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Weak Cayley Table Groups of Crystallographic Groups

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ABSTRACT

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Let G be a group. A weak Cayley table isomorphism $\varphi : G \to G$ is a bijection satisfying two conditions: (i) φ sends conjugacy classes to conjugacy classes; and (ii) $\varphi(g_1)\varphi(g_2)$ is conjugate to $\varphi(g_1g_2)$ for all $g_1, g_2 \in G$. The set of all such mappings forms a group $\mathcal{W}(G)$ under composition. We study $\mathcal{W}(G)$ for fifty-six of the two hundred nineteen three-dimensional crystallographic groups G as well as some other groups. These fifty-six groups are related to our previous work on wallpaper groups [HP].

Keywords: crystallographic groups, automorphisms, weak Cayley table isomorphisms

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Chapter 1. Introduction

Let G and H be groups. As defined in [JS, Hu], a *weak Cayley table morphism* is a function $\varphi : G \to H$ satisfying two conditions: (i) for $g, g' \in G$, $\varphi(g)\varphi(g')$ is conjugate to $\varphi(gg')$; and (ii) g is conjugate to g' in G if and only if $\varphi(g)$ is conjugate to $\varphi(g')$ in H. A *weak Cayley table isomorphism* is a bijective weak Cayley table morphism. In the situation where φ is bijective and $G = H, \varphi$ is a generalization of an automorphism, and we call these mappings *weak Cayley table maps* or *wcts*. The set of all such mappings $\varphi : G \to G$ forms the *weak Cayley table group* $\mathcal{W}(G) = \mathcal{W}$ under composition and we note that the automorphism group $\mathrm{Aut}(G)$ of G is a subgroup of $\mathcal{W}(G)$. The inverse map $\iota : g \mapsto g^{-1}$ is also an element in $\mathcal{W}$. We define $\mathcal{W}_0 = \langle \mathrm{Aut}(G), \iota \rangle$, and we call the wcts in this subgroup *trivial.* If $\mathcal{W} = \mathcal{W}_0$ we say $\mathcal{W}(G)$ is *trivial.*

Although this will not be relevant to this thesis, we now explain where this idea comes from. If $G = \{g_1 = 1, g_2, \ldots\}$, then the *weak Cayley table* of G is the $|G| \times |G|$ matrix whose ij entry is the conjugacy class of $g_i g_j$. Two finite groups have the same weak Cayley table if and only if they have the same 1- and 2-characters, in the sense of Frobenius [JMS]. Here, for a complex character χ, the corresponding 1-character is $\chi^{(1)} = \chi$, and the 2-character is $\chi^{(2)} : G^2 \to \mathbb{C}, \chi^{(2)}(x, y) = \chi(x)\chi(y) - \chi(xy)$. The group $\mathcal{W}(G)$ is the group of symmetries of the weak Cayley table of G [JMS]. We note that the notion of a k-character only makes sense in the situation where G is finite; however, the weak Cayley table is defined for any group, and $\mathcal{W}(G)$ makes sense for any group.

Given a group G one would like to determine whether or not $\mathcal{W}(G)$ is trivial and to find the *non-trivial* wcts in $\mathcal{W} \setminus \mathcal{W}_0$. Previous research has determined the weak Cayley table groups of various finite and infinite groups. For example, dihedral groups, symmetric groups, most finite irreducible Coxeter groups, most alternating groups, and $\mathrm{PSL}(2, p^n)$ all have trivial weak Cayley table groups [Hu, HN, HN2]. In [HP] we studied the weak Cayley table groups of the seventeen two-dimensional crystallographic groups, also known as *wallpaper* *groups* or *plane groups*. We found that thirteen wallpaper groups have trivial weak Cayley table groups while four have non-trivial weak Cayley table groups. In that paper we were able to generalize one of these results to show that if $G = A \rtimes_\theta \mathcal{C}_p$ (here A is abelian, p is an odd prime, and θ is not trivial) then $\mathcal{W}(G)$ is non-trivial.

In this thesis we study the weak Cayley table groups of some of the three-dimensional crystallographic groups. Elements of an n-dimensional crystallographic group, also known as a *space group*, are isometries that act on Euclidean space $\mathbb{E}^n$. There are 219 three-dimensional space groups, up to isomorphism. As explained in [CFHT], 184 of these space groups consist of isometries that preserve one direction (up to orientation) and consequently, the space group can be given a *fibration*. (See §4.4 for a definition.) If a three-dimensional space group can be fibered, then the action of the space group on the set of fibers, a subspace isomorphic to $\mathbb{E}^2$, gives the action of some wallpaper group on $\mathbb{E}^2$. Thus there is a way to associate any of these 184 space groups to some wallpaper group.

In this thesis we chose to study the fifty-six space groups that correspond to one of the four wallpaper groups that have non-trivial weak Cayley table groups. We found that twenty have trivial weak Cayley table groups while thirty-six of them have non-trivial weak Cayley table groups.

Several of the groups examined here have cyclic quotients. Our study of these cases motivated us to study the general case where a group G contains an abelian normal subgroup A such that G/A is cyclic. We were able to prove that if $2 < |G/A| < \infty$ and if the conjugation action of G/A on A is faithful, then $\mathcal{W}(G)$ will be non-trivial (see Theorem 3.3).

1.1 Properties of weak Cayley table isomorphisms

The following properties of weak Cayley table isomorphisms in $\mathcal{W}(G)$ will be helpful as we determine $\mathcal{W}(G)$. In this section, G, H and K are groups. For $g, g' \in G$ we will write g is conjugate to g' in G as $g \sim_G g'$, or $g \sim g'$ if the context is clear. We will write g^G to denote the conjugacy class of $g \in G$.

Recall that a wct φ by definition satisfies $\varphi(g^G) = \varphi(g)^H$ for all $g \in G$. We will say that φ *preserves conjugacy classes* when we refer to this property of wcts.

Proposition 1.1. *Let $\varphi : G \to H$ be a weak Cayley table isomorphism. Then*

(i) φ maps the identity in G to the identity in H : $\varphi(1_G) = 1_H$.

(ii) φ respects inverses: $\varphi(g^{-1}) = \varphi(g)^{-1}$.

(iii) $\varphi^{-1} : H \to G$ is a weak Cayley table isomorphism.

(iv) For the centers of groups we have: $\varphi(Z(G)) = Z(H)$.

(v) φ maps involutions to involutions: $g^2 = 1$ implies $\varphi(g)^2 = 1$.

(vi) φ maps normal subgroups to normal subgroups: $N \trianglelefteq G$ implies $\varphi(N) \trianglelefteq H$.

(vii) If $N \trianglelefteq G$ and $\varphi(N) = M$, then φ maps cosets of N to cosets of M. In other words, $\varphi(Ng) = \varphi(N)\,\varphi(g)$ for all $g \in G$.

(viii) Let $N \trianglelefteq G$. Then φ induces a map $\bar{\varphi} : G/N \to H/\varphi(N)$ which is also a weak Cayley table isomorphism.

Proof. Proofs of these same results in the case where G and H are finite can also be found in [JMS, p. 398]. (i) Let $\varphi(\alpha) = 1$. Then $\varphi(\alpha \cdot \alpha) \sim 1$. Then $\varphi(\alpha^2) = 1$. Since φ is a bijection this implies $\alpha^2 = \alpha$; thus $\alpha = 1$.
(ii) Here $1 = \varphi(g \cdot g^{-1}) \sim \varphi(g)\varphi(g^{-1})$ implies $\varphi(g^{-1}) = \varphi(g)^{-1}$.
(iii) First we note that since φ preserves conjugacy classes it is clear that φ^{-1} also preserves conjugacy classes. It remains to show that φ^{-1} respects the group operation, up to conjugacy. Let $f, g \in H$. Since φ is bijective, there exists some $f', g' \in G$ such that $f = \varphi(f')$ and $g = \varphi(g')$. Using $\varphi(f')\varphi(g') \sim \varphi(f'g')$, we have

$$\varphi^{-1}(fg) = \varphi^{-1}(\varphi(f')\varphi(g')) \sim \varphi^{-1}(\varphi(f'g')) = f'g' = \varphi^{-1}(f)\varphi^{-1}(g).$$

(iv) For $g \in G$, we have $|g^G| = |\varphi(g^G)| = |\varphi(g)^H|$. The first equality follows from the bijectivity of φ and the second is a consequence of φ preserving conjugacy classes. It follows that $|g^G| = 1$ if and only if $|\varphi(g)^H| = 1$, i.e. $g \in Z(G)$ if and only if $\varphi(g) \in Z(H)$.

(v) Here $1 = g^2$ implies $\varphi(1) = \varphi(g \cdot g) \sim \varphi(g)\varphi(g)$. So $\varphi(g)^2 = 1$.

(vi) Since φ preserves conjugacy classes, (i) implies that φ will map a normal subgroup to a union of conjugacy classes that contains 1. By the definition of a weak Cayley table map this union is closed under the group operation and by (ii) we have inverses, thus it is a normal subgroup.

(vii) Let $x, y \in G$ satisfy $Nx = Ny$ and so $xy^{-1} \in N$. Then $\varphi(xy^{-1}) \in M$ implies $\varphi(x)\varphi(y^{-1}) = \varphi(x)\varphi(y)^{-1} \in M$ and thus $M\varphi(x) = M\varphi(y)$.

$(viii)$ Let $\varphi(N) = M$. Using (vii) we define $\bar{\varphi} : G/N \to H/M$ by $\bar{\varphi} : Ng \mapsto M\varphi(g)$. First we will show that $\bar{\varphi}$ maps conjugacy classes to conjugacy classes. Let $Ng, Nh \in G/N$ and suppose $Ng \sim_{G/N} Nh$. It follows that $g \sim_G hn$ for some $n \in N$. Since φ preserves conjugacy classes, this gives $\varphi(g) \sim_H \varphi(nh) \sim_H \varphi(n)\varphi(h)$. It follows that

$$\varphi(N)\varphi(g) \sim_{H/M} \varphi(N)\varphi(n)\varphi(h) = \varphi(N)\varphi(h).$$

In other words, $\bar{\varphi}(Ng) \sim_{H/M} \bar{\varphi}(Nh)$.

Now we show that that the converse also holds, i.e. that $\bar{\varphi}(Ng) \sim_{H/M} \bar{\varphi}(Nh)$ implies that $Ng \sim_{G/N} Nh$. We assume $\bar{\varphi}(Ng) \sim_{H/M} \bar{\varphi}(Nh)$, in other words, $\varphi(N)\varphi(g) \sim_{H/M} \varphi(N)\varphi(h)$. It follows that for some $n \in N$, $\varphi(g) \sim_H \varphi(n)\varphi(h) \sim_H \varphi(nh)$. Since φ preserves conjugacy classes, this implies $g \sim_G nh$, thus $Ng \sim_{G/N} Nnh = Nh$.

Lastly we show that for $Nx, Ny \in G/N$, $\bar{\varphi}(Nx \cdot Ny) \sim_{H/M} \bar{\varphi}(Nx) \cdot \bar{\varphi}(Ny)$. We have $\varphi(xy) \sim_H \varphi(x)\varphi(y)$ which implies that $\varphi(N)\varphi(xy) \sim_{H/M} \varphi(N)\varphi(x)\varphi(y)$. Therefore,

$$\bar{\varphi}(Nx \cdot Ny) = \bar{\varphi}(Nxy) = \varphi(N)\varphi(xy) \sim_{H/M} \varphi(N)\varphi(x)\varphi(y) = \bar{\varphi}(Nx)\bar{\varphi}(Ny),$$

which shows that $\bar{\varphi}$ is a weak Cayley table map. □

Lemma 1.2. *Let $\varphi_1 : G \to H$, $\varphi_2 : H \to K$ be weak Cayley table morphisms. Then $\varphi_2 \circ \varphi_1 : G \to K$ is also a weak Cayley table morphism.*

Proof. Since φ_1 and φ_2 preserve conjugacy classes, it is clear that $\varphi_1 \circ \varphi_2$ also preserves conjugacy classes. It remains to show that $\varphi_1 \circ \varphi_2$ respects the group operation, up to conjugacy. Let $g, h \in G$. Since $\varphi_2(g \cdot h) \sim \varphi_2(g)\varphi_2(h)$ and φ_1 preserves conjugacy classes, we have

$$(\varphi_1 \circ \varphi_2)(g \cdot h) \sim \varphi_1(\varphi_2(g)\varphi_2(h)).$$

The above is conjugate to $(\varphi_1 \circ \varphi_2)(g) \cdot (\varphi_1 \circ \varphi_2)(h)$ because φ_1 respects the group operation up to conjugacy. □

This result, together with Proposition 1.1 (*iii*), shows that $\mathcal{W}(G)$ is a group.

Lemma 1.3. *The inverse map $\iota : g \mapsto g^{-1}$ is in the center of $\mathcal{W}(G)$.*

Proof. Let $g, h \in G$. It is clear that $g \sim h$ if and only if $g^{-1} \sim h^{-1}$, thus ι preserves conjugacy classes. We also have

$$\iota(gh) = h^{-1}g^{-1} \sim g^{-1}h^{-1} = \iota(g)\iota(h).$$

We conclude that $\iota \in \mathcal{W}(G)$.

The fact that ι commutes with any $\varphi \in \mathcal{W}$ follows from Proposition 1.1 (*ii*): $(\varphi \circ \iota)(g) = \varphi(g^{-1}) = \varphi(g)^{-1} = (\iota \circ \varphi)(g)$. □

An *anti-automorphism* is a bijective map $\alpha : G \to G$ that satisfies $\alpha(gh) = \alpha(h)\alpha(g)$ for all $g, h \in G$. Let α be an anti-automorphism of G and let $\psi = \iota \circ \alpha$. Then for any $g, h \in G$,

$$\psi(gh) = \alpha(gh)^{-1} = (\alpha(h)\alpha(g))^{-1} = \alpha(g)^{-1}\alpha(h)^{-1} = \psi(g)\psi(h).$$

Thus ψ is an automorphism. It follows that any anti-automorphism is the composition of an automorphism with the inverse map. By Lemma 1.2 an anti-automorphism is a wct. This shows that $\mathcal{W}_0(G)$ is the group of all automorphisms and anti-automorphisms of G.

Chapter 2. Preliminary results

2.1 Commutators and commutator subgroups

For $a, b \in G$ we will write $a^b = b^{-1}ab$. Also, we define the commutator $(a, b) = a^{-1}b^{-1}ab = a^{-1}a^b$. For subgroups $H, K \leq G$, we define $[H, K] = \langle (h, k) \,:\, h \in H, k \in K \rangle$.

Throughout this thesis, whenever we have a group G that contains a normal abelian subgroup A then we will let F denote a set of coset representatives for G/A. We will also assume that A is countably generated with generators $x_1, x_2, \cdots$.

In what follows we will frequently use the Witt-Hall identities, which can be found in [MKS, p. 290]. These are

$$(a, b) =(b, a)^{-1}; \tag{2.1}$$

$$(a, b \cdot c) =(a, c) \cdot (a, b) \cdot ((a, b), c) \tag{2.2}$$

$$=(a, c) \cdot (a, b)^c; \tag{2.3}$$

$$(a \cdot b, c) =(a, c) \cdot ((a, c),\, b) \cdot (b, c) \tag{2.4}$$

$$=(a, c)^b \cdot (b, c). \tag{2.5}$$

Definitions For G a group with an abelian normal subgroup $A = \langle x_1, x_2, \cdots \rangle$ we define

$$K = \langle (x_i, h) \,:\, i \in \{1, 2, \cdots\},\, h \in F\} \rangle.$$

We will show later that K does not depend on F. For $g \in G$, we define

$$K_g = \langle (x_i, g) \,:\, i \in \{1, 2, \cdots\} \rangle.$$

We will see that an equivalent definition of K is $K = \{(a, h) \,:\, a \in A, h \in F\}$, and also that an equivalent definition of K_g is $K_g = \{(a, g) \,:\, a \in A\}$. It will frequently be helpful to think of K_g this way. To show that the definitions are equivalent, we will first prove a lemma.

Lemma 2.1. *Let G be a group with an abelian subgroup $A \trianglelefteq G$. For $a, b \in A, g \in G$ we have*

$$(ab, g) = (a, g) \cdot (b, g).$$

It follows that for $k \in \mathbb{Z}$, $(a, g)^k = (a^k, g)$.

Proof. First we note that since A is normal, $(a, g) = a^{-1}a^g \in A$. Since A is abelian, $((a, g), b) = 1$. Then by Eq. (2.4) we have

$$(a \cdot b, g) = (a, g) \cdot ((a, g), b) \cdot (b, g) = (a, g) \cdot (b, g).$$

The second statement can be proven for $k \in \mathbb{N}$ by letting $b = a$ and applying an inductive argument. Putting $b = a^{-1}$ we see that $(a, g)^{-1} = (a^{-1}, g)$ and thus for $k \in \mathbb{Z}$ we have $(a, g)^k = (a^k, g)$. □

We are now ready to prove the equivalence of the two definitions of K_g and K.

Lemma 2.2. *An equivalent definition of K_g is $K_g = \{(a, g) : a \in A\}$. An equivalent definition of K is $K = \{(a, h) : a \in A, h \in F\}$.*

Proof. Since K_g is generated by commutators of the form (x_i, g) where $\langle x_1, x_2, \cdots \rangle = A$, an arbitrary element of K_g is a word in $\{(x_i, g) : i \in \mathbb{N}\}$. By Lemma 2.1, this word can be written as the commutator (a, g) where a is a word in $\{x_i^{\pm 1} : i \in \mathbb{N}\}$. It follows that the two definitions of K_g are equivalent. The same argument shows that the two definitions of K are equivalent. □

Clarification about notation: In Lemma 2.3 below we show that $K_f = K_{af}$ for any $a \in A$. It follows that each K_f subgroup corresponds to a coset $Af \in G/A$. Thus, whenever possible, we may denote each K_g subgroup by K_f where $f \in F$ and $Af = Ag$. However, in general, when we write K_g that does not necessarily imply that $g \in F$.

Lemma 2.3. *Let G be a group with normal abelian subgroup A. If f_1 and f_2 are in the same coset of G/A (i.e. $Af_1 = Af_2$) then for $a \in A$ we have $(a, f_1) = (a, f_2)$. This implies that $K_{f_1} = K_{f_2}$. In other words, K_f does not depend on which coset representative is used. This also shows that $K = [A, G]$.*

Proof. Assume $Af_1 = Af_2$. Then $f_2 = bf_1$ for some $b \in A$. Then by Eq. (2.2), for $a \in A$, (since A is abelian),

$$(a, f_2), = (a, bf_1) = (a, f_1)(a, b)((a, b), f_1) = (a, f_1),$$

and the result follows by Lemma 2.2. □

In Lemmas 2.4 through 2.11 we prove results about commutators and K_f subgroups that will be helpful in various upcoming proofs.

