,207,209<br>211,215,216,217<br>221,225,229 | $y_0$ | $-y_0^2$ | $0$ |
| 195,196,197,200<br>202,204,207,209<br>211,215,216,217<br>221,225,229 | $y_0$ | $y_0^2$ | $0$ |
| 195,196,197,200<br>202,204,207,209<br>211,215,216,217<br>221,225,229 | $y_0$ | $y_0^2$ | $2\,y_0$ |
| 198,199,201,203<br>205,206,208,218<br>219,220,222,223<br>224,226,227,228 | $-2\,y_0-1$ | $-4\,y_0^2-4\,y_0-1$ | $0$ |
| 198,201,203,208<br>210,214,218,219<br>220,222,223,224<br>226,227,228,230 | $2\,y_0-1$ | $-4\,y_0^2+4\,y_0-1$ | $0$ |
| 198,199,201,203<br>206,208,210,214<br>218,219,220,222<br>223,227,228,230 | $2\,y_0+1$ | $4\,y_0^2+4\,y_0+1$ | $0$ |
| 198,199,201,203<br>205,206,208,218<br>220,223,224,227 | $2\,y_0+1$ | $4\,y_0^2+4\,y_0+1$ | $4\,y_0+2$ |
| 198,199,201,203<br>206,208,210,214<br>218,219,220,222<br>223,224,226,227<br>228,230 | $-2\,y_0+1$ | $4\,y_0^2-4\,y_0+1$ | $0$ |
| 198,199,201,205<br>206,208,210,214<br>218,219,220,222<br>223,224,228,230 | $2\,y_0-1$ | $4\,y_0^2-4\,y_0+1$ | $-4\,y_0+2$ |
| 198,199,206,210<br>226,227,228 | $-2\,y_0+3$ | $-4\,y_0^2+12\,y_0-9$ | $0$ |
| 199,206,210,220<br>226 | $-2\,y_0-3$ | $4\,y_0^2+12\,y_0+9$ | $-4\,y_0-6$ |
| 199,206,214,220<br>227,230 | $-2\,y_0+5$ | $4\,y_0^2-20\,y_0+25$ | $0$ |
| 199,206,210,214<br>219,220,226,227<br>228,230 | $2\,y_0+3$ | $-4\,y_0^2-12\,y_0-9$ | $0$ |
| 199,206 | $2\,y_0-15$ | $4\,y_0^2-60\,y_0+225$ | $-4\,y_0+30$ |
| 210,227,228 | $-2\,y_0+5$ | $-4\,y_0^2+20\,y_0-25$ | $0$ |
| 210 | $-2\,y_0-7$ | $-4\,y_0^2-28\,y_0-49$ | $0$ |
| 210 | $-2\,y_0-13$ | $4\,y_0^2+52\,y_0+169$ | $0$ |
| 210,214,219,220<br>230 | $-2\,y_0+3$ | $4\,y_0^2-12\,y_0+9$ | $0$ |
| 212,213 | $-4\,y_0+3$ | $-16\,y_0^2+24\,y_0-9$ | $0$ |
| 212,213 | $4\,y_0-1$ | $-16\,y_0^2+8\,y_0-1$ | $0$ |
| 212 | $4\,y_0-11$ | $16\,y_0^2-88\,y_0+121$ | $0$ |
| 212 | $4\,y_0+9$ | $16\,y_0^2+72\,y_0+81$ | $8\,y_0+18$ |
| 212,213 | $4\,y_0-3$ | $16\,y_0^2-24\,y_0+9$ | $0$ |
| 212,213 | $4\,y_0+3$ | $-16\,y_0^2-24\,y_0-9$ | $0$ |
| 212 | $-4\,y_0-1$ | $-16\,y_0^2-8\,y_0-1$ | $0$ |
| 212 | $4\,y_0-5$ | $-16\,y_0^2+40\,y_0-25$ | $0$ |
| 212 | $-4\,y_0+1$ | $16\,y_0^2-8\,y_0+1$ | $0$ |
| 212 | $4\,y_0-7$ | $16\,y_0^2-56\,y_0+49$ | $0$ |
| 212 | $-4\,y_0+1$ | $16\,y_0^2-8\,y_0+1$ | $8\,y_0-2$ |

Table 7: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 181–212

| Groups No. | $p_\sigma$ | $q_\sigma$ | $g_\sigma$ |
|---|---|---|---|
| 213 | $4\,y_0+5$ | $16\,y_0^2+40\,y_0+25$ | 0 |
| 213 | $4\,y_0+1$ | $16\,y_0^2+8\,y_0+1$ | $8\,y_0+2$ |
| 213 | $4\,y_0-15$ | $16\,y_0^2-120\,y_0+225$ | 0 |
| 213 | $4\,y_0-9$ | $-16\,y_0^2+72\,y_0-81$ | 0 |
| 213 | $-4\,y_0+9$ | $16\,y_0^2-72\,y_0+81$ | 0 |
| 213 | $4\,y_0-3$ | $16\,y_0^2-24\,y_0+9$ | $-8\,y_0+6$ |
| 214,220,226,230 | $2\,y_0-3$ | $4\,y_0^2-12\,y_0+9$ | $4\,y_0-6$ |
| 214,230 | $2\,y_0-13$ | $4\,y_0^2-52\,y_0+169$ | $-4\,y_0+26$ |
| 214,230 | $-2\,y_0-5$ | $-4\,y_0^2-20\,y_0-25$ | 0 |
| 226,227,228 | $2\,y_0+3$ | $4\,y_0^2+12\,y_0+9$ | 0 |
| 227,228 | $2\,y_0-9$ | $4\,y_0^2-36\,y_0+81$ | 0 |
| 227 | $2\,y_0-5$ | $4\,y_0^2-20\,y_0+25$ | $4\,y_0-10$ |
| 227 | $-2\,y_0-7$ | $4\,y_0^2+28\,y_0+49$ | 0 |