Lemma 2.4. *Let G be a group with normal abelian subgroup A. If G/A is abelian, then for $f, g \in G$ and $a \in A$, $(a, f)^g = (a^g, f)$.*

Proof. Since G/A is abelian, $f^g = bf$ for some $b \in A$. Thus

$$(a, f)^g = (a^g, f^g) = (a^g, bf) = (a^g, f).$$

The last equality follows from Lemma 2.3. □

Lemma 2.5. *Let G be a group with normal abelian subgroup A. For $f \in F$ we have $K_f \leq K \leq A$. Additionally, $K \trianglelefteq G$. If G/A is abelian, then $K_f \trianglelefteq G$.*

Proof. It is clear from the definition of K_f and K that $K_f \leq K$. By Lemma 2.2 any element of K can be written as (a, f) for some $a \in A, f \in F$. Since $A \trianglelefteq G$ the commutator $(a, f) = a^{-1}a^f \in A$, thus $K \leq A$.

Now we show that $K \trianglelefteq G$. An arbitrary element of K is (b, h) for some $b \in A$, and $h \in G$. For $g \in G$, we have $h^g \in A\tilde{h}$ for some $\tilde{h} \in F$. Then by Lemma 2.3,

$$(b, h)^g = (b^g, h^g) = (b^g, \tilde{h}),$$

which is contained in K by Lemma 2.2. Thus any conjugate of an element of K is in K, proving $K \trianglelefteq G$.

To prove the second statement we now assume G/A is abelian. Let $a \in A$ so (a, f) is an arbitrary element of K_f by Lemma 2.2. By Lemma 2.4, a conjugate of a commutator $(a, f)^h$ can be written as (a^h, f) which is also in K_f, thus $K_f \trianglelefteq G$. □

Lemma 2.6. *Let G be a group with normal abelian subgroup A. Let $f \in G$. Any commutator of the form (a, f) with $a \in A$ can be written as (b, f^{-1}) where $b = (a^f)^{-1}$. This implies that $K_f = K_{f^{-1}}$.*

Proof. We have

$$\begin{aligned}
(a, f) =& f^{-1}f(a^{-1}f^{-1}af) \\
=& f^{-1}(fa^{-1}f^{-1}a)f \\
=& (f^{-1}, a)^f \\
=& (f^{-1}, a^f) \\
=& (f^{-1}, b^{-1}) && \text{because } a^f = b^{-1} \\
=& (b^{-1}, f^{-1})^{-1} && \text{by Eq. (2.1)} \\
=& (b, f^{-1}) && \text{by Lemma 2.1.}
\end{aligned}$$

It follows by Lemma 2.2 that $K_f = K_{f^{-1}}$. □

If $H \leq G$ then $C_G(H)$ will denote the centralizer of H in G.

Lemma 2.7. *Let G be a group with normal abelian subgroup A. Assume that G/A is abelian. Let $f, h \in G$ and let $a \in A$. Then*

$$((a, f), h) = ((a, h), f).$$

This implies that $h \in C_G(K_f)$ if and only if $f \in C_G(K_h)$.

Proof. We have

$$\begin{aligned}
((a, f), h) &= (a, f)^{-1}(a, f)^h \\
&= (a^{-1}, f)(a^h, f) && \text{by Lemmas 2.1 and 2.4} \\
&= (a^{-1}a^h, f) && \text{by Lemma 2.1} \\
&= ((a, h), f).
\end{aligned}$$

The second statement can be deduced by using the definition of K_f found in Lemma 2.2 and noting that if $((a, f), h) = 1$ for all $a \in A$ then $((a, h), f) = 1$ for all $a \in A$. The converse follows from a similar argument. ☐

Lemma 2.8. *Let G be a group with normal abelian subgroup A. Assume that G/A is abelian. Let $f \in G$. Let $j, k \in \mathbb{N}$. If $j \mid k$ then $K_{f^j} \geq K_{f^k}$.*

Proof. We proceed by proving these statements:

(i) For $h \in G$, $K_{fh} \leq K_f K_h$.

(ii) For $n \in \mathbb{N}$, $K_{f^n} \leq K_f K_{f^{n-1}}$;

(iii) For $n \in \mathbb{N}$, $K_{f^n} \leq K_f$.

Recall that by Lemma 2.2 an arbitrary element of K_g is (a, g) for $a \in A$. We will use this throughout the proof.

We first prove (i). Since G/A is abelian we have $hf \in Afh$, thus by Lemma 2.3 and Eq. (2.3) we have

$$(a, fh) = (a, hf) = (a, f)(a, h)^f.$$

By Lemma 2.5 K_h is normal thus $(a, h)^f \in K_h$. This shows that (a, fh) (i.e. an arbitrary element of K_{fh}) is a product of a commutator in K_f and a commutator in K_h, proving (i). To prove (ii) we apply (i) with $h = f^{n-1}$. We prove (iii) by induction. When $n = 1$ there is nothing to prove. We assume inductively that it is true for $n = k - 1$, i.e. $K_{f^{k-1}} \leq K_f$. Thus we have $K_{f^k} \leq K_f K_{f^{k-1}} \leq K_f K_f = K_f$ where the first containment follows from (ii) and the second containment follows by our inductive assumption. Thus (iii) is true for $n = k$.

Now to prove Lemma 2.8 we apply (iii), supposing that $n = k/j$ (so $k = nj$) and replacing f in (iii) with f^j. This gives

$$K_{(f^j)^n} \leq K_{f^j} \text{ i.e. } K_{f^{jn}} \leq K_{f^j} \text{ i.e. } K_{f^k} \leq K_{f^j}.$$ ☐

Lemma 2.9. *Let G be a group with normal abelian subgroup A. Assume G/A be abelian. Let $f \in F, f \notin A$, satisfy $f^n \in A$ for some $n \in \mathbb{N}$. (Assume $f^i \notin A$ for all $1 \leq i < n$.) Let $m \in \mathbb{N}$. If $\gcd(m, n) = d$ then $K_{f^m} = K_{f^d}$.*

Proof. We have $\gcd(m, n) = d$, thus (by Bezout's identity) there exists $m' \in \mathbb{Z}$ such that $mm' \equiv d \bmod n$. It follows that $K_{f^{mm'}} = K_{f^d}$. Now we apply Lemma 2.8 twice, (noting that

$d\,|\,m$):

$$K_{f^d} \geq K_{f^m} \geq K_{f^{mm'}} = K_{f^d}.$$

We conclude that $K_{f^d} = K_{f^m}$. □

Lemma 2.10. *Let G be a group with normal abelian subgroup A. Let $g_1, g_2 \in G$ and suppose $g_1, g_2 \in Af$ for some $f \in F$. Then $g_1 g_2^{-1} \in K_f$ if and only if there exists $\alpha \in A$ such that $g_2 = g_1^{\alpha}$.*

Proof. Let $g_1 = af$ and $g_2 = bf$ for some $a, b \in A$. Note that $g_1 g_2^{-1} = (af) \cdot (bf)^{-1} = ab^{-1}$. Then by Lemma 2.6 and Lemma 2.2,

$$\begin{aligned} g_1 g_2^{-1} = ab^{-1} \in K_f &\iff a^{-1}b \in K_{f^{-1}} \\ &\iff \text{there exists } \alpha \in A \text{ such that } a^{-1}b = (\alpha, f^{-1}) \\ &\iff \text{there exists } \alpha \in A \text{ such that} \\ &\qquad bf = a(a^{-1}b)f = a(\alpha^{-1} f \alpha f^{-1})f = af^{\alpha} = (af)^{\alpha}. \end{aligned}$$

□

Lemma 2.11. *Let $G' = [G, G]$ denote the commutator subgroup of a group G and let $\varphi \in \mathcal{W}(G)$. If $c \in G'$ is a commutator, then $\varphi(c)$ is also a commutator. In particular, $\varphi(G') = G'$. In other words, $a \in G'$ if and only if $\varphi(a) \in G'$. Also, $\varphi(K) = K$.*

Proof. Let $c \in G'$; thus $c = g^{-1}g^h$ for some $g, h \in G$. Then since φ preserves conjugacy classes, there exists some $f \in G$ such that

$$\varphi(c) = \varphi(g^{-1} \cdot g^h) \sim \varphi(g^{-1})\varphi(g^h) = \varphi(g)^{-1}\varphi(g)^f = (\varphi(g), f). \tag{2.6}$$

This shows that $\varphi(c)$ is conjugate to a commutator. Since the conjugate of a commutator is a commutator, $\varphi(c)$ is a commutator. To prove the converse, we note that $\varphi^{-1} \in \mathcal{W}(G)$; thus φ^{-1} will also map a commutator to a commutator. Thus if we assume $\varphi(c) \in G'$, then $\varphi^{-1}(\varphi(c)) = c \in G'$. We have shown that $\varphi(G') = G'$.

By Lemma 2.2 we have $K = \langle (a, h) \,:\, a \in A, h \in F \rangle$. Then using Eq. (2.6) with $g = a \in A$ we see that φ sends any generator (a, h) of K to the commutator $(\varphi(a), f)$ for some $f \in G$.

By Lemma (2.3) we may assume $f \in F$. Since φ is a bijection, the set $\{(a,h) : a \in A, h \in F\}$ is mapped to itself. It follows that $\varphi(K) = K$. □

2.2 Maps defined using $\mathcal{C}$ and $\mathcal{F}$

The non-trivial wcts described in Theorems 3.3, 5.1, 5.2, 5.3, 5.4, 5.7, 5.8, and 5.9 may be defined as bijections that conjugate group elements in certain cosets of G/A by a fixed element but fix elements in other cosets. This motivates the following definitions:

Definitions For $\lambda \in G$ and $\mathcal{C} \subseteq G/A$, we define a map $\tau(\lambda, \mathcal{C}) : G \to G$ as follows:

$$\tau(\lambda, \mathcal{C}) : \begin{cases} g \mapsto g^{\lambda} & \text{if } Ag \in \mathcal{C}, \\ g \mapsto g & \text{if } Ag \in \mathcal{F}, \end{cases} \tag{2.7}$$

where $\mathcal{F} = (G/A) \setminus \mathcal{C}$. When $\mathcal{C}$ has been made clear we may simply write τ_λ to denote the function. We define $\mathcal{P} \subseteq G/A$ to be

$$\mathcal{P} = \{Af \in G/A : Af = Af_1 \cdot Af_2 \text{ for some } Af_1 \in \mathcal{C}, Af_2 \in \mathcal{F}\}.$$

Lastly we define $\mathcal{I} = \bigcap_{Af \in \mathcal{P}} K_f$. We note that $\mathcal{P}$ and $\mathcal{I}$ are determined by $\mathcal{C}$, thus we may write $\mathcal{P}(\mathcal{C})$ and $\mathcal{I}(\mathcal{C})$ when we want to distinguish between $\mathcal{P}$ subsets (or $\mathcal{I}$ subgroups) that correspond to different $\mathcal{C}$ subsets.

The non-trivial wcts defined in this thesis are all $\tau(\lambda, \mathcal{C})$ maps such that the cosets of G/A in either $\mathcal{C}$ or $\mathcal{F}$ form a proper subgroup $N \leq G/A$. Note that by composing $\tau(\lambda, \mathcal{C}) \in \mathcal{W}$ with the inner automorphism $I_{\lambda^{-1}} : g \mapsto g^{\lambda^{-1}}$ we effectively interchange $\mathcal{C}$ and $\mathcal{F}$. Thus, it is somewhat of an arbitrary choice whether to put $N = \mathcal{C}$ or $N = \mathcal{F}$. However, for most of the τ_λ maps we define in this thesis we found it advantageous to put $N = \mathcal{F}$, as this made it easier to prove that $\tau_\lambda \in \mathcal{W}$ or to prove that $\tau_\lambda \in \mathcal{W} \setminus \mathcal{W}_0$.

The following theorem gives sufficient conditions for a $\tau(\lambda, \mathcal{C})$ map to be a wct.

Theorem 2.12. *Let G be a group with an abelian normal subgroup A. Suppose $\tau(\lambda, \mathcal{C}) : G \to G$ is a map of the form given in Eq. (2.7) and that $\tau_\lambda(Af) = Af$ for all $Af \in G/A$. (In*

Lemma 2.13 we show that the latter requirement is satisfied if G/A is abelian or if $\lambda \in A$.)

If we have $(\lambda, g^{-1}) \in \mathcal{I}$ for every $g \in G$ such that $Ag \in \mathcal{C}$, then $\tau_\lambda \in \mathcal{W}(G)$.

Proof. Note that since τ_λ acts by conjugation, for any conjugacy class C in G we have $\tau_\lambda(C) = C$. Therefore it is clear that τ_λ preserves conjugacy classes. By assumption $\tau_\lambda(Af) = Af$ for all $Af \in G/A$. This implies that $\tau_\lambda(\mathcal{C}) = \mathcal{C}$. It follows that τ_λ is a bijection. Then to prove that $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$ it remains to show that for any $g_1, g_2 \in G$ we have $\tau_\lambda(g_1)\tau_\lambda(g_2) \sim \tau_\lambda(g_1 g_2)$.

Case 1: $Ag_1, Ag_2 \in \mathcal{C}$: Then

$$\tau_\lambda(g_1)\tau_\lambda(g_2) = g_1^\lambda g_2^\lambda = (g_1 g_2)^\lambda \begin{cases} = \tau_\lambda(g_1 g_2) & \text{if } Ag_1 g_2 \in \mathcal{C} \\ \sim \tau_\lambda(g_1 g_2) & \text{if } Ag_1 g_2 \in \mathcal{F}. \end{cases}$$

Case 2: $Ag_1, Ag_2 \in \mathcal{F}$: Then

$$\tau_\lambda(g_1)\tau_\lambda(g_2) = g_1 g_2 \begin{cases} = \tau_\lambda(g_1 g_2) & \text{if } Ag_1 g_2 \in \mathcal{F} \\ \sim \tau_\lambda(g_1 g_2) & \text{if } Ag_1 g_2 \in \mathcal{C}. \end{cases}$$

Case 3: $Ag_1 \in \mathcal{C}$ and $Ag_2 \in \mathcal{F}$:

We have $\tau_\lambda(g_1)\tau_\lambda(g_2) = g_1^\lambda g_2$ and we wish to show this is conjugate to $g_1 g_2$. (Whether $Ag_1 g_2$ is in $\mathcal{C}$ or $\mathcal{F}$, this suffices.) By hypothesis $\tau_\lambda(Af) = Af$ for all $Af \in G/A$, thus $\tau_\lambda(g_1) \in Ag_1$ so $g_1^\lambda g_2 \in Ag_1 g_2$. Lemma 2.10 asserts that to show $g_1^\lambda g_2 \sim g_1 g_2$ it suffices to show that $(g_1^\lambda g_2)(g_1 g_2)^{-1} \in K_{g_1 g_2}$. We simplify this product:

$$(g_1^\lambda g_2) \cdot (g_1 g_2)^{-1} = g_1^\lambda g_2 \cdot g_2^{-1} g_1^{-1} = g_1^\lambda \cdot (g_2 g_2^{-1}) \cdot g_1^{-1} = \lambda^{-1} g_1 \lambda g_1^{-1} = (\lambda, g_1^{-1}).$$

We are assuming that $(\lambda, g_1^{-1}) \in \mathcal{I}$, which, by the definitions of $\mathcal{I}$ and $\mathcal{P}$, implies (since $Ag_1 g_2 \in \mathcal{P}$) that $(\lambda, g_1^{-1}) \in K_{g_1 g_2}$. Thus by Lemma 2.10 we conclude that $g_1 g_2 \sim g_1^\lambda g_2$ which proves this case.

Case 4: g_1 satisfies $Ag_1 \in \mathcal{F}$ while g_2 satisfies $Ag_2 \in \mathcal{C}$:

Since $\tau(g_1)\tau(g_2) = g_1 g_2^\lambda \sim g_2^\lambda g_1$ this case reduces to Case 3 so we are done. $\square$

Lemma 2.13. *Let G be a group with subgroup $A \trianglelefteq G$. Let $f, \lambda \in G$. If G/A is abelian or if $\lambda \in A$, then $f^\lambda \in Af$.*

Proof. Let $g = f^\lambda$. Then $Ag = Af^{A\lambda}$. If G/A is abelian or if $A\lambda = A$, then $Ag = Af$, i.e. $g = f^\lambda \in Af$. □

When $\mathcal{I} \trianglelefteq G$, the key hypothesis in Theorem 2.12 that $(\lambda, g^{-1}) \in \mathcal{I}$ can be rephrased more simply as $(\lambda, g) \in \mathcal{I}$. (By Lemma 2.5, $\mathcal{I} \trianglelefteq G$ when G/A is abelian.) The equivalence of the two is shown by the following result:

Lemma 2.14. *Let G be a group with an abelian subgroup $A \trianglelefteq G$. Let $g \in G$ and $a \in A$. Let $N \trianglelefteq G$. Then $(a, g) \in N$ if and only if $(a, g^{-1}) \in N$.*

Proof. We have

$$\begin{aligned} (a, g) &= ((a^g)^{-1}, g^{-1}) && \text{by Lemma 2.6} \\ &= (a^g, g^{-1})^{-1} && \text{by Lemma 2.1} \\ &= ((a, g^{-1})^g)^{-1}. \end{aligned}$$

□

Every group G we consider in this thesis has an abelian normal subgroup A such that G/A is abelian. Thus by Theorem 2.12 and Lemma 2.13, to show that $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$, it suffices to show that $(\lambda, g^{-1}) \in \mathcal{I}$ for every $g \in G$ such that $Ag \in \mathcal{C}$. For the groups we are studying, there are infinitely many such group elements g, so it is not practical to check each (λ, g) one by one. The following two corollaries give us sufficient conditions to satisfy $(\lambda, g^{-1}) \in \mathcal{I}$ that can be verified easily. Corollary 2.15 (ii) and Corollary 2.16 (ii) will be applied repeatedly in Ch. 5.

Corollary 2.15. *Let G be a group with an abelian normal subgroup A and let $\lambda \in A$. Let $\tau(\lambda, \mathcal{C}) : G \to G$ where $\tau_\lambda(Af) = Af$ for all $Af \in G/A$.*

(i) If $(\lambda, f^{-1}) \in \mathcal{I}$ for all $f \in F$ such that $Af \in \mathcal{C}$, then $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$. (Rather than verifying that $(\lambda, g^{-1}) \in \mathcal{I}$ for every $g \in Af \in \mathcal{C}$ (as required by Theorem 2.12), it suffices to show $(\lambda, f^{-1}) \in \mathcal{I}$ where $f \in F$ satisfies $Af \in \mathcal{C}$.)

(ii) If $\lambda \in \mathcal{I}$ *and* $\mathcal{I} \trianglelefteq G$ *then* $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$.

Proof. Lemma 2.3 states that when $\lambda \in A$, for any $g \in Af$ we have $(\lambda, g^{-1}) = (\lambda, f^{-1})$. Thus $(\lambda, f^{-1}) \in \mathcal{I}$ implies $(\lambda, g^{-1}) \in \mathcal{I}$ for all $g \in Af \in \mathcal{C}$. Statement (i) then follows from Theorem 2.12.

Now to prove (ii), assume $\lambda \in \mathcal{I}$. Then for any $g \in G$ (since $\mathcal{I}$ is normal by hypothesis) we have $\lambda^{-1}\lambda^{g^{-1}} = (\lambda, g^{-1}) \in \mathcal{I}$ as well. This holds in particular when $g \in Ag \in \mathcal{C}$, as required for Theorem 2.12. Then by that result we have $\tau_\lambda \in \mathcal{W}(G)$. □

Corollary 2.16. *Let* G *be a group with an abelian normal subgroup* A *and let* $\tau(\lambda, \mathcal{C}) : G \to G$ *be a map of the form given in Eq. (2.7). Suppose that* λ *commutes with every element* $f \in F$ *such that* $Af \in \mathcal{C}$.

(i) If $(\lambda, a) \in \mathcal{I}$ *for all* $a \in A$ *then* $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$. *Equivalently,* $(\lambda, x_i) \in \mathcal{I}$ *for all generators* x_i *of* A, $1 \leq i \leq n$, *implies* $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$.

(ii) If we have $K_\lambda \leq \mathcal{I}$ *then* $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$.

Proof. This follows from Theorem 2.12. Note that since λ commutes with every $f \in F$ such that $Af \in \mathcal{C}$, we have $\tau_\lambda(Af) = Af$ for all $Af \in G/A$. Thus to show $\tau_\lambda \in \mathcal{W}(G)$ is suffices to show that $(\lambda, g^{-1}) \in I$ for every $g \in G$ such that $Ag \in \mathcal{C}$.

We first prove (i). Let $f \in F$ satisfiy $Af \in \mathcal{C}$. For $g \in Af$ we can write $g = a^{-1}f$ for some $a \in A$. By hypothesis λ commutes with f, thus $(\lambda, f^{-1}) = 1$. Then using Eq. (2.2) we have

$$\begin{aligned}(\lambda, g^{-1}) =&(\lambda, f^{-1}a)\\ =&(\lambda, a) \cdot (\lambda, f^{-1}) \cdot ((\lambda, f^{-1}), a)\\ =&(\lambda, a).\end{aligned}$$

By assumption $(\lambda, a) \in \mathcal{I}$ for all $a \in A$ therefore $(\lambda, g^{-1}) \in \mathcal{I}$ for all $g \in Af \in \mathcal{C}$. By Theorem 2.12, $\tau_\lambda \in \mathcal{W}(G)$. The second statement in (i) follows from Lemma 2.1.

To prove (ii) we will show that $(\lambda, a) \in \mathcal{I}$ for $a \in A$ and then our result follows from (i). Recall $K_\lambda = \langle (a, \lambda) \ : \ a \in A \rangle$ by Lemma 2.2, thus an arbitrary element of K_λ can be written as (a, λ) for $a \in A$. We are assuming $K_\lambda \leq \mathcal{I}$ thus we have (a, λ) and its inverse (λ, a) contained in $\mathcal{I}$, so we are done. □

Chapter 3. Generally applicable results

In this chapter we include results that may be applied to groups that are not necessarily crystallographic.

3.1 Sufficient conditions for a WCT to be non-trivial

Theorem 3.1. *Let G be a group with an abelian normal subgroup A. Assume that the conjugation action of G/A on A defined by $a \cdot (Ag) = a^g$ is faithful. Let $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G)$ be a wct of the form given in Eq. (2.7). Also assume that $\mathcal{F}$ and $\mathcal{C}$ are not empty.*

(i) If $\lambda \notin A$ then $\tau(\lambda, \mathcal{C})$ is not an automorphism, i.e. $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G) \setminus \mathrm{Aut}(G)$.

(ii) If $|G/A| \geq 3$ then $\tau(\lambda, \mathcal{C})$ is not an anti-automorphism, i.e. either $\tau(\lambda, \mathcal{C}) \in \mathrm{Aut}(G)$ or $\tau(\lambda, \mathcal{C}) \in \mathcal{W}(G) \setminus \mathcal{W}_0(G)$.

Proof. We prove (i) by contradiction. Suppose that τ_λ is an automorphism, and let $a \in A$ satisfy $(a, \lambda) \neq 1$. (Since the conjugation action of G/A is faithful and $\lambda \notin A$ we know such an a exists.) Let $\tau_\lambda = \tau(\lambda, \mathcal{C})$. We consider two cases:

Case 1: $A \in \mathcal{F}$: Then for $f \in Af \in \mathcal{C}$ we have

$$af^\lambda = \tau_\lambda(a)\tau_\lambda(f) = \tau_\lambda(a \cdot f) = (af)^\lambda = a^\lambda f^\lambda.$$

Case 2: $A \in \mathcal{C}$: Then for $f \in Af \in \mathcal{F}$ we have

$$a^\lambda f = \tau_\lambda(a)\tau_\lambda(f) = \tau_\lambda(a \cdot f) = af.$$

In either case we arrive at $a = a^\lambda$, contradicting $(a, \lambda) \neq 1$. We conclude that τ_λ is not an automorphism, proving (i).

To prove (ii) we assume that $|G/A| \geq 3$ thus (since $\mathcal{C}$ and $\mathcal{F}$ each contain at least one coset) $\mathcal{C}$ or $\mathcal{F}$ contains at least two cosets. We consider two cases with $A \in \mathcal{F}$ and two cases with $A \in \mathcal{C}$. In all four cases we assume by way of contradiction that $\tau(\lambda, \mathcal{C})$ is an anti-automorphism and use the fact that the action of G/A on A is faithful (i.e. $a^f = a$ for all $a \in A$ implies $f \in A$) to arrive at a contradiction.

Case 1: $\mathcal{F} = \{A\}$: Let $a \in A$ and let $f \in G$ satisfy $Af \in \mathcal{C}$. Note $Af^{-1} \in \mathcal{C}$. (We do not assume Af and Af^{-1} are distinct.) Since we assume τ_λ is an anti-automorphism. Then for $a \in A$,

$$a = \tau_\lambda(a) = \tau_\lambda(af \cdot f^{-1}) = \tau_\lambda(f^{-1})\tau_\lambda(af) = (f^{-1})^\lambda (af)^\lambda = (f^{-1}af)^\lambda = a^{f\lambda}.$$

This implies that $f\lambda$ commutes with a for all $a \in A$. Since the action of G/A is faithful we conclude $f\lambda \in A$, i.e. $\lambda \in Af^{-1}$. This must hold for all $Af \in \mathcal{C}$, which is a contradiction since $|\mathcal{C}| \geq 2$ in this case.

Case 2: $A \in \mathcal{F}$ and $|\mathcal{F}| \geq 2$: Let $g \in G$ satisfy $g \notin A, Ag \in \mathcal{F}$. Let $a \in A$. Assuming that τ_λ is an anti-automorphism, we have

$$ag = \tau_\lambda(a \cdot g) = \tau_\lambda(g)\tau_\lambda(a) = g \cdot a.$$

This shows that g commutes with any $a \in A$, which by the faithfulness of the action of G/A on A, indicates $g \in A$, a contradiction.

Case 3: $\mathcal{C} = \{A\}$: Let $a \in A$ and let $h \in G$ satisfy $Ah \in \mathcal{F}$. Note $Ah^{-1} \in \mathcal{F}$. Again we assume τ_λ is an anti-automorphism, and so we have

$$a^\lambda = \tau_\lambda(a) = \tau_\lambda(ah \cdot h^{-1}) = \tau_\lambda(h^{-1})\tau_\lambda(ah) = h^{-1} \cdot ah = a^h.$$

We have $a^\lambda = a^h$ for arbitrary $a \in A$. The faithful action of G/A tells us that $A\lambda = Ah$ so $\lambda \in Ah$. This must be true for all $Ah \in \mathcal{F}$, which is a contradiction since we have $|\mathcal{F}| \geq 2$ in this case.

Case 4: $A \in \mathcal{C}$ and $|\mathcal{C}| \geq 2$: Let $a \in A$. Let $f \in G, f \notin A$ satisfy $Af \in \mathcal{C}$. Assuming that τ_λ is an anti-automorphism gives

$$(af)^\lambda = \tau_\lambda(a \cdot f) = \tau_\lambda(f)\tau_\lambda(a) = f^\lambda a^\lambda = (fa)^\lambda.$$

This shows that f commutes with any $a \in A$ thus we must have $f \in A$, a contradiction. □

Theorem 3.2. *Let N be a normal subgroup in a group G. Assume that $\tau \in \mathcal{W}(G)$ satisfies $\tau(N) = N$ and suppose it induces the map $\overline{\tau} : G/N \to G/N$. If $\overline{\tau}$ is a non-trivial wct then τ is also a non-trivial wct.*

Proof. We prove the contrapositive: If τ is a trivial wct then $\overline{\tau}$ is also a trivial wct. We consider two cases: either τ is an automorphism or τ is an anti-automorphism.

First we suppose that $\tau \in \operatorname{Aut}(G)$, i.e. for $g_1, g_2 \in G$ we have $\tau(g_1 g_2) = \tau(g_1)\tau(g_2)$. It follows that

$$\overline{\tau}(g_1 N \cdot g_2 N) = \overline{\tau}(g_1 g_2 N) = \overline{\tau}(g_1 N)\overline{\tau}(g_2 N),$$

thus $\overline{\tau}$ is an automorphism.

The second case follows from a similar argument. If τ is an anti-automorphism then for $g_1, g_2 \in G$ we have $\tau(g_1 g_2) = \tau(g_2)\tau(g_1)$. In this case,

$$\overline{\tau}(g_1 N \cdot g_2 N) = \overline{\tau}(g_1 g_2 N) = \overline{\tau}(g_2 N)\overline{\tau}(g_1 N),$$

thus $\overline{\tau}$ is an anti-automorphism. In either case, $\overline{\tau}$ is a trivial wct. □

3.2 Groups with cyclic quotients

Theorem 3.3. *Let G be a group with an abelian normal subgroup A such that $G/A \cong \mathcal{C}_n$ where $2 < n \in \mathbb{N}$. Assume that the conjugation action of G/A on A defined by $a \cdot (Ag) = a^g$ is faithful. Then $\mathcal{W}(G) \neq \mathcal{W}_0(G)$.*

Proof. Suppose that $G/A = \langle A\rho \rangle$ where $\rho \in G$ satisfies $\rho^n \in A$. Without loss, we put $F = \{\rho^j \,:\, 0 < j \leq n\}$. Accordingly we will write $G/A = \{A\rho^j \,:\, 0 < j \leq n\}$.

Let q be a prime divisor of n and let $m \in \mathbb{N}$ satisfy $q^m \mid n$ and $q^{m+1} \nmid n$. Let $c = n/q^m$ (thus c is relatively prime to q and $n = cq^m$). Fix $1 \leq k \leq m$. Note that there exists an index q^k subgroup $\langle A\rho^{q^k} \rangle \leq G/A$. Let $N = n/q^{m-k+1} = cq^{k-1}$. Let $\mathcal{F} = \langle A\rho^{q^k} \rangle$ and let $\mathcal{C} = (G/A) \setminus \mathcal{F}$. We will show that $\tau(\rho^N, \mathcal{C}) \in \mathcal{W}(G) \setminus \mathcal{W}_0(G)$. To prove $\tau(\rho^N, \mathcal{C}) \in \mathcal{W}(G)$ we will use Corollary 2.16 (*ii*). It is clear that ρ^N commutes with every element of F. By the corollary it suffices to show that $K_{\rho^N} \leq \mathcal{I}$.

Since $\mathcal{F}$ is a subgroup of G/A, we have $\mathcal{P}(\mathcal{C}) = \mathcal{C}$ thus

$$\mathcal{I} = \bigcap_{Af \in \mathcal{C}} K_f.$$

Note that $\mathcal{F} = \{A\rho^j \in G/A : q^k \mid j\}$. Therefore its complement

$$\begin{aligned}
\mathcal{C} &= \{A\rho^j \in G/A : q^k \nmid j\} \\
&= \{A\rho^j \in G/A : \gcd(j, q^k) \in \{1, q, q^2, \dots, q^{k-1}\}\} && \text{since } q \text{ is prime} \\
&= \{A\rho^j \in G/A : \gcd(j, q^m) \in \{1, q, q^2, \dots, q^{k-1}\}\} && \text{since } k \leq m \\
&= \{A\rho^j \in G/A : \gcd(j, q^m) \mid q^{k-1}\} \\
&= \{A\rho^j \in G/A : \gcd(j, n) \mid cq^{k-1}\} && \text{since } n = cq^m \\
&= \{A\rho^j \in G/A : \gcd(j, n) \mid N\} && \text{since } N = cq^{k-1} \\
&= \{A\rho^j \in G/A : K_{\rho^{\gcd(j,n)}} \geq K_{\rho^N}\} && \text{by Lemma 2.8} \\
&= \{A\rho^j \in G/A : K_{\rho^j} \geq K_{\rho^N}\} && \text{by Lemma 2.9.}
\end{aligned}$$

This shows that K_{ρ^N} is contained in K_{ρ^j} for all $A\rho^j \in \mathcal{P}$, thus $K_{\rho^N} \leq \mathcal{I}$ as desired. By Corollary 2.16 (*ii*), τ_{ρ^N} is a wct. By Theorem 3.1 this map is a non-trivial wct. □

The next result uses notation for crystallographic groups that will be explained in §4.2.

Corollary 3.4. *The following seventeen space groups have non-trivial wct groups:* $G_{143}, G_{144}, G_{146}, G_{75}, G_{76}, G_{77}, G_{79}, G_{80}, G_{81}, G_{82}, G_{147}, G_{148}, G_{168}, G_{169}, G_{171}, G_{173},$ *and* G_{174}.

Proof. Groups G_{143}, G_{144}, and G_{146} satisfy $G/A \cong \mathcal{C}_3$.

Groups $G_{75}, G_{76}, G_{77}, G_{79}, G_{80}, G_{81}$, and G_{82} satisfy $G/A \cong \mathcal{C}_4$.

Groups $G_{147}, G_{148}, G_{168}, G_{169}, G_{171}, G_{173}$, and G_{174} satisfy $G/A \cong \mathcal{C}_6$.

The result follows from Theorem 3.3. □

Chapter 4. Three-dimensional space groups

A *lattice* in n-dimensional Euclidean space $\mathbb{E}^n$ is a subgroup $\mathfrak{L}$ of $\mathbb{E}^n$ isomorphic to $\mathbb{Z}^n$ [E, p. 25]. The set of translation symmetries of $\mathfrak{L}$ is a group (under composition) that is isomorphic to $\mathbb{Z}^n$. We will denote this group as A. An n-dimensional *crystallographic point group* P is a finite group of symmetries of $\mathfrak{L}$ that fix one point in $\mathbb{E}^n$ [E, p. 90]. An n-dimensional *crystallographic group*, or *space group* G is an extension of A by the point group P [Ja, p.127], [E, p. 155]. In other words, we have the short exact sequence

$$1 \longrightarrow A \longrightarrow G \longrightarrow P \longrightarrow 1.$$

Thus, P is isomorphic to G/A and A has finite index in G [E, p. 154]. Consequently, a space group element $g \in G$ acts on $\mathbf{v} \in \mathbb{E}^n$ in a manner that such that $g(\mathbf{v}) = p(\mathbf{v}) + \mathbf{t}$ for some $p \in P$ and some $\mathbf{t} \in \mathbb{E}^n$. [Ja, p. 108], [E, p. 153].

The symmetries in a crystallographic point group of a three-dimensional space group may include inversions, rotations, improper rotations, and reflections [I], [E], [Ja]. Inversions and reflections in a crystallographic point group have order 2. The *crystallographic restriction* states that for $n \in \{2, 3\}$, the symmetries of a lattice in $\mathbb{E}^n$ must have order $1, 2, 3, 4$, or 6 [L]. A consequence of this restriction, together with the fact that only seven distinct lattice structures exist that tile $\mathbb{E}^3$, is that there exist 219 three-dimensional space groups [Ja, p. 119]. The International Union of Crystallography (IUC) has assigned each three-dimensional space group a number from 1 to 230 [I]. (There are 11 isomorphic pairs that are numbered separately.)

4.1 Space group elements

There are seven types of elements in three-dimensional space groups. These are: translations, reflections, glide reflections, rotations, screw rotations, inversions, and improper rotations (also known as rotoinversions) [E], [I]. We may think of these group elements as symmetries of an arrangement of atoms in a crystal in $\mathbb{E}^3$. They are also *isometries* of $\mathbb{E}^3$, meaning they are bijections that preserve distances.

A *translation* is an orientation-preserving isometry that maps a vector $\mathbf{v}$ to $\mathbf{v} + \mathbf{a}$ for some fixed $\mathbf{a} \in \mathfrak{L}$. It is easy to see that any two translations commute, and it is also true that any conjugate of a translation is a translation. Thus the set of translations is a normal abelian subgroup of the crystallographic group [E, p. 153]. We will denote the translation subgroup A because it is abelian. For a three-dimensional space group, $A \cong \mathbb{Z}^3$ and there is a standard choice of standard generators which we denote as x, y, and z. Note that each non-trivial translation in a crystallographic group has infinite order. There is a one-to-one correspondence between the elements in A and the points on the lattice $\mathfrak{L}$, and this will be useful in the proofs of Theorems 6.1 and 6.21.

A *reflection* is an order 2, orientation-reversing isometry. Let s be a reflection in $\mathbb{E}^3$, thus it is a reflection across a plane $\mathcal{P}(s)$, the *mirror plane* of s. Suppose that $\mathcal{P}(s)$ is a plane that contains the origin and let $\mathbf{u}_{\mathcal{P}(s)} = \mathbf{u}$ be a unit normal vector to $\mathcal{P}(s)$. Then for $\mathbf{v} \in \mathbb{E}^3$, s maps $\mathbf{v}$ to the vector $\mathbf{v} - 2(\mathbf{v} \cdot \mathbf{u})\mathbf{u}$. Note that for any vector $\mathbf{w} \in \mathcal{P}(s)$, $\mathbf{w} \cdot \mathbf{u} = 0$ so $s(\mathbf{w}) = \mathbf{w}$. Thus s fixes every vector in its mirror plane, $\mathcal{P}(s)$.