Table 8: The polynomials $p_\sigma$, $q_\sigma$, and $g_\sigma$ for space groups Nos. 213–227

| No. | $f_\sigma$ | Groups No. |
|---|---|---|
| 1 | $y_0y_1y_2$ | 16,47 |
| 2 | $2\,(2\,y_0-1)y_1+2\,(2\,(2\,y_0-1)y_1-2\,y_0+1)y_2-2\,y_0+1$ | 19 |
| 3 | $-2\,(2\,y_0+1)y_1+2\,(2\,(2\,y_0+1)y_1-2\,y_0-1)y_2+2\,y_0+1$ | 19 |
| 4 | $4\,y_0y_1y_2$ | 21,65 |
| 5 | $y_0^3+2\,y_0^2y_1+2\,\big(y_0^2+2\,y_0y_1\big)y_2$ | 22,23,69,71 |
| 6 | $y_0^3+4\,y_0^2y_1+4\,y_0y_1^2+2\,\big(y_0^2+2\,y_0y_1\big)y_2$ | 22,69 |
| 7 | $4\,(2\,y_0-1)y_2^2+4\,y_0^2+2\,(2\,y_0-1)y_1+4\,\big(2\,y_0^2+(2\,y_0-1)y_1+y_0-1\big)y_2-1$ | 24 |
| 8 | $-16\,y_0^3-4\,(2\,y_0-3)y_1^2+12\,y_0^2-12\,\big(2\,y_0^2-3\,y_0\big)y_1-2\,\big(4\,y_0^2+2\,(2\,y_0-3)y_1-9\big)y_2+36\,y_0-27$ | 24 |
| 9 | $-2\,(2\,y_0+1)y_1-2\,(2\,(2\,y_0+1)y_1-2\,y_0-1)y_2+2\,y_0+1$ | 48,61 |
| 10 | $2\,(2\,y_0+1)y_1-2\,(2\,(2\,y_0+1)y_1+2\,y_0+1)y_2+2\,y_0+1$ | 48 |
| 11 | $-12\,(y_0-3)y_1-12\,y_1^2-2\,\big(4\,(y_0-3)y_1+4\,y_1^2-6\,y_0+9\big)y_2+18\,y_0-27$ | 70 |
| 12 | $-8\,y_0^3-4\,(2\,y_0-3)y_1^2+12\,y_0^2+8\,\big(2\,y_0^2-3\,y_0\big)y_1-2\,\big(4\,y_0^2-2\,(2\,y_0-3)y_1-9\big)y_2+18\,y_0-27$ | 70 |
| 13 | $-4\,y_0^2-2\,(2\,y_0+1)y_1-2\,\big(4\,y_0^2+2\,(2\,y_0+1)y_1-1\big)y_2+1$ | 73 |
| 14 | $-4\,(2\,y_0-3)y_1^2+12\,(2\,y_0-3)y_1+2\,(2\,(2\,y_0-3)y_1-6\,y_0+9)y_2-18\,y_0+27$ | 73 |
| 15 | $y_0^3$ | 195,196,197,200<br>202,204,207,209<br>211,215,216,217<br>221,225,229 |
| 16 | $-8\,y_0^3-12\,y_0^2-6\,y_0-1$ | 198,199,201,203<br>205,206,208,210<br>214,218,219,220<br>222,223,224,226<br>228,230 |
| 17 | $-8\,y_0^3+12\,y_0^2-6\,y_0+1$ | 198,199,201,203<br>205,206,208,210<br>214,218,219,220<br>222,223,224,226<br>227,228,230 |
| 18 | $8\,y_0^3+36\,y_0^2+54\,y_0+27$ | 198,199,205,206<br>214,219,220,226<br>227,228,230 |
| 19 | $8\,y_0^3-36\,y_0^2+54\,y_0-27$ | 198,210,219,220<br>227,228 |
| 20 | $-8\,y_0^3+108\,y_0^2-486\,y_0+729$ | 199,206 |
| 21 | $8\,y_0^3-60\,y_0^2+150\,y_0-125$ | 210,220,227 |
| 22 | $8\,y_0^3-84\,y_0^2+294\,y_0-343$ | 210 |
| 23 | $-64\,y_0^3-144\,y_0^2-108\,y_0-27$ | 212,213 |
| 24 | $64\,y_0^3+48\,y_0^2+12\,y_0+1$ | 212,213 |
| 25 | $64\,y_0^3-336\,y_0^2+588\,y_0-343$ | 212 |
| 26 | $-64\,y_0^3-912\,y_0^2-4332\,y_0-6859$ | 212 |
| 27 | $-64\,y_0^3+48\,y_0^2-12\,y_0+1$ | 212,213 |
| 28 | $64\,y_0^3-144\,y_0^2+108\,y_0-27$ | 213 |
| 29 | $-64\,y_0^3+432\,y_0^2-972\,y_0+729$ | 213 |
| 30 | $64\,y_0^3+432\,y_0^2+972\,y_0+729$ | 213 |
| 31 | $-8\,y_0^3+252\,y_0^2-2646\,y_0+9261$ | 214,230 |
| 32 | $8\,y_0^3+108\,y_0^2+486\,y_0+729$ | 214,227,230 |
| 33 | $-8\,y_0^3+132\,y_0^2-726\,y_0+1331$ | 227 |

Table 9: The polynomials $f_\sigma$ for space groups

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