A *glide reflection* γ reflects across a plane $\mathcal{P}(\gamma)$ and then translates in a direction parallel to some vector in $\mathcal{P}(\gamma)$. A glide reflection fixes $\mathcal{P}(\gamma)$ but not the vectors in $\mathcal{P}(\gamma)$. A glide reflection is orientation-reversing. The distance of the translation is half of a unit vector in $\mathfrak{L}$, or some multiple of that distance. The square of a glide reflection is a non-trivial translation. Hence, glide reflections have infinite order. If a reflection s commutes with a translation x then their product xs is one example of a glide reflection [Ja, p. 109-10].

In a three-dimensional space group, a *rotation* ρ is a finite order, orientation-preserving isometry that fixes every point on a line in $\mathbb{E}^3$. This line is the *axis of rotation* and if $\rho \neq \mathrm{Id}$ then this axis is unique. Suppose ρ is rotation about a line ℓ that contains the origin, with *turning angle* θ. (If $|\rho| = m$ then $\theta = 2\pi k/m$ where $\gcd(k, m) = 1$.) Then $\rho(\mathbf{v}) = \mathbf{w}$ implies that $|\mathbf{v}| = |\mathbf{w}|$ and also that the distance from $\mathbf{v}$ to the line ℓ is equal to the distance from

$\mathbf{w}$ to ℓ. By the crystallographic restriction, ρ must have order 1, 2, 3, 4, or 6.

A *screw rotation* r is a rotation about an axis ℓ together with translation in the direction of ℓ. Thus it fixes the line ℓ but it does not fix the vectors in ℓ. Like translations and rotations, a screw rotation is orientation-preserving. If θ is the turning angle of a screw rotation r in $\mathbb{E}^3$, then by the crystallographic restriction, $\theta \in \{\pi/3, \pi/2, 2\pi/3, \pi, 2\pi\}$ and $r^{2\pi/\theta}$ is a nontrivial translation in A in the direction of ℓ, [Ja, p. 109-10]. Hence, screw rotations have infinite order. If a rotation ρ commutes with a translation x then their product $x\rho$ is one example of a screw rotation.

An *inversion* through a point $\mathbf{p}$ is an order 2, orientation-reversing isometry that maps a vector $\mathbf{v}$ to $2\mathbf{p} - \mathbf{v}$. It follows that $\mathbf{p}$ is the only point fixed by the inversion. Inversions are also known as *point inversions* or *point reflections*. Inversions that fix the origin are known as *central inversions* [Ja, p. 71].

Lastly we have *improper rotations*, which are also referred to as *rotoreflections* or *rotoinversions*. The latter two designations are indicative of the fact that there are two ways to think of this symmetry element. The first is to consider it a rotation with turning angle θ through an axis ℓ, followed by a reflection across a plane $\mathcal{P}$ perpendicular to ℓ. The second is to consider it a rotation with turning angle $\theta \pm \pi$ through an axis ℓ, followed by an inversion through the point where ℓ intersects $\mathcal{P}$. By the crystallographic restriction, $\theta \in \{\pi/3, \pi/2, \pi\}$, however when $\theta = \pi$ then this symmetry could be regarded as a point inversion. Thus an improper rotation that is not an inversion will have order 4 or order 6 [Ja, p. 70].

We prove a lemma about the cardinality of conjugacy classes in a crystallographic group.

Lemma 4.1. *Let G be a crystallographic group with translation subgroup A.*

(i) If $a \in A$ then $|a^G| \leq |G/A|$.

(ii) If $h \in G \setminus A$ then $|h^G| = \infty$.

Proof. Recall $A \trianglelefteq G$. To prove (i) we note that every $g \in G$ can be written $g = bf$ for some $b \in A, f \in F$. Therefore,

$$a^G = \{a^g : g \in G\} = \{a^{bf} : b \in A, f \in F\} = \{a^f : f \in F\}.$$

Since there are at most $|G/A|$ elements in F, we have $|a^G| \leq |G/A|$.

To prove (ii) we note that the conjugation action of G/A on elements of A is faithful. Thus for fixed $h \in G$ there exists some $b \in A$ (depending on h) such that $(h, b) \neq 1$. Note that for $k \in \mathbb{Z}$, $h^{b^k} = hh^{-1}b^{-k}hb^k = h(h, b^k)$. Thus

$$h^G = \{h^g : g \in G\} \supseteq \{h^{b^k} : k \in \mathbb{Z}\} = \{h(h, b^k) : k \in \mathbb{Z}\} = \{h(h, b)^k : k \in \mathbb{Z}\},$$

where the last equality follows from Lemma 2.1. Since $1 \neq (h, b) \in A$ and therefore has infinite order, we see that h^G contains an infinite number of elements in the Ah coset. □

4.2 Naming conventions

There are at least ten different naming systems or naming conventions commonly used to identify space groups and their point groups. In our previous work [HP] we used Hermann-Mauguin notation to represent the seventeen wallpaper groups. Here we will continue to use Hermann-Mauguin notation when referring to a wallpaper group and we will also use it when identifying the crystallographic point group of a space group. However, when referring to a three-dimensional space group we will identify it by the number assigned to it by The International Union of Crystallography. (Recall that IUC has assigned each three-dimensional space group a number from 1 to 230.) We will write the group represented by IUC number n as "G_n."

4.3 The four wallpaper groups

In [HP] we find that the wallpaper groups that have non-trivial wct groups are **p3, p4, p6,** and **p2mm**. In this section we will briefly describe these four groups. A wallpaper group is a 2-dimensional crystallographic group. We think of a wallpaper pattern corresponding to a wallpaper group G as a subset of $\mathbb{E}^2$. The action of the group elements on $\mathbb{E}^2$ leaves the pattern unchanged. The translation subgroup $A = \langle x, y \rangle$ is a finite index normal subgroup $A \cong \mathbb{Z}^2$. We think of x as horizontal translation (to the right) and y as either vertical translation upwards for groups **p4** or **p2mm** or translation at an angle of $\pi/3$ from the horizontal for groups **p3** and **p6**. The other generators of G will be denoted ρ (for a rotation) and σ (for a reflection).

Each of these four groups are a semi-direct products, $G = A \rtimes_\theta P$ where P is the corresponding crystallographic point group. For **p3**, the point group contains only order 3 rotations and is isomorphic to $\mathcal{C}_3$. For **p4**, the point group contains only two order 4 rotations and one order 2 rotation. It is isomorphic to $\mathcal{C}_4$. Similarly, **p6** has point group isomorphic to $\mathcal{C}_6$ and contains rotations of order $6, 3$, and 2. The point group for **p2mm** contains two reflections and their product, an order 2 rotation. It is isomorphic to $\mathcal{C}_2^2$.

The group presentations we used as we studied these groups are:

$$\mathbf{p3} : \langle x, y, \rho \,|\, (x, y), x^\rho = x^{-1}y, y^\rho = x^{-1}, \rho^3 \rangle;$$

$$\mathbf{p4} : \langle x, y, \rho \,|\, (x, y), x^\rho = y, y^\rho = x^{-1}, \rho^4 \rangle;$$

$$\mathbf{p6} : \langle x, y, \rho \,|\, (x, y), x^\rho = y, y^\rho = x^{-1}y, \rho^6 \rangle;$$

$$\mathbf{p2mm} : \langle x, y, \rho, \sigma \,|\, (x, y), \rho^2, \sigma^2, (\rho, \sigma), x^\rho = x^{-1}, y^\rho = y^{-1}, x^\sigma = x, y^\sigma = y^{-1} \rangle.$$

4.4 The fifty-six groups

If G is a group that acts on $\mathbb{E}^n$, then a *fibration of* G is determined by a decomposition of $\mathbb{E}^n$ as a direct product: $\mathbb{E}^n = \mathbb{E}^{n-1} \times \mathbb{E}^1$ such that for all $x \in \mathbb{E}^{n-1}, g \in G$, there exists an $x' \in \mathbb{E}^{n-1}$ such that $g(\{x\} \times \mathbb{E}^1) = \{x'\} \times \mathbb{E}^1$. In the case where $n = 3$, the action of G on the subspace $\mathbb{E}^2$ corresponds to the action of some wallpaper group on $\mathbb{E}^2$. In this situation, [CFHT] say that the space group G *can be obtained as a fibration over the corresponding wallpaper group.*

In [CFHT] Conway et al. show which three-dimensional space groups may be obtained as a fibration over some wallpaper group, i.e. a two-dimensional crystallographic group or *plane group*. For each plane group they list all fibrations that exist over it and the space group that corresponds to each fibration. Accordingly, we focus our attention on the fifty-six space groups that may be obtained as a fibration over one of these four wallpaper groups, i.e. the wallpaper groups described in the previous section. These fifty-six groups are listed in Tables 4.1, 4.2, 4.3, 4.4, and 4.5.

4.5 Twelve crystallographic point groups

This section has been taken from Table 10.1.2 which begins on page 752 of [I]. It will be convenient to partition the fifty-six space groups according to their crystallographic point group. There exist thirty-two crystallographic point groups in $\mathbb{E}^3$ but only twelve of those will be of interest to us in this thesis. These twelve groups are (using Hermann-Mauguin notation):

$$\mathbf{\tfrac{2}{m}},\ \mathbf{222},\ \mathbf{mm2},\ \mathbf{\tfrac{2}{m}\tfrac{2}{m}\tfrac{2}{m}},\ \mathbf{4},\ \mathbf{\overline{4}},\ \mathbf{\tfrac{4}{m}},\ \mathbf{3},\ \mathbf{\overline{3}},\ \mathbf{6},\ \mathbf{\overline{6}},\ \text{and}\ \mathbf{\tfrac{6}{m}}.$$

Here we will give a description of the non-identity elements that are contained in each of these point groups.

The point groups $\mathbf{\frac{2}{m}}$, **222**, and **mm2** are isomorphic to $\mathcal{C}_2^2$. The point group $\mathbf{\frac{2}{m}}$ contains a rotation, a reflection, and an inversion. The point group **222** contains three rotations. The point group **mm2** contains one rotation and two reflections. The point group $\mathbf{\frac{2}{m}\frac{2}{m}\frac{2}{m}}$ is isomorphic to $\mathcal{C}_2^3$. This point group contains one inversion, three rotations, and three reflections. These four point groups correspond to space groups that may be obtained from the wallpaper group **p2mm**.

The next three point groups listed, $\mathbf{4}, \mathbf{\overline{4}}$, and $\mathbf{\frac{4}{m}}$ correspond to space groups that may be obtained from the wallpaper group **p4**. They are isomorphic to $\mathcal{C}_4, \mathcal{C}_4$, and $\mathcal{C}_4 \times \mathcal{C}_2$, respectively. The point group **4** contains three rotations. The point group $\mathbf{\overline{4}}$ contains two improper rotations as well as one rotation. The point group $\frac{\mathbf{4}}{\mathbf{m}}$ contains three rotations, two improper rotations, one reflection and one inversion.

Point groups **3** and $\overline{\mathbf{6}}$ correspond to space groups that may be obtained from **p3**. They are isomorphic to $\mathcal{C}_3$ and $\mathcal{C}_6$, respectively. The point group **3** contains two rotations. The point group $\overline{\mathbf{6}}$ consists of two rotations, two improper rotations, and one reflection.

The point groups $\overline{\mathbf{3}}$, **6**, and $\frac{\mathbf{6}}{\mathbf{m}}$ correspond to space groups that may be obtained from **p6**. The first two are isomorphic to $\mathcal{C}_6$. The point group $\overline{\mathbf{3}}$ consists of two improper rotations, two rotations, and one inversion. The point group **6** contains five rotations. Lastly we have the point group $\frac{\mathbf{6}}{\mathbf{m}}$ which is isomorphic to $\mathcal{C}_6 \times \mathcal{C}_2$. This point group contains five rotations, four improper rotations, one reflection, and one inversion.

4.6 Choosing generators for group presentations

From [SHC, SCC] we have irreducible representations for each of the 219 three-dimensional space groups. These are 4×4 orthogonal matrices over $\mathbb{Q}$. For each space group, [SHC] gives a sequence of matrices that generates a group isomorphic to that space group. Using Magma, [BCP] we use these matrices to find presentations for the fifty-six space groups of interest to us. For twenty-nine of the fifty-six groups we examined, the matrices we use to define group generators for the presentations are simply the set of matrices given in the file. (Such groups will not be mentioned in the discussion below.) However for twenty-seven space groups there are advantages to using other generators, which will be explained here.

We denote the ith matrix in the set corresponding to a space group as M_i.

For Groups 75, 76, and 77 we define: $\rho = M_2;\ x = M_3;\ y = M_4;\ z = M_5$.

For Groups 79 and 80 we define: $\rho = M_2;\ x = M_3;\ y = M_3^{-1}M_4;\ z = M_5$.

For Group 81 we define: $\rho = M_2^{-1};\ x = M_3;\ y = M_4;\ z = M_5$.

For Group 82 we define: $\rho = M_2;\ x = M_3;\ y = M_3M_4^{-1};\ z = M_5$.

For Groups 83, 84, 85, and 86 we define: $\rho = M_2;\ t = M_3;\ x = M_4;\ y = M_5;\ z = M_6$.

For Groups 87 and 88 we define: $\rho = M_2;\ t = M_3;\ x = M_4;\ y = M_4^{-1}M_5;\ z = M_6$.

For Groups 147, 168, 169, and 173, define: $\rho = M_1^{-1}M_2;\ x = M_3;\ y = M_3M_4;\ z = M_5$.

For Group 148 we define: $\rho = M_1^{-1}M_2;\ x = M_3;\ y = M_3^{-1}M_4;\ z = M_5$.

For Group 171 we define: $\rho = M_1^{-1}M_2M_5;\ x = M_3;\ y = M_3M_4;\ z = M_5$.

For Groups 175 and 176, define: $\rho = M_1^{-1}M_2;\ t = M_3;\ x = M_4;\ y = M_4M_5;\ z = M_6$.

For Groups 143 and 144 we define: $\rho = M_1;\ x = M_2;\ y = M_2M_3;\ z = M_4$.

For Group 146 we define: $\rho = M_1;\ x = M_2;\ y = M_2^{-1}M_3;\ z = M_4$.

For Group 174 we define: $\rho = M_1;\ s = M_2;\ x = M_3;\ y = M_3M_4;\ z = M_5$.

In the first twenty-one groups listed above (including Groups 175 and 176), we use the single generator ρ in our presentations instead of the two generators M_1 and M_2. By doing so we reduce the number of generators in the presentation, a helpful simplification. We will show that in all cases, this does not yield a proper subgroup of the space group, therefore nothing is lost in this simplification. It suffices to show that M_1 and M_2 are contained in $\langle \rho, x, y, z\rangle$. (Note that for Groups numbered 88 or lower we have $M_2 = \rho^{\pm 1}$ thus we need only show that $M_1 \in \langle \rho, x, y, z\rangle$.)

In Groups 75, 76, 79, 81, 82, 83, 85, and 87 we have $M_1 = \rho^2$. In Groups 77 and 84 we have $M_1 = z^{-1}\rho^2$. In Group 80 we have $M_1 = x^{-2}yz\rho^2$. In Group 86 we have $M_1 = x^{-1}z^{-1}\rho^2$. In Group 88 we have $M_1 = y\rho^2$. In Groups 147, 148, 168, 169, and 175 we have $M_1 = \rho^2$ and $M_2 = \rho^3$. In Group 171 we have $M_1 = \rho^2$ and $M_2 = z^{-1}\rho^3$; in Groups 173 and 176 we have $M_1 = z^{-1}\rho^2$ and $M_2 = z^{-1}\rho^3$.

In most of the twenty-five groups listed above we have defined y as a product of matrices. This is so that specific relations would be included in the group presentations. (This is also the reason ρ is defined as M_2^{-1} in Group 81.) For spacegroups numbered between 75 and 88, these relations are $x^\rho = yz^\delta$ for $\delta \in \{-1, 0, 1\}$ and $y^\rho = x^{-1}$. For spacegroups numbered between 147 and 176 (except 174) these relations are $x^\rho = y$ and $y^\rho = x^{-1}yz^\delta$, for $\delta \in \{0, 2\}$. For spacegroups numbered between 143 and 146 and also for group 174 these relations are $x^\rho = x^{-1}y$ and $y^\rho = x^{-1}$. Taking a quotient of the space group mod $\langle z\rangle$ (this subgroup is normal in all twenty-five of these space groups) these relations are identical to the relations found in the presentation of wallpaper groups of type **p3, p4** or **p6** in our previous work, [HP]. This consistency will be particularly helpful when applying Theorem 3.2.

For Group 13 we define: $r = M_1;\ t = M_2;\ x = M_3;\ y = M_4;\ z = M_5^{-1}$. For merely aesthetic reasons we chose to use the inverse of M_5 instead of M_5. This affects only one change in the group presentation: it gives $(rt)^2 = z$ rather than $(rt)^2 = z^{-1}$.

For Group 39 we define: $p = M_4^{-1}M_5M_1;\ s = M_2;\ x = M_3;\ y = M_4;\ z = M_5$. The simplest way to define p would be to choose $p = M_1$. This would result in the group presentation for Group 39 including the relations $(p,s) = (ps)^2 = y^2z^{-1}$. The relation $(ps)^2 = y^2z^{-1} \notin Z(G) = \langle z\rangle$ is problematic because it does not satisfy the hypotheses of Proposition 6.13. By defining $p = M_4^{-1}M_5M_1$ we have the nicer group relations $(p,s) = 1$ and $(ps)^2 = z$. With $(ps)^2$ in the center of the group the proposition is applicable, which is a significant advantage.

4.7 The group presentations

According to Table 1 in [CFHT], there are thirty-one space groups that can be obtained as a fibration over a wallpaper group of type **p2mm**. These thirty-one groups are listed in Tables 4.1 and 4.2.

The three groups G_{10}, G_{12}, and G_{13} have presentations of the form

$$G = \langle x, y, z, r, t \,|\, (x,y), (y,z), (x,z), r^2, t^2, (rt)^2 = \alpha_{rt}, \\ x^r = x^{-1}y^{\delta}, (y,r), z^r = z^{-1}, (xt)^2, (yt)^2, (zt)^2\rangle, \tag{4.1}$$

where $\alpha_{rt} \in A = \langle z\rangle$ and $\delta \in \{0,1\}$.

The four groups G_{16}, G_{17}, G_{21}, and G_{22} have presentations of the form

$$G = \langle x, y, z, p, r \,|\, (x,y), (y,z), (x,z), p^2 = \alpha_p, r^2, (pr)^2, \\ x^p = x^{-1}z^{\delta}, y^p = y^{-1}z^{\delta}, (z,p), x^r = x^{-1}y^{\gamma}, y^r = yz^{-\delta}, z^r = z^{-1}\rangle, \tag{4.2}$$

where $\alpha_p, \in A = \langle z\rangle$ and $\delta, \gamma \in \{0,1\}$.

The six groups $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42} have presentations of the form

$$G = \langle x, y, z, p, s \,|\, (x, y), (y, z), (x, z), p^2 = \alpha_p, s^2 = \alpha_s, (p, s), \quad x^p = x^{-1}z^\delta, y^p = y^{-1}z^\gamma, (z, p), (x, s), y^s = y^{-1}z^\gamma, (z, s)\rangle, \tag{4.3}$$

where $\alpha_p, \alpha_s, \in A = \langle x, y, z\rangle$ and $\delta, \gamma \in \{0, 1\}$.

Table 4.1: Parameters in the presentations of some space groups G with point groups $\frac{\mathbf{2}}{\mathbf{m}}$, **222**, or **mm2**

Point group	**Group number**	**Equation number**	α_{rt}	α_p	α_s	δ	γ
2/m	10	(4.1)	1			0	
2/m	12	(4.1)	1			1	
2/m	13	(4.1)	z			0	
222	16	(4.2)		1		0	0
222	17	(4.2)		z		0	0
222	21	(4.2)		1		0	1
222	22	(4.2)		1		1	0
mm2	25	(4.3)		1	1	0	0
mm2	26	(4.3)		z	z	0	0
mm2	27	(4.3)		1	z	0	0
mm2	38	(4.3)		1	1	0	1
mm2	39	(4.3)		z	1	0	1
mm2	42	(4.3)		1	1	1	1

The fourteen groups $G_{47}, G_{49}, G_{50}, G_{51}, G_{53}, G_{54}, G_{55}, G_{57}, G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68} have presentations of the form

$$G = \langle x, y, z, p, r, t |\, (x, y), (y, z), (x, z), p^2 = \alpha_p, r^2 = \alpha_r, t^2, (pr)^2 = \alpha_{pr}, (pt)^2 = \alpha_{pt}, \quad (rt)^2 = \alpha_{rt}, x^p = x^{-1}, y^p = y^{-1}, (z, p), x^r = x^{-1}y^\delta, (y, r), z^r = z^{-1}, (xt)^2, (yt)^2, (zt)^2\rangle, \tag{4.4}$$

where $\alpha_p \in \langle z\rangle, \alpha_r \in \langle y\rangle, \alpha_{pr}, \alpha_{pt}, \alpha_{rt} \in A = \langle x, y, z\rangle$ and $\delta \in \{0, 1\}$.

The four groups G_{69}, G_{72}, G_{73}, and G_{74} have presentations of the form

$$G = \langle x, y, z, p, r, t |\, (x, y), (y, z), (x, z), p^2 = \alpha_p, r^2 = \alpha_r, t^2, (pr)^2 = \alpha_{pr}, (pt)^2 = \alpha_{pt}, \quad (rt)^2 = \alpha_{rt}, x^p = x^{-1}z, y^p = y^{-1}z^{1-\delta}, (z, p), x^r = x^{-1}y^\delta, y^r = yz^{\delta-1}, z^r z, (xt)^2, (yt)^2, (zt)^2\rangle, \tag{4.5}$$

where $\alpha_p \in \langle z\rangle, \alpha_r \in \langle y\rangle, \alpha_{pr}, \alpha_{pt}, \alpha_{rt} \in A = \langle x, y, z\rangle$ and $\delta \in \{0, 1\}$.

Table 4.2: Parameters in the presentations of some space groups with point group $\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}$

Group number	**Equation number**	α_p	α_r	α_{pr}	α_{pt}	α_{rt}	δ
47	(4.4)	1	1	1	1	1	0
49	(4.4)	1	1	1	1	z^{-1}	0
50	(4.4)	1	1	1	$x^{-1}y^{-1}$	x^{-1}	0
51	(4.4)	1	1	x^{-1}	x^{-1}	1	0
53	(4.4)	z	1	1	x^{-1}	$x^{-1}z^{-1}$	0
54	(4.4)	1	1	x^{-1}	x^{-1}	z^{-1}	0
55	(4.4)	1	y	x	1	x^{-1}	0
57	(4.4)	z	y	1	1	z^{-1}	0
63	(4.4)	z	1	1	1	z^{-1}	1
64	(4.4)	z	y	1	y^{-1}	z^{-1}	1
65	(4.4)	1	1	1	1	1	1
66	(4.4)	1	1	1	1	z^{-1}	1
67	(4.4)	1	y	1	y^{-1}	1	1
68	(4.4)	1	1	$x^{-2}y$	$x^{-2}y$	z^{-1}	1
69	(4.5)	1	1	1	1	1	0
72	(4.5)	1	y	$x^2y^{-1}z^{-1}$	1	$x^{-2}yz$	1
73	(4.5)	z	y	$x^{-2}yz$	$x^{-2}yz$	z^{-1}	1
74	(4.5)	1	y	1	y^{-1}	1	1

In [CFHT] they find that there are thirteen space groups that can be obtained as a fibration over a wallpaper group of type **p4**. These thirteen groups are listed in Table 4.3.

The seven groups $G_{75}, G_{76}, G_{77}, G_{79}, G_{80}, G_{81}$, and G_{82} have presentations of the form

$$G = \langle x, y, z, \rho \,|\, (x, y), (y, z), (x, z),\ \rho^4 = \alpha_\rho, x^\rho = yz^\delta, y^\rho = x^{-1}, z^\rho = z^\gamma \rangle, \tag{4.6}$$

where $\alpha_\rho \in A = \langle z \rangle, \delta \in \{-1, 0, 1\}$, and $\gamma \in \{-1, 1\}$.

The six groups $G_{83}, G_{84}, G_{85}, G_{86}, G_{87}$, and G_{88} have presentations of the form

$$G = \langle x, y, z, \rho, t \,|\, (x, y), (y, z), (x, z),\ \rho^4 = \alpha_\rho, t^2, (\rho, t) = \eta, \tag{4.7}$$
$$x^\rho = yz^\delta, y^\rho = x^{-1}, (z, \rho), (xt)^2, (yt)^2, (zt)^2 \rangle,$$

where $\alpha_\rho \in \langle z \rangle, \eta \in A = \langle x, y, z \rangle$ and $\delta \in \{0, 1\}$.

There are four space groups that can be obtained from a wallpaper group of type **p3** [CFHT]. These are groups $G_{143}, G_{144}, G_{146}$, and G_{174}. The first three have a point group **3**.

Table 4.3: Parameters in the presentations of groups with point groups $\mathbf{4}, \overline{\mathbf{4}}$, or $\frac{\mathbf{4}}{\mathbf{m}}$

Point group	**Group number**	**Equation number**	α_ρ	η	δ	γ
4	75	(4.6)	1		0	1
4	76	(4.6)	z		0	1
4	77	(4.6)	z^2		0	1
4	79	(4.6)	1		1	1
4	80	(4.6)	z		1	1
$\overline{\mathbf{4}}$	81	(4.6)	1		0	-1
$\overline{\mathbf{4}}$	82	(4.6)	1		-1	-1
4/m	83	(4.7)	1	1	0	
4/m	84	(4.7)	z^2	z^{-1}	0	
4/m	85	(4.7)	1	x^{-1}	0	
4/m	86	(4.7)	z^2	$y^{-1}z^{-1}$	0	
4/m	87	(4.7)	1	1	1	
4/m	88	(4.7)	z	$x^{-2}yz$	1	

Group G_{174} has point group $\overline{\mathbf{6}}$. The space groups G_{143}, G_{144}, and G_{146} have presentations of the form

$$G = \langle x, y, z, \rho \,|\, (x, y), (y, z), (x, z), \rho^3 = \alpha_\rho, x^\rho = x^{-1}yz^\delta, y^\rho = x^{-1}, (z, \rho)\rangle, \qquad (4.8)$$

where $\alpha_\rho \in \langle z\rangle$ and $\delta \in \{0, 2\}$.

Table 4.4: Parameters in the presentations of groups with point group **3**

Group number	**Equation number**	α_ρ	δ
143	(4.8)	1	0
144	(4.8)	z	0
146	(4.8)	1	2

The group G_{174} has presentation

$$G = \langle x, y, z, \rho, s \,|\, (x, y),(y, z), (x, z), \rho^3, s^2, (\rho, s),$$
$$x^\rho = x^{-1}y, y^\rho = x^{-1}, (z, \rho), (x, s), (y, s), z^s = z^{-1}\rangle. \qquad (4.9)$$

We again refer to [CFHT] to determine which space groups may be obtained from the wallpaper group of type **p6**. According to Table 1 there are eight such groups. These are listed in Table 4.5. $G_{168}, G_{169}, G_{171}, G_{173}$ which have point group $\mathbf{6} \cong \mathcal{C}_6$.

The six groups $G_{147}, G_{148}, G_{168}, G_{169}, G_{171}$, and G_{173} have presentations of the form

$$G = \langle x, y, z, \rho \,|\, (x,y), (y,z), (x,z), \rho^6 = \alpha_\rho, x^\rho = y, y^\rho = x^{-1}yz^\delta, z^\rho = z^\gamma \rangle, \tag{4.10}$$

where $\alpha_\rho \in A = \langle z \rangle, \delta \in \{0, 2\}$, and $\gamma \in \{-1, 1\}$.

The two groups G_{175} and G_{176} have presentations of the form

$$G = \langle x, y, z, \rho, t \,|\, (x,y), (y,z), (x,z), \rho^6 = \alpha_\rho, t^2, (\rho, t) = \eta, \tag{4.11}$$

$$x^\rho = y, y^\rho = x^{-1}y, (\rho, z), (xt)^2, (yt)^2, (zt)^2 \rangle,$$

where $\alpha_\rho, \eta \in \langle z \rangle$.

Table 4.5: Parameters in the presentations of groups with point groups $\overline{\mathbf{3}}, \mathbf{6}$, or $\frac{\mathbf{6}}{\mathbf{m}}$

Point group	**Group number**	**Equation number**	α_ρ	η	δ	γ
$\overline{\mathbf{3}}$	147	(4.10)	1		0	-1
$\overline{\mathbf{3}}$	148	(4.10)	1		2	-1
6	168	(4.10)	1		0	1
6	169	(4.10)	z		0	1
6	171	(4.10)	z^2		0	1
6	173	(4.10)	z^3		0	1
6/m	175	(4.11)	1	1		
6/m	176	(4.11)	z^3	z^{-1}		

Chapter 5. Space groups with non-trivial WCT groups

5.1 Groups having point group **3** or $\overline{\mathbf{6}}$

The following applies to G_{143}, G_{144}, and G_{146}.

Theorem 5.1. *Let G be a group with presentation of the form given in Eq. (4.8). Then $\tau(\rho, \mathcal{C})$, with $\mathcal{C} = \{A\rho, A\rho^2\}$, is a non-trivial wct map.*

Proof. For this map we have $\mathcal{P} = \{A\rho, A\rho^2\}$ and so by Lemma 2.6 we have $\mathcal{I} = K_\rho$. It is clear that ρ commutes with every element of F, thus we may apply Corollary 2.16 (ii). Since $\mathcal{I} = K_\rho$, we see that τ_ρ is a wct map.

We may use Theorem 3.2 to verify that τ_ρ is a non-trivial wct. Note that $Z(G) = \langle z \rangle \trianglelefteq G$. The quotient

$$G/Z(G) = \langle x, y, \rho \,|\, (x, y), \rho^3, x^\rho = x^{-1}y, y^\rho = x^{-1} \rangle,$$

is a wallpaper group of type **p3**. Now τ_ρ induces a map on the quotient $G/Z(G)$:

$$\overline{\tau_\rho} \begin{cases} g \mapsto g^\rho & \text{if } \overline{Ag} \in \overline{\mathcal{C}} = \{\overline{A\rho}, \overline{A\rho^2}\}, \\ g \mapsto g & \text{if } \overline{Ag} \in \overline{\mathcal{F}} = \{\overline{A}\}. \end{cases}$$

This is precisely the non-trivial wct that exists in the wallpaper groups of type **p3** [HP]. It follows by Theorem 3.2 that $\tau_\rho \in \mathcal{W}(G) \setminus \mathcal{W}_0(G)$. □

The following applies to G_{174}.

Theorem 5.2. *Let G be a group with presentation of the form given in Eq. (4.9). The following are non-trivial wct maps:*

(i) $\tau(\rho, \mathcal{C}_1), \mathcal{C}_1 = \{A\rho, A\rho^2, A\rho s, A\rho^2 s\}$; *and*

(ii) $\tau(s, \mathcal{C}_2), \mathcal{C}_2 = \{As, A\rho s, A\rho^2 s\}$.

Proof. For the map τ_ρ we have $\mathcal{P}(\mathcal{C}_1) = \{A\rho, A\rho^2, A\rho s, A\rho^2 s\}$ and applying Lemma 2.6 we have $\mathcal{I}(\mathcal{C}_1) = K_\rho \cap K_{\rho s}$. Now the relations in the presentation of G give $K_\rho = \langle x^2y^{-1}, xy\rangle$ and $K_{\rho s} = \langle x^2y^{-1}, xy, z^2\rangle$, therefore $\mathcal{I}(\mathcal{C}_1) = K_\rho$. Since $F = \langle \rho, s\rangle$ is an abelian subgroup of G, we see that ρ commutes with every element of F. By Corollary 2.16 (*ii*) we conclude that $\tau_\rho \in \mathcal{W}(G)$.

Now $\langle z, s\rangle \trianglelefteq G$. (In fact, $G = \langle x, y, \rho\rangle \times \langle z, s\rangle$.) Consider the quotient $G/\langle z, s\rangle$:

$$G/\langle z, s\rangle = \langle x, y, \rho \,|\, (x, y), \rho^3, x^\rho = x^{-1}y, y^\rho = x^{-1}\rangle.$$

This is the wallpaper group **p3**. The map τ_ρ induces a map on the quotient $\overline{\tau_\rho} : G/\langle z, s\rangle \to G/\langle z, s\rangle$ defined as

$$\overline{\tau_\rho} : \begin{cases} g \mapsto g^\rho & \text{if } \overline{Ag} \in \overline{\mathcal{C}} = \{\overline{A\rho}, \overline{A\rho^2}\}, \\ g \mapsto g & \text{if } \overline{Ag} \in \overline{\mathcal{F}} = \{\overline{A}\} \end{cases}$$

which we know to be a non-trivial map [HP]. It follows by Theorem 3.2 that $\tau(\rho, \mathcal{C})$ is also a non-trivial wct.

We now consider the map τ_s. We will show that this is a wct by applying Corollary 2.16 (*ii*). We have $F = \langle \rho, s\rangle$, an abelian subgroup of G, thus s commutes with every element of F. For this map we have $\mathcal{P} = K_s \cap K_{\rho s} \cap K_{\rho^2 s}$. The relations in the group presentation give us $K_{\rho s} = K_{\rho^2 s} = \langle x^2y^{-1}, xy, z^2\rangle$ and $K_s = \langle z^2\rangle$. Therefore $\mathcal{I}(\mathcal{C}_2) = K_s$. By Corollary 2.16 (*ii*) we conclude that $\tau_s \in \mathcal{W}(G)$. By Theorem 3.1 $\tau_s \in \mathcal{W}(G) \setminus \mathcal{W}_0(G)$. □

5.2 Groups having point group $\mathbf{4}, \overline{\mathbf{4}}$, or $\frac{\mathbf{4}}{\mathbf{m}}$

The following two theorems apply to space groups with point group **4** or $\overline{\mathbf{4}}$.

Theorem 5.3. *Let G be a group with a presentation of the form given in Eq. (4.7). Then for $\lambda \in \langle x, y, \rho\rangle$, the map $\tau(\lambda, \{A\rho, A\rho^3\})$ is a non-trivial wct.*

Proof. For this map $\mathcal{P} = \{A\rho, A\rho^3\}$. By Lemma 2.6 $K_\rho = K_{\rho^3}$, thus we have $\mathcal{I} = K_\rho$. For any $\lambda \in \langle x, y\rangle \leq A$ we clearly have (λ, ρ) and (λ, ρ^3) contained in $K_\rho = K_{\rho^3} = \mathcal{I}$. Thus by

Lemma 2.14 and Corollary 2.15 (i), τ_λ is a wct.

For $\lambda = \rho$ we may apply Corollary 2.16 (ii) since ρ commutes with every element of F. Clearly we have $K_\lambda \leq \mathcal{I}$; thus τ_ρ is also a wct.

Notice that $Z = \langle z \rangle \trianglelefteq G$; thus we may consider the quotient

$$G/Z = \langle x, y, \rho \,|\, (x, y), \rho^4, x^\rho = y, y^\rho = x^{-1} \rangle.$$

This is a wallpaper group of type **p4**. The map τ_λ induces a map on the quotient, $\overline{\tau_\lambda} : G/Z \to G/Z$ defined as

$$\overline{\tau_\lambda} : (g) = \begin{cases} g^\lambda & \text{if } \overline{Ag} \in \{\overline{A\rho}, \overline{A\rho^3}\}, \\ g & \text{if } \overline{Ag} \in \{\overline{A}, \overline{A\rho^2}\}, \end{cases}$$

which we know to be a non-trivial wct [HP]. It follows by Theorem 3.2 that τ_λ is also a non-trivial wct. □

Theorem 5.4. *Let G be a group with a presentation of the form given in Eq. (4.7). For these groups we have $K_\rho = \langle xy, x^{-1}yz^\delta \rangle$, with $\delta \in \{0, 1\}$. Then for $\lambda \in K_\rho$ the map $\tau(\lambda, \mathcal{C}), \mathcal{C} = \{A\rho, A\rho^3, A\rho t, A\rho^3 t\}$ is a non-trivial wct.*

Proof. From the relations in the presentation of the group one can check that $K_\rho = \langle xy, x^{-1}yz^\delta \rangle$.

Now for this map we have $\mathcal{P} = \{A\rho, A\rho^3, A\rho t, A\rho^3 t\}$ and so

$$\mathcal{I} = K_\rho \cap K_{\rho^3} \cap K_{\rho t} \cap K_{\rho^3 t} = K_\rho \cap K_{\rho t},$$

the last equality being justified by Lemma 2.6. Note also that $\mathcal{I} \trianglelefteq G$ since it is the intersection of normal subgroups by Lemma 2.5.

We will use Corollary 2.15 (i) to show that τ_λ is a wct. Accordingly, we need to show that $\{(\lambda, f^{-1}) \,|\, f \in \{\rho, \rho^3, \rho t, \rho^3 t\}\} \subseteq \mathcal{I}$. By Lemmas 2.3 and 2.14, it suffices to show that (λ, ρ) and $(\lambda, \rho t)$ are contained in $\mathcal{I} = K_\rho \cap K_{\rho t}$. Obviously $(\lambda, \rho) \in K_\rho$ and $(\lambda, \rho t) \in K_{\rho t}$.

It is also easy to see that $(\lambda, \rho t) \in K_\rho$ since $\lambda \in K_\rho$ and by Lemma 2.5 K_ρ is normal, thus $(\lambda, \rho t) = \lambda^{-1}\lambda^{\rho t}$ is a product of two elements in K_ρ. It remains to show that $(\lambda, \rho) \in K_{\rho t}$.

First we prove a lemma.

Lemma 5.5.

$$\textit{For } b \in A,\ (b^{\rho^2}, \rho) = (b, \rho)^{-1}. \tag{5.1}$$

Proof. From the relations in the group presentation we have $K_{\rho^2 t} = \langle z^\delta, z^2 \rangle$. Since $(z, \rho) = 1$ this implies that $\rho \in C_G(K_{\rho^2 t})$. It follows by Lemma 2.7 that $\rho^2 t \in C_G(K_\rho)$. In other words, for $b \in A$, $(b, \rho)^{\rho^2 t} = (b, \rho)$. By Lemma 2.4 the left hand side is $(b^{\rho^2}, \rho)^t$. Recall that for $\alpha \in A$ we have $\alpha^t = \alpha^{-1}$ and so we have $(b^{\rho^2}, \rho)^{-1} = (b, \rho)$, which proves the lemma. □

Now we will show that $(\lambda, \rho) \in K_{\rho t}$ by showing that (λ, ρ) can be written as a commutator $(c, \rho t)$ for some $c \in A$. Let $\lambda = (a, \rho)$ for some $a \in A$. Let $b = a^{\rho^{-1}}$ so that $\lambda = (b^\rho, \rho)$. Then

$$\begin{aligned}
(\lambda, \rho) = ((a, \rho), \rho) &= (a^\rho \cdot a^{-1}, \rho) \\
&= (a^\rho, \rho)(a^{-1}, \rho) && \text{by Lemma 2.1} \\
&= (b^{\rho^2}, \rho)(b^{\rho t}, \rho) && a^\rho = b^{\rho^2} \text{ and } a^{-1} = b^{\rho t} \\
&= (b, \rho)^{-1}(b^{\rho t}, \rho) && \text{using Eq. (5.1)} \\
&= (b, \rho)^{-1}(b, \rho)^{\rho t} && \text{by Lemma 2.4} \\
&= ((b, \rho), \rho t).
\end{aligned}$$

We conclude that τ_λ is a wct.

Now we show that τ_{xy} and $\tau_{x^{-1}yz^\delta}$ are non-trivial wcts:

$$\tau_{xy}(\rho) \cdot \tau_{xy}(\rho) = x^{-2}y^{-2}\rho^2 \neq \rho^2 = \tau_{xy}(\rho^2).$$

$$\tau_{x^{-1}yz^\delta}(\rho)\tau_{x^{-1}yz^\delta}(\rho) = x^2y^{-2}z^{-2\delta}\rho^2 = (x^2z^{-\delta}\rho)^2 \neq \rho^2 = \tau_{x^{-1}yz^\delta}(\rho^2).$$ □

5.3 Groups having point group $\overline{\mathbf{3}}, \mathbf{6}$ or $\frac{\mathbf{6}}{\mathbf{m}}$

Proposition 5.6. *We define $\alpha = xy$, and $\beta = x^{-2}y$. For groups having a presentation of the form given in Eq. (4.10) (and assuming that $\delta = 0$ or $\gamma = -1$) we have*

$$K_\rho = K_{\rho^5} = \langle x, y, z^{1-\gamma}\rangle;$$
$$K_{\rho^2} = K_{\rho^4} = \langle \alpha, \beta z^\delta\rangle;$$
$$K_{\rho^3} = \langle x^2, y^2, z^{1-\gamma}\rangle.$$

For groups having a presentation of the form given in Eq. (4.11) we have

$$K_\rho = K_{\rho^5} = \langle x, y\rangle;$$
$$K_{\rho^2} = K_{\rho^4} = \langle \alpha, \beta\rangle;$$
$$K_{\rho^3} = \langle x^2, y^2\rangle;$$
$$K_t = \langle x^2, y^2, z^2\rangle$$
$$K_{\rho t} = K_{\rho^5 t} = \langle \alpha, \beta, z^2\rangle;$$
$$K_{\rho^2 t} = K_{\rho^4 t} = \langle x, y, z^2\rangle;$$
$$K_{\rho^3 t} = \langle z^2\rangle.$$

Each of these subgroups is normal.

Proof. From the given presentations and the definition of the K_f subgroups one can calculate the K_f subgroups to be as given above. Lemma 2.6 may also be applied. Since G/A is abelian, we know by Lemma 2.5 that the K_f subgroups are normal. □

The following applies to $G_{147}, G_{148}, G_{168}, G_{169}, G_{171}$, and G_{173}.

Theorem 5.7. *Assume $\lambda \neq 1$. Let $\alpha = xy$, and $\beta = x^{-2}y$. Groups with presentations of the form described in Eq. (4.10) with $\delta = 0$ or $\gamma = -1$ have the following non-trivial wct maps:*

(i) For $\lambda \in \langle x^2, y^2, \rho^3\rangle$, $\tau(\lambda, \mathcal{C}_1), \mathcal{C}_1 = \{A, A\rho^2, A\rho^4\}$; and

(ii) For $\lambda \in \langle \alpha, \beta z^\delta, \rho^2\rangle$, $\tau(\lambda, \mathcal{C}_2), \mathcal{C}_2 = \{A, A\rho^3\}$.

Proof. We will use Corollaries 2.15 and 2.16 to show that these two maps are wcts. For the first map $\tau(\lambda, \mathcal{C}_1)$ we have $\mathcal{P}(\mathcal{C}_1) = \{A\rho, A\rho^3, A\rho^5\}$. By Proposition 5.6, $K_{\rho^3} \subseteq K_\rho = K_{\rho^5}$, thus $\mathcal{I}(\mathcal{C}_1) = K_{\rho^3}$. Since x^2 and y^2 are contained in $K_{\rho^3} = \mathcal{I}(\mathcal{C}_1)$, by Corollary 2.15 (*ii*) $\tau(x^2, \mathcal{C}_1)$ and $\tau(y^2, \mathcal{C}_1)$ are wct maps. Now clearly ρ^3 commutes with every element of F and K_{ρ^3} is contained in $\mathcal{I}(\mathcal{C}_1)$. Then by Corollary 2.16 (*ii*), $\tau(\rho^3, \mathcal{C}_1)$ is also a wct map.

For the second map $\tau(\lambda, \mathcal{C}_2)$ we have $\mathcal{P}(\mathcal{C}_2) = \{A\rho, A\rho^2, A\rho^4, A\rho^5\}$. By Proposition 5.6 $K_{\rho^2} = K_{\rho^4} \subseteq K_\rho = K_{\rho^5}$, thus $\mathcal{I}(\mathcal{C}_2) = K_{\rho^2}$. Since α and βz^δ are in $K_{\rho^2} = \mathcal{I}(\mathcal{C}_2)$, by Corollary 2.15 (*ii*) $\tau(\alpha, \mathcal{C}_2)$ and $\tau(\beta z^\delta, \mathcal{C}_2)$ are wct maps. Of course ρ^2 commutes with every element of F and K_{ρ^2} is contained in $\mathcal{I}(\mathcal{C}_2)$, so by Corollary 2.16 (*ii*) $\tau(\rho^2, \mathcal{C}_2)$ is also a wct map.

Note that $\langle z \rangle \trianglelefteq G$. The image of these maps in $G/\langle z \rangle$ are the non-trivial wcts in wallpaper group **p6**. By Theorem 3.2 these maps are also non-trivial wcts. □

The following applies to G_{175} and G_{176}.

Theorem 5.8. *Assume $\lambda \neq 1$. Let $\alpha = xy$, $\beta = x^{-2}y$. Groups with presentations of the form described in Eq. (4.11) have following non-trivial wcts maps:*

(i) For $\lambda \in \langle x^2, y^2 \rangle$, $\tau(\lambda, \mathcal{C}_1), \mathcal{C}_1 = \{A, A\rho^2, A\rho^4, A\rho t, A\rho^3 t, A\rho^5 t\}$; and

(ii) For $\lambda \in \langle \alpha, \beta \rangle$, $\tau(\lambda, \mathcal{C}_2), \mathcal{C}_2 = \{A, A\rho^3, At, A\rho^3 t\}$.

Additionally, if $\eta = 1$ (which is the case for G_{175}), then $\tau(\rho^3, \mathcal{C}_1)$ and $\tau(\rho^2, \mathcal{C}_2)$ are non-trivial wcts.

Proof. We will use Corollaries 2.15 and 2.16 to show that these two maps are wcts. For the first map $\tau(\lambda, \mathcal{C}_1)$ we have $\mathcal{P}(\mathcal{C}_1) = \{A\rho, A\rho^3, A\rho^5, At, A\rho^2 t, A\rho^4 t\}$ thus by Proposition 5.6

$$\mathcal{I}(\mathcal{C}_1) = \langle x, y \rangle \cap \langle x^2, y^2 \rangle \cap \langle x^2, y^2, z^2 \rangle \cap \langle x, y, z^2 \rangle = \langle x^2, y^2 \rangle = K_{\rho^3}.$$

Since x^2 and y^2 are contained in $K_{\rho^3} = \mathcal{I}(\mathcal{C}_1)$, by Corollary 2.15 (*ii*), $\tau(x^2, \mathcal{C}_1)$ and $\tau(y^2, \mathcal{C}_1)$ are wcts.

For the second map, τ_λ we have $\mathcal{P}(\mathcal{C}_2) = (G/A) \setminus \{A, A\rho^3, At, A\rho^3 t\}$; thus by Proposition 5.6

$$\mathcal{I}(\mathcal{C}_2) = \langle x, y\rangle \cap \langle \alpha, \beta\rangle \cap \langle \alpha, \beta, z^2\rangle \cap \langle x, y, z^2\rangle = \langle \alpha, \beta\rangle = K_{\rho^2}.$$

Since α and β are contained in $K_{\rho^2} = \mathcal{I}(\mathcal{C}_2)$, by Corollary 2.15 (ii) $\tau(\alpha, \mathcal{C}_2)$ and $\tau(\beta, \mathcal{C}_2)$ are wcts.

Now we consider the maps $\tau(\rho^3, \mathcal{C}_1)$ and $\tau(\rho^2, \mathcal{C}_2)$. Here F consists of elements $\rho^j t^k$ for $j \in \{0, 1, 2, 3, 4, 5\}$ and $k \in \{0, 1\}$. Since we are assuming $\eta = 1$ it is clear that $\rho^2, \rho^3 \in F$ commute with every element of F. Thus by Corollary 2.16 (ii), since $\mathcal{I}(\mathcal{C}_1) = K_{\rho^3}$ and $\mathcal{I}(\mathcal{C}_2) = K_{\rho^2}$ we know that $\tau(\rho^3, \mathcal{C}_1)$ and $\tau(\rho^2, \mathcal{C}_2)$ are wct maps.

Next we show that $\tau_{x^2}, \tau_{y^2}, \tau_\alpha$, and τ_β are not homomorphisms:

$$\tau_{x^2}(\rho) \cdot \tau_{x^2}(\rho) = \rho \cdot \rho \neq x^{-2} y^{-2} \rho^2 = \tau_{x^2}(\rho \cdot \rho);$$

$$\tau_{y^2}(\rho) \cdot \tau_{y^2}(\rho) = \rho \cdot \rho \neq x^{2} y^{-4} \rho^2 = \tau_{y^2}(\rho \cdot \rho);$$

$$\tau_\alpha(\rho) \cdot \tau_\alpha(\rho^2) = \rho \cdot \rho^2 \neq \alpha^{-2} \rho^3 = \tau_\alpha(\rho \cdot \rho^2);$$

$$\tau_\beta(\rho) \cdot \tau_\beta(\rho^2) = \rho \cdot \rho^2 \neq \beta^{-2} \rho^3 = \tau_\beta(\rho \cdot \rho^2).$$

It follows by Theorem 3.1 (ii) that these are non-trivial wcts. This theorem also tells us (since $\rho^2, \rho^3 \notin A$) that τ_{ρ^2} and τ_{ρ^3} are non-trivial wcts. □

5.4 Some groups that have point group $\frac{\mathbf{2}}{\mathbf{m}}$, $\mathbf{mm2}$, or $\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}$

Theorem 5.9. *The following are non-trivial wcts:*

(i) *For* $G_{10} : \tau(r, \{Ar, At\})$ *and* $\tau(rt, \{Art, At\})$;

(ii) *For* $G_{25}, G_{26}, G_{27}, G_{38}, G_{39},$ *and* $G_{42} : \tau(ps, \{Ap, Aps\})$ *and* $\tau(s, \{Ap, As\})$;

(iii) *For* $G_{47} : \tau(prt, \{Aprt, At, Ap, Ar\})$;

(iv) *For* G_{47} *and* $G_{51} : \tau(rt, \{Art, At, Apr, Ap\})$;

(v) *For* $G_{47}, G_{55},$ *and* $G_{65} : \tau(pt, \{Apt, At, Ar, Apr\})$.

Proof. Note that each of these maps are of the form given in Eq. (2.7). To show that such a map (a $\tau(\lambda, \mathcal{C})$ map) is a wct of the indicated space group, Corollary 2.16 (*ii*) asserts that it suffices to show that two conditions are met. The first is that $(\lambda, f) = 1$ for every $f \in F$ such that $Af \in \mathcal{C}$. The second is that $K_\lambda \leq \mathcal{I}$. Also note that for each of the maps here, $\mathcal{I} = \bigcap_{Af \in \mathcal{C}} K_f$. The relations in the presentations of each of these groups show that the first condition is met. Proposition A.1 gives the K_f subgroups for each of these groups and shows that the second condition (the containment of K_λ) is also met. Thus we conclude that each of these maps are wcts. By Theorem 3.1 they are non-trivial wcts. □

Chapter 6. To determine $\mathcal{W}(G)$

6.1 Method

For the thirty-one groups listed in Tables 4.1 and 4.2 we will determine a set of generators of $\mathcal{W}(G)$. We do so in six steps which we also used in [HP]. These are:

Step one: For an arbitrary wct φ, we show that $\varphi|_A$ is an automorphism.

Step two: We show that we may compose φ with trivial weak Cayley table maps so that $\varphi|_A$ is the identity map on A.

Step three: We show that we may again compose φ with trivial wcts so that φ fixes each coset in G/A.

Step four: We determine elements of $\mathcal{W}(G)$ that we may compose φ with so as to have $\varphi(t) = t$ for all $t \in F$.

Step five: We show that for $t \in F$ there is an $f \in F$ such that $\varphi(at) = a^f t$ for $a \in A$.

Step six: We determine elements of $\mathcal{W}(G)$ that we may compose φ with so as to have $\varphi = \mathrm{Id}$.

In our work here we found it advantageous to combine steps two and three. Note that Theorem 6.1 shows that step one is true for any crystallographic group and similarly, Theorem 6.21 shows that step five is true for any crystallographic group. Also note also that in steps two, three, four, and six we frequently will compose with inner automorphisms. We will denote the automorphism that conjugates each group element by $g \in G$ as I_g.

6.2 Step one

Here we show that step one is true for any n-dimensional crystallographic group.

Theorem 6.1. *Let G be a crystallographic group with translation subgroup $A \cong \mathbb{Z}^n$ for $n \in \mathbb{N}$. Let $\varphi \in \mathcal{W}(G)$. Then $\varphi|_A$ is an automorphism.*

Proof. By Lemma 4.1, the only elements of G that have finite conjugacy classes are in A. Since φ preserves conjugacy classes and is bijective, φ maps finite conjugacy classes to finite conjugacy classes. We therefore have $\varphi(A) = A$. Because A is abelian, in this proof we will denote the group operation for A additively. Also, to denote the conjugation action of $g \in G$ on $a \in A$ we will write $g(a)$.

Let $a, b \in A$. Using the fact that φ respects inverses, we have

$$\varphi(a+b) \sim \varphi(a) + \varphi(b); \tag{6.1}$$

$$\varphi(b) = \varphi(a+b-a) \sim \varphi(a+b) - \varphi(a); \tag{6.2}$$

$$\varphi(a) = \varphi(a+b-b) \sim \varphi(a+b) - \varphi(b). \tag{6.3}$$

Eq. (6.1) implies there exists some $g_1 \in G$ such that $\varphi(a+b) = g_1(\varphi(a) + \varphi(b))$. Similarly, Eq. (6.2) implies there exists some $g_2 \in G$ such that $g_2(\varphi(b)) = \varphi(a+b) - \varphi(a)$ and Eq. (6.3) implies there exists some $g_3 \in G$ such that $g_3(\varphi(a)) = \varphi(a+b) - \varphi(b)$. Solving for $\varphi(a+b)$ we have the following three equations:

$$\varphi(a+b) = g_1(\varphi(a) + \varphi(b)); \tag{6.4}$$

$$= \varphi(a) + g_2(\varphi(b)); \tag{6.5}$$

$$= \varphi(b) + g_3(\varphi(a)). \tag{6.6}$$

Recall that every element of A corresponds to a translation in Euclidean $n-$space, $n \in \mathbb{N}$, and thus to a point on the lattice $\mathfrak{L}$. We may think of $a \in A$ translating the lattice $\mathfrak{L}$ by a distance of $|a|$ and so it follows that $c \in a^G$ will also translate by a distance of $|a|$. Thus for $g \in G$, we can think of $g(a)$ as being some point on an $(n-1)$-sphere of radius $|a|$ centered at the origin. From this we see that Eq. (6.4) indicates that $\varphi(a+b)$ lies on an $(n-1)$-sphere of radius $|\varphi(a) + \varphi(b)|$ centered at the origin. Next we see that Eq. (6.5) indicates that $\varphi(a+b)$ lies on an $(n-1)$-sphere of radius $|\varphi(b)|$ centered at $\varphi(a)$. Lastly Eq. (6.6) implies

$\varphi(a+b)$ lies on an $(n-1)$-sphere of radius $|\varphi(a)|$ centered at $\varphi(b)$.

Therefore $\varphi(a+b)$ lies in the intersection of these three spheres. By Lemma 6.2 this intersection is $\varphi(a)+\varphi(b)$. In other words, $\varphi(a+b)=\varphi(a)+\varphi(b)$.

Lemma 6.2. *Let* $\mathbf{a} \neq \mathbf{0}$ *and* $\mathbf{b} \neq \mathbf{0}$ *be vectors in* $\mathbb{E}^n$. *Let* $\mathcal{S}_0$ *be an* $(n-1)$*-sphere of radius* $||\mathbf{a}+\mathbf{b}||$ *centered at the origin. Let* $\mathcal{S}_a$ *be an* $(n-1)$*-sphere of radius* $||\mathbf{b}||$ *with center* $\mathbf{a}$ *and similarly let* $\mathcal{S}_b$ *be an* $(n-1)$*-sphere of radius* $||\mathbf{a}||$ *with center* $\mathbf{b}$. *Then the intersection of the three spheres is one point, namely* $\mathbf{a}+\mathbf{b}$.

Proof. Clearly $\mathbf{a}+\mathbf{b}$ is contained in each of $\mathcal{S}_a, \mathcal{S}_b$, and $\mathcal{S}_0$ thus we have $\{\mathbf{a}+\mathbf{b}\} \subseteq \mathcal{S}_a \cap \mathcal{S}_b \cap \mathcal{S}_0$. It remains to show the reverse containment: $\mathcal{S}_a \cap \mathcal{S}_b \cap \mathcal{S}_0 \subseteq \{\mathbf{a}+\mathbf{b}\}$.

We note that if $\mathbf{a}+\mathbf{b}=\mathbf{0}$, then $\mathcal{S}_0=\{\mathbf{0}\}$ so $\mathcal{S}_0 \cap \mathcal{S}_a \cap \mathcal{S}_b=\{\mathbf{0}\}$ is one point, proving this case. So now we assume $\mathbf{a}+\mathbf{b} \neq \mathbf{0}$.

We have $\mathcal{S}_0=\{\mathbf{x} \in \mathbb{E}^n : ||\mathbf{x}||^2=||\mathbf{a}+\mathbf{b}||^2\}$, $\mathcal{S}_a=\{\mathbf{x} \in \mathbb{E}^n : ||(\mathbf{x}-\mathbf{a})||^2=||\mathbf{b}||^2\}$, and $\mathcal{S}_b=\{\mathbf{x} \in \mathbb{E}^n : ||\mathbf{x}-\mathbf{b}||^2=||\mathbf{a}||^2\}$. Also, let $\mathcal{P}$ be the hyperplane that is tangent to $\mathcal{S}_0$ at the point $\mathbf{a}+\mathbf{b}$.

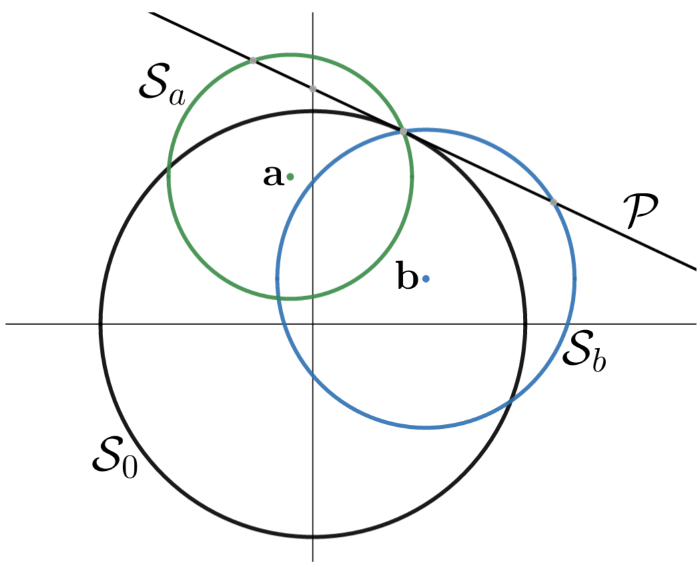

Figure 6.1: The spheres $\mathcal{S}_0, \mathcal{S}_a, \mathcal{S}_b$ with the plane $\mathcal{P}$ in $\mathbb{E}^2$

Now any $\mathbf{x} \in \mathcal{S}_0$ must satisfy

$$\mathbf{x} \cdot \mathbf{x} - (\mathbf{a} + \mathbf{b}) \cdot (\mathbf{a} + \mathbf{b}) = 0. \tag{6.7}$$

Also, any $\mathbf{x} \in \mathcal{S}_a$ must satisfy

$$(\mathbf{x} - \mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) - \mathbf{b} \cdot \mathbf{b} = 0. \tag{6.8}$$

Any $\mathbf{x} \in \mathcal{S}_0 \cap \mathcal{S}_a$ must satisfy both of these equations. Subtracting Eq. (6.7) from Eq. (6.8) and expanding we have

$$(\mathbf{x} \cdot \mathbf{x} - 2\mathbf{a} \cdot \mathbf{x} + \mathbf{a} \cdot \mathbf{a}) - \mathbf{b} \cdot \mathbf{b} - (\mathbf{x} \cdot \mathbf{x} - (\mathbf{a} \cdot \mathbf{a} + 2\mathbf{a} \cdot \mathbf{b} + \mathbf{b} \cdot \mathbf{b})) = 0.$$

Canceling gives

$$(-2\mathbf{a} \cdot \mathbf{x} + \mathbf{a} \cdot \mathbf{a}) + (\mathbf{a} \cdot \mathbf{a} + 2\mathbf{a} \cdot \mathbf{b}) = 0.$$

Simplifying and dividing by 2 gives

$$\mathbf{a} \cdot ((\mathbf{a} + \mathbf{b}) - \mathbf{x}) = 0.$$

Using $\mathbf{x} \in \mathcal{S}_0 \cap \mathcal{S}_b$, a similar argument gives

$$\mathbf{b} \cdot ((\mathbf{a} + \mathbf{b}) - \mathbf{x}) = 0.$$

It follows that any $\mathbf{x} \in \mathcal{S}_0 \cap \mathcal{S}_a \cap \mathcal{S}_b$ satisfies

$$(\mathbf{a} + \mathbf{b}) \cdot ((\mathbf{a} + \mathbf{b}) - \mathbf{x}) = 0,$$

The set of all $\mathbf{x}$ that satisfy this equation is the hyperplane that has normal vector $\mathbf{a} + \mathbf{b}$ and contains the point $\mathbf{a} + \mathbf{b}$. This is the plane $\mathcal{P}$ that is tangent to $\mathcal{S}_0$ at the point $\mathbf{a} + \mathbf{b}$. Recall that we also have $\mathbf{x} \in \mathcal{S}_0$, thus $\mathbf{x} \in \mathcal{P} \cap \mathcal{S}_0$. Of course, this intersection is just one point (the point of tangency), which is $\mathbf{a} + \mathbf{b}$. □

6.3 Steps two and three

In this section we will prove results useful for proving step two and step three. These results will be applied in Ch. 7 and Ch. 8 to the thirty-one space groups listed in Tables 4.1 and

4.2.

Definition For a group G with abelian normal subgroup A we define the set

$$\mathbf{C}_2 = \mathbf{C}_2(G) = \{a \in A : a^G = \{a, a^{-1}\}\}.$$

Proposition 6.3. *In Table 6.1 we have the* $\mathbf{C}_2$ *subsets for the space groups that have a presentation of the form given in Eqs. (4.1), (4.2), (4.3), (4.4), or (4.5).*

Table 6.1: $\mathbf{C}_2$ for thirty-one groups

Group number(s)	$\mathbf{C}_2$
10, 13	$\langle x, z\rangle \cup \langle y\rangle$
12	$\langle x^2y^{-1}, z\rangle \cup \langle y\rangle$
16, 17	$\langle x\rangle \cup \langle y\rangle \cup \langle z\rangle$
21	$\langle x^2y^{-1}\rangle \cup \langle y\rangle \cup \langle z\rangle$
22	$\langle x^2z^{-1}\rangle \cup \langle y^2z^{-1}\rangle \cup \langle z\rangle$
25, 26, 27	$\langle x\rangle \cup \langle y\rangle$
38, 39	$\langle x\rangle \cup \langle y^2z^{-1}\rangle$
42	$\langle x^2z^{-1}\rangle \cup \langle y^2z^{-1}\rangle$
47-57	$\langle x\rangle \cup \langle y\rangle \cup \langle z\rangle$
63-68	$\langle x^2y^{-1}\rangle \cup \langle y\rangle \cup \langle z\rangle$
69	$\langle x^2z^{-1}\rangle \cup \langle y^2z^{-1}\rangle \cup \langle z\rangle$
72-74	$\langle x^2y^{-1}z^{-1}\rangle \cup \langle y\rangle \cup \langle z\rangle$

Proof. This follows from the relations found in the presentation of the respective groups. (For brevity we write "47-57" to represent groups $G_{47}, G_{49}, G_{50}, G_{51}, G_{53}, G_{54}, G_{55}$, and G_{57} (note we are not including G_{48} and G_{56}); we write "63-68" to represent $G_{63}, G_{64}, G_{65}, G_{66}$, G_{67}, and G_{68}.) □

Lemma 6.4. *Let* G *be a crystallographic group. Let* $\varphi \in \mathcal{W}(G)$ *and* $a \in A$. *Let* $g \in G$ *satisfy* $g^2 \in A$. *Then*

$$a^g = a^{-1} \text{ implies that } \varphi(a)^{\varphi(g)} = \varphi(a)^{-1}.$$

Proof. By Theorem 6.1 we know that $\varphi|_A$ is a homomorphism thus for $k \in \mathbb{Z}, \varphi(a^k) = \varphi(a)^k$. Then $\varphi(a^k \cdot g) \sim \varphi(a)^k\varphi(g)$. Squaring both sides we have

$$\varphi(g^2) = \varphi(a^k g{\cdot}a^k g) \sim \varphi(a)^k\varphi(g)\varphi(a)^k\varphi(g) = \varphi(a)^k\varphi(g)^2(\varphi(a)^k)^{\varphi(g)} = \varphi(g)^2(\varphi(a)\varphi(a)^{\varphi(g)})^k.$$

Since $g^2 \in A$ its image $\varphi(g^2)$ has finitely many conjugates, thus $\varphi(a)\varphi(a)^{\varphi(g)} = 1$, in other words, $\varphi(a)^{\varphi(g)} = \varphi(a)^{-1}$. □

Proposition 6.5. *Let G be a crystallographic group. Let $\varphi \in \mathcal{W}(G)$. Then*

(i) $Z(G) \cap \mathbf{C}_2 = \{1\}$.

(ii) $\varphi(\mathbf{C}_2) = \mathbf{C}_2$.

(iii) $\varphi(\langle \mathbf{C}_2 \rangle) = \langle \mathbf{C}_2 \rangle$.

(iv) Let $j \in \mathbb{N}$. If there exists a set $B = \{\beta_i\}_{i=1}^{j} \subseteq \mathbf{C}_2$ such that $\mathbf{C}_2 = \bigcup_{i=1}^{j} \langle \beta_i \rangle$ and $\langle \mathbf{C}_2 \rangle$ is a free abelian group of rank j with generating set B, then for $\beta \in B$ we have $\varphi(\beta) \in \{a \in A : a \in B \text{ or } a^{-1} \in B\}$.

Proof. Statement (i) is clear since $a^{-1} = a \in A$ is only possible if a is the identity. Now to prove (ii) we recall that φ maps conjugacy classes to conjugacy classes bijectively, therefore any nontrivial element in $\mathbf{C}_2$ is mapped to a conjugacy class containing exactly two elements of A. By Proposition 1.1 (ii), φ also respects inverses, thus we conclude that $\varphi(\mathbf{C}_2) = \mathbf{C}_2$. By Theorem 6.1 $\varphi|_A$ is an automorphism of A thus (iii) follows immediately from (ii).

To prove (iv), we will assume there exists $B = \{\beta_i\}_{i=1}^{j} \subseteq \mathbf{C}_2$ such that $\mathbf{C}_2 = \bigcup_{i=1}^{j} \langle \beta_i \rangle$ and $\langle \mathbf{C}_2 \rangle$ is a free abelian group of rank j with generating set B. Let $\beta \in B$. As $\beta \in \mathbf{C}_2$, we have $\varphi(\beta) \in \mathbf{C}_2$ by (ii). Our assumption that $\mathbf{C}_2 = \bigcup_{i=1}^{j} \langle \beta_i \rangle$ implies that $\varphi(\beta) = \beta_i^k$ for some $1 \leq i \leq j$ and $k \in \mathbb{Z}$. Since $\varphi|_A$ is an automorphism of A, we see that (iii) implies $\varphi(B)$ must be a free generating set for $\langle \mathbf{C}_2 \rangle$. We therefore must have $\varphi(\beta) = \beta_i^k$ for $k \in \{1, -1\}$ and we are done. □

The following applies to G_{10}, G_{12}, and G_{13}. This result is analogous to (i) and (ii) of Proposition 6.9 (which does not apply to these three groups because here $\mathbf{C}_2$ is not a union of cyclic subgroups).

Proposition 6.6. *Let G be a crystallographic group with presentation of the form given in Eq. (4.1). (Therefore $A = \langle x, y, z \rangle$.) Let $\varphi \in \mathcal{W}(G)$. Then $\varphi(y) \in \{y, y^{-1}\}$ and $\varphi(Af) = Af$ for all $f \in F$.*

Proof. The generators used in the group presentation are x, y, z, r, t and we define $F = \{r, rt, t, 1\}$. Every element in the At coset is an involution, and this is not the case for any other coset. This implies $\varphi(At) = At$, and therefore $\varphi(Art) \in \{Ar, Art\}$.

By Proposition 6.5 (ii) we know $\varphi(\mathbf{C}_2) = \mathbf{C}_2$ and here $\mathbf{C}_2$ is the union of a free abelian subgroup of rank two and a cyclic subgroup. Since $\varphi|_A$ is a bijective homomorphism, it must preserve this structure and in particular, it must map the cyclic subgroup to itself. The cyclic subgroup contained in $\mathbf{C}_2$ is $\langle y \rangle$. We may therefore assume $\varphi(y) = y^\delta$ for $\delta \in \{-1, 1\}$.

Now $(rt)^2 \in A$ and $y^{rt} = y^{-1}$, thus by Lemma 6.4 we have $\varphi(y)^{\varphi(rt)} = \varphi(y)^{-1}$, i.e. $(y^\delta)^{\varphi(rt)} = y^{-\delta}$. If $\varphi(rt) \in Ar$ we would have a contradiction since y commutes with every element in Ar. We conclude that $\varphi(Art) = Art$ and thus $\varphi(Ar) = Ar$. □

The following corollary applies to $G_{21}, G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68}.

Corollary 6.7. *Let G be a crystallographic group with translation subgroup $A = \langle x, y, z \rangle \cong \mathbb{Z}^3$ and $\mathbf{C}_2 = \langle x^2y^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$. Let $\varphi \in \mathcal{W}(G)$. For $\beta \in \{x^2y^{-1}, y\}$ we have $\varphi(\beta) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$. We also have $\varphi(z) \in \{z, z^{-1}\}$.*

Proof. By Proposition 6.5 (iv) with $B = \{x^2y^{-1}, y, z\}$ we have

$$\{\varphi(x^2y^{-1}), \varphi(y), \varphi(z)\} \subseteq \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}.$$

Now since $\varphi|_A$ is a homomorphism,

$$\varphi(x^2y^{-1})\varphi(y) = \varphi(x^2y^{-1} \cdot y) = \varphi(x^2) = \varphi(x)^2$$

must be a square of an element in A. The bijectivity of φ requires $\varphi(x^2y^{-1})\varphi(y)$ to be a product of two distinct elements in $\{(x^2y^{-1})^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. In order for this product to be a square, one of the two factors must be in $\{(x^2y^{-1})^{\pm 1}\}$ and the other must be in $\{y^{\pm 1}\}$. In other words, $\varphi(x^2y^{-1})\varphi(y)$ cannot be a square if either of $\varphi(x^2y^{-1})$ or $\varphi(y)$ is in $\{z^{\pm 1}\}$. Therefore by bijectivity we must have $\varphi(z) \in \{z^{\pm 1}\}$. □

The following applies to $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42}.

Lemma 6.8. *Let G be a group with presentation of the form given in Eq. (4.3). We define $F = \{1, p, s, ps\}$. Let $\varphi \in \mathcal{W}(G)$. Then*

(i) $Z(G) = \langle z \rangle$.

(ii) $a \in \mathbf{C}_2$ *if and only if both* $a^p = a^{-1}$ *and* $a \in \{a^s, a^{ps}\}$.

(iii) $\mathbf{C}_2$ *is the union of two cyclic groups.*

(iv) $\langle \mathbf{C}_2 \rangle \cap Z(G) = 1$.

(v) $\varphi(z) \in \{z^{\pm 1}\}$.

(vi) There exists an outer automorphism $\psi_\iota : G \to G$ *such that*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1}).$$

Composing φ *with this map if necessary we may assume that* $\varphi(z) = z$.

Proof. The relations given in the group presentation indicate that for $i, j, k \in \mathbb{Z}$ we have $(x^i y^j z^k)^p = x^{-i} y^{-j} z^u$ where $u \in \{k, j+k, i+j+k\}$. This shows that for $a \in A$,

$$\text{if } a^p = a, \text{ then } a \in \langle z \rangle. \tag{6.9}$$

It follows that $Z(G) \subseteq \{a \in A \;:\; (a, p) = 1\} = \langle z \rangle$. The reverse inclusion is clear since the relations in the presentation of G state that z commutes with x, y, p and s. This proves (i).

Recall that $\mathbf{C}_2$ is the set of elements $a \in G$ such that $a^G = \{a, a^{-1}\}$. Therefore, $1 \neq a \in \mathbf{C}_2$ is inverted by the action of two of the elements of F and fixed by the action of the other two elements of F, one of which is of course the identity. Eq. (6.9) shows that p cannot be the non-identity element of F that fixes $a \in \mathbf{C}_2$, since any element fixed by p is central and by Proposition 6.5 (i), the only central element contained in $\mathbf{C}_2$ is the identity. Hence we have (ii).

Statement (iii) follows from (ii). The set of elements fixed by s is a cyclic subgroup and the set of elements fixed by ps is another cyclic subgroup. Any element in one of these two cyclic subgroups is inverted by p. Therefore, $\mathbf{C}_2$ is comprised of the union of these two cyclic subgroups The relations in the presentation of G determine which elements generate the two cyclic subgroups. (Refer to Table 6.1.)

To prove (iv) we use the facts given in Proposition 6.3, specifically, the generators of the cyclic subgroups that comprise $\mathbf{C}_2$. Thus we see that for groups G_{25}, G_{26}, and G_{27}, we have $\langle \mathbf{C}_2 \rangle = \langle x, y \rangle$. For groups G_{38} and G_{39}, we have $\langle \mathbf{C}_2 \rangle = \langle x, y^2 z^{-1} \rangle$. For group G_{42}, we have $\langle \mathbf{C}_2 \rangle = \langle x^2 z^{-1}, y^2 z^{-1} \rangle$. Each of these subgroups intersects the cyclic subgroup $\langle z \rangle = Z(G)$ trivially.

We will show that $\varphi(z) \in \{z, z^{-1}\}$ results from the fact that $\varphi|_A$ is a bijective homomorphism. We have $\varphi(Z(G)) = Z(G)$, by Proposition 1.1 (iv), thus $\varphi(z) \in \langle z \rangle$. Let $\varphi(z) = z^k$ for some $k \in \mathbb{Z}$, then as $\varphi|_A$ is a homomorphism $\langle \varphi(z) \rangle = \langle z^k \rangle$. If $k \notin \{\pm 1\}$ then $\langle \varphi(z) \rangle$ would be a proper subgroup of $\langle z \rangle$, contradicting the surjectivity of φ. This proves (v).

The map ψ_ι satisfies the relations in each of the six presentations of these groups thus it is in Aut(G). Since $\psi_\iota(z) = z^{-1}$, and $\varphi(z) \in \{z, z^{-1}\}$ by (v), we therefore have (vi). □

Definition Let $j \in \mathbb{N}$. Given a set $B = \{\beta_i\}_{i=1}^{j} \subseteq A$ and $f \in F$ we define

$$\mathrm{Inv}(B, f) = \{\beta \in B \,:\, \beta^f = \beta^{-1}\}.$$

When B is understood then we may write $\mathrm{Inv}(B, f)$ simply as $\mathrm{Inv}(f)$.

The following proposition applies to twenty-eight of the thirty-one groups listed in Tables 4.1 and 4.2. (It does not apply to G_{10}, G_{12}, and G_{13}.) Result (iii) applies to the twenty-four groups that have presentations of the form given in Eqs. (4.3), (4.4), or (4.5). Result (iv) applies only to the eighteen groups listed on Table 4.2.

Proposition 6.9. *For $m, n \in \mathbb{N}$, such that $2 \leq m \leq n$ let G be a group with normal abelian subgroup $A \cong \mathbb{Z}^n$ and $G/A \cong C_2^m$. Suppose that for some $2 \leq j \leq n$ there exists a set $B = \{\beta_i\}_{i=1}^{j} \subseteq \mathbf{C}_2$ such that $\mathbf{C}_2 = \bigcup_{i=1}^{j} \langle \beta_i \rangle$. Assume also that B is a free generating set for $\langle \mathbf{C}_2 \rangle \cong \mathbb{Z}^j$. Lastly we assume that the action of G/A on B defined by $\beta \cdot (Ag) = \beta^g$ is* *well-defined and faithful, so that* $\beta^{g_1} = \beta^{g_2}$ *holds for all* $\beta \in B$ *if and only if* $Ag_1 = Ag_2$*. Let* $\varphi \in \mathcal{W}(G)$*.*

(i) For $f, g \in F$*, if* $\varphi(Af) = Ag$*, then* $|\mathrm{Inv}(B, f)| = |\mathrm{Inv}(B, g)|$*.*

(ii) $\varphi(\beta) \in \beta^G$ *for all* $\beta \in B$ *if and only if* $\varphi(Af) = Af$ *for all* $f \in F$*.*

(iii) If $j = m$ *and* $\varphi(\beta) \in \beta^G$ *for all* $\beta \in B$*, then there exists* I_f *for some* $f \in F$ *so that* $(I_f \circ \varphi)|_{\langle \mathbf{C}_2 \rangle} = \mathrm{Id}$*.*

(iv) If $j = m = n$ *and* $\varphi(\beta) \in \beta^G$ *for all* $\beta \in B$*, then there exists* I_f *for some* $f \in F$ *so that* $(I_f \circ \varphi)|_A = \mathrm{Id}$*.*

Proof. We prove (i) using Lemma 6.4. Let $f, g \in F$. Fix $\beta \in \mathrm{Inv}(f)$, so that $\beta^f = \beta^{-1}$. By the Lemma, $\varphi(\beta)^{\varphi(f)} = \varphi(\beta)^{-1}$. By assumption $\varphi(Af) = Ag$, thus the action of $\varphi(f)$ on A must be equal to the action of g on A so we have $\varphi(\beta)^g = \varphi(\beta)^{-1}$. By Proposition 6.5 (iv) we have $\varphi(\beta) \in \{(\beta')^{\pm 1}\}$ for some $\beta' \in B$. As φ respects inverses we see that the statement $\varphi(\beta) \in \{(\beta')^{\pm 1}\}$ implies $(\beta')^g = (\beta')^{-1}$. Thus $\beta' \in \mathrm{Inv}(g)$. Since φ is bijective, this shows that for every $\beta \in \mathrm{Inv}(f)$ there exists a $\beta' \in \mathrm{Inv}(g)$ and therefore $|\mathrm{Inv}(f)| \leq |\mathrm{Inv}(g)|$. To prove that $|\mathrm{Inv}(f)| \geq |\mathrm{Inv}(g)|$ we note that $\varphi \in \mathcal{W}(G)$ implies $\varphi^{-1} \in \mathcal{W}(G)$, $\varphi^{-1}(Ag) = Af$ and apply the previous argument. Therefore $|\mathrm{Inv}(f)| = |\mathrm{Inv}(g)|$, proving (i).

We prove (ii). ($\Longrightarrow$) Suppose contrapositively that $\varphi(f_1) \in Af_2$ for some $f_1, f_2 \in F$, with $f_1 \neq f_2$. Since $f_1 \neq f_2$, by interchanging f_1 and f_2 if necessary we may assume there exists some $\beta \in B$ such that $\beta \in \mathrm{Inv}(f_1), \beta \notin \mathrm{Inv}(f_2)$; thus $\beta^{f_2} = \beta$ but $\beta^{f_1} = \beta^{-1}$. Using $\varphi(f_1) \in Af_2$ and applying Lemma 6.4 to the statement $\beta^{f_1} = \beta^{-1}$, we have $\varphi(\beta)^{f_2} = \varphi(\beta)^{\varphi(f_1)} = \varphi(\beta)^{-1}$. This shows $\varphi(\beta)$ is inverted by the action of f_2, although we know β and its inverse are not (because $\beta \notin \mathrm{Inv}(f_2)$). From this we conclude that $\varphi(\beta) \notin \{\beta^{\pm 1}\} = \beta^G$.

($\Longleftarrow$) Conversely, assume that $\varphi(Af) = Af$ for all $f \in F$ and suppose to the contrary that there exists $\beta \in B$ such that $\varphi(\beta) \notin \beta^G$. By Proposition 6.5 (iv) we know $\varphi(\beta) \in (\hat{\beta})^G = \{\hat{\beta}^{\pm 1}\}$ for some $\hat{\beta} \in B$. In other words, φ permutes the conjugacy classes in the collection $\{\beta^G : \beta \in B\}$. Define the subset $B' \subseteq B$ to be

$$B' = \{\beta \in B : \varphi(\beta^G) \neq \beta^G\},$$

and define a function $\lambda : B' \to \mathbb{N}$ to be

$$\lambda : \beta \mapsto |\{f \in F : \beta \in \text{Inv}(f)\}|.$$

(Note that the codomain of λ does not include zero because $\lambda(\beta) = 0$ means β commutes with every element of F, which would imply β is central, a contradiction.) Choose $\beta_1 \in B'$ so that $\lambda(\beta_1)$ is maximal, i.e. $\lambda(\beta_1) = \max\{\lambda(\beta) : \beta \in B'\}$. Let $\varphi(\beta_1^G) = \beta_2^G$. Note that $\beta_2 \in B'$ (because φ is bijective) and thus $\lambda(\beta_1) \geq \lambda(\beta_2)$. In other words, β_1 is inverted by at least as many elements of F as β_2 is. This, combined with the fact that the action of G/A on B is faithful, ensures that there exists an $h \in F$ such that $\beta_1 \in \text{Inv}(h)$ but $\beta_2 \notin \text{Inv}(h)$. We will show that $\beta_1 \in \text{Inv}(h)$ implies that $\beta_2 \in \text{Inv}(h)$, thus arriving at a contradiction.

We have $\beta_1 \in \text{Inv}(h)$ i.e. $\beta_1^h = \beta_1^{-1}$, and applying Lemma 6.4 to this equation gives $\varphi(\beta_1)^{\varphi(h)} = \varphi(\beta_1)^{-1}$. Since φ respects inverses, $\beta_2^{\varphi(h)} = \beta_2^{-1}$. We are assuming $\varphi(Ah) = Ah$ so we know $\varphi(h) \in Ah$, thus $\beta_2^h = \beta_2^{-1}$. This shows that $\beta_2 \in \text{Inv}(h)$, giving the needed contradiction.

Before we can prove (iii) we will first need to prove that when $j = m$, the collection $\{\text{Inv}(f)\}_{f \in F}$ is $\mathcal{P}(B)$, the power set of B. By definition $\{\text{Inv}(f)\}_{f \in F}$ is a subset of the power set of B, thus it suffices to show that the cardinality of $\{\text{Inv}(f)\}_{f \in F}$ is at least $|\mathcal{P}(B)|$. We will use the fact that G/A acts faithfully on B. If $f, g \in F$ and $f \neq g$, then $j = m$ shows that there exists some $\beta \in B$ such that $\beta^f \neq \beta^g$ thus $\text{Inv}(f) \neq \text{Inv}(g)$. This shows that

$$|\{\text{Inv}(f) : f \in F\}| \geq |F| = |G/A| = 2^m = 2^j = |\mathcal{P}(B)|.$$

We are now ready to prove (iii). By assumption we have $j = m$ and $\varphi(\beta_i) \in \beta_i^G = \{\beta_i, \beta_i^{-1}\}$ for $1 \leq i \leq j$. Thus there exists some subset $B_{\text{Inv}} = \{\beta \in B : \varphi(\beta) = \beta^{-1}\}$, but also, φ fixes all elements in $B \setminus B_{\text{Inv}}$. Since $\{\text{Inv}(f)\}_{f \in F}$ is the power set of B, we know there exists an $f \in F$ such that $\text{Inv}(f) = B_{\text{Inv}}$. In other words, there exists an $f \in F$ such that $(\varphi \circ I_f) : \beta_i \mapsto \beta_i$ for $1 \leq i \leq n$. Composing we have $\varphi|_B = \text{Id}$ and since $\varphi|_A$ is a homomorphism and B is a generating set for $\langle \mathbf{C}_2 \rangle$, we now have $\varphi|_{\langle \mathbf{C}_2 \rangle} = \mathrm{Id}$ and we are done.

Lastly we show that statement (iv) follows from (iii) when $n = j = m$. Recall that both A and $\langle \mathbf{C}_2 \rangle$ are free abelian groups and $j = n$ means that $\mathrm{rank}(\langle \mathbf{C}_2 \rangle) = \mathrm{rank}(A)$. It follows that $\langle \mathbf{C}_2 \rangle$ has finite index in A so we may write $|A : \langle \mathbf{C}_2 \rangle| = \ell$ for some $\ell \in \mathbb{N}$. Let $A = \langle x_1, x_2, \ldots, x_n \rangle$. Note that for every generator x_i we have $x_i^\ell \in \langle \mathbf{C}_2 \rangle$, and so by (iii) we may assume $\varphi(x_i^\ell) = x_i^\ell$. Since $\varphi|_A$ is a homomorphism, we have

$$\varphi(x_i)^\ell = \varphi(x_i^\ell) = x_i^\ell,$$

which can only be true if $\varphi(x_i) = x_i$, since $A \cong \mathbb{Z}^n$. This is true for all generators x_i of A, proving (iv). $\square$

The following is a corollary to Proposition 6.9 and it applies to $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42}.

Corollary 6.10. *Let G be a group with a presentation of the form given in Eq. (4.3). Define $F = \{1, p, s, ps\}$. Let $\varphi \in \mathcal{W}(G)$. Then*

(i) $\varphi(Ap) = Ap$.

(ii) *If $\varphi(Af) = Af$ for all $f \in F$ and $\varphi(z) = z$, then composing with inner automorphisms as necessary we may assume that $\varphi|_A = \mathrm{Id}$.*

Proof. By Lemma 6.8 (iii) there exist $\beta_1, \beta_2 \in \mathbf{C}_2$ so that $\mathbf{C}_2 = \langle \beta_1 \rangle \cup \langle \beta_2 \rangle$. To prove (i) we apply Proposition 6.9 (i) with $B = \{\beta_1, \beta_2\}$. For these groups we have $|\mathrm{Inv}(p)| = 2$ but $|\mathrm{Inv}(s)| = |\mathrm{Inv}(ps)| = 1$. Thus φ must map the Ap coset to itself.

To prove (ii) we assume that $\varphi(Af) = Af$ for all $f \in F$ and we apply Proposition 6.9 (ii). This gives $\varphi(\beta) \in \beta^G$ for all $\beta \in B$. Then applying Proposition 6.9 (iii) we know there exist inner automorphisms so that composing φ with these automorphisms we have $\varphi|_{\langle \mathbf{C}_2 \rangle} = \mathrm{Id}$. Now by hypothesis $\varphi(z) = z$ so, since $\varphi|_A$ is an isomorphism, we have $\varphi|_{\langle \mathbf{C}_2, z \rangle} = \mathrm{Id}$. We will show that $\langle \mathbf{C}_2, z\rangle$ is a finite index subgroup of A. Since $\varphi|_A$ is an isomorphism, this implies that $\varphi|_A = \mathrm{Id}$.

By Lemma 6.8 (i), we have $Z(G) = \langle z\rangle$ and by Proposition 6.5 (i), $\langle z\rangle$ intersects $\langle \mathbf{C}_2\rangle$ trivially. Statement (iii) of Lemma 6.8 indicates that $\langle \mathbf{C}_2\rangle$ has rank two. Thus $\langle \mathbf{C}_2, z\rangle$ has rank three, which implies it has finite index in A, and we are done. □

The following is a corollary to Proposition 6.9 and it applies to the space groups numbered between 47 and 74 which are listed in Table 4.2.

Corollary 6.11. *Let G be a group with a presentation of the form given in Eqs. (4.4) or (4.5). We write the presentation of G using generators x, y, z, p, r, t and we define $F = \{p, r, pr, prt, rt, pt, t, 1\}$. Let $\varphi \in \mathcal{W}(G)$. Then we have*

(i) $\varphi(At) = At$.

(ii) For $f \in \{p, r, pr\}$ we have $\varphi(Af) = Ag$ for some $g \in \{p, r, pr\}$.

(iii) For $f \in \{prt, rt, pt\}$ we have $\varphi(Af) = Ag$ for some $g \in \{prt, rt, pt\}$.

Proof. For these groups we have

$$|\mathrm{Inv}(t)| = 3;\ |\mathrm{Inv}(p)| = |\mathrm{Inv}(r)| = |\mathrm{Inv}(pr)| = 2;\ |\mathrm{Inv}(prt)| = |\mathrm{Inv}(rt)| = |\mathrm{Inv}(pt)| = 1.$$

Applying statement (i) of Proposition 6.9 gives the result. □

In step three it is often helpful to consider which cosets contain elements of order 2 since cosets containing involutions may only be mapped to cosets that contain involutions. When $f \in F$ has order 2 it is clear that Af contains order 2 elements. However, it is possible to have $f^2 \neq 1$ and yet have involutions in Af. The following Lemma makes it easy to determine whether or not a given coset contains involutions. (Note that it only applies to groups having presentations of the form given in Eqs. (4.1), (4.4), or (4.5).)

Lemma 6.12. *Let G be a group with an abelian normal subgroup A and suppose $t \in G$ satisfies $t^2 = 1$ and $a^t = a^{-1}$ for any $a \in A$. Let $f \in F$ and assume $f^2 \in A$. Then the Af coset contains elements of order 2 if and only if $f^2 \in K_{ft}$.*

Proof. Let $a \in A$. Note that as $f^2 \in A$, $a^{f^{-1}} = a^f$. Then

$$(af)^2 = 1 \iff afaf = aa^f(f^2) = 1$$
$$\iff f^2 = a^{-1}(a^f)^{-1} = a^{-1}a^{ft} = (a, ft).$$

This shows that there exists an $a \in A$ such that (af) has order 2 if and only if there exists an $a \in A$ such that $f^2 = (a, ft)$. By Lemma 2.2 this is equivalent to $f^2 \in K_{ft}$. □

6.4 Step four

In this section we will prove results useful for proving step 4. These results will be applied in Ch. 7 and Ch. 8 to the thirty-one space groups listed in Tables 4.1 and 4.2.

The following applies to $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42}.

Proposition 6.13. *Let G be a group with a presentation of the form given in Eq. (4.3). We define $F = \{1, p, s, ps\}$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $\varphi(p) = p$. Then $\varphi(f) = f$ for all $f \in F$.*

Proof. We will prove two results and then use them to prove the proposition.

Claim 1: For $b \in A$, if $b^s = b^{ps} = b^{-1}$, then $b = 1$.

To prove this we first note that $b^s = b^{ps}$ implies that b commutes with p and therefore $b^G = \{b, b^{-1}\}$, so $b \in \mathbf{C}_2$. By Lemma 6.8 (iii) we know that $\mathbf{C}_2$ is the union of two cyclic subgroups that intersect trivially. By Lemma 6.8 (ii) we know one cyclic subgroup contains all elements of $\mathbf{C}_2$ that are inverted by the action of ps, and the other contains all elements of $\mathbf{C}_2$ that are inverted by the action of s. It follows that the only element of $\mathbf{C}_2$ (and therefore any element of A) that is inverted by both s and ps is the identity. This proves Claim 1.

Claim 2: For $f \in F$ we have $f^2 \in Z(G)$.

Now recall that for $f \in F$ we have defined $\alpha_f = f^2$. We have $Z(G) = \langle z \rangle$ by Lemma 6.8 (i), and the relations in the presentation of G state that α_p, α_s and $\alpha_{ps} = \alpha_p\alpha_s$ are all contained in $\langle z \rangle$. (See Table 4.1.) This proves Claim 2.

We now show that $\varphi|_A = \mathrm{Id}$ and $\varphi(p) = p$ imply that $\varphi(f) = f$ for all $f \in F$. By Proposition 6.9 (ii) we have $\varphi(Af) = Af$ for all $f \in F$. Therefore $\varphi(ps) = bps$ and $\varphi(s) = cs$ for some $b, c \in A$.

Squaring both sides of $\varphi(ps) = bps$ we have

$$\alpha_{ps} = \varphi(\alpha_{ps}) = \varphi((ps)^2) \sim (bps)^2 = bb^{ps}psps = bb^{ps}\alpha_{ps}.$$

Since α_{ps} is central, conjugacy implies equality; therefore $\alpha_{ps} = bb^{ps}\alpha_{ps}$ and so $b^{ps} = b^{-1}$. We also have $\varphi(p^{-1} \cdot ps) \sim p^{-1}bps$ and squaring both sides of this relation gives

$$\alpha_s = \varphi(\alpha_s) = \varphi(s^2) \sim (p^{-1}bps)^2 = (b^p s)^2 = b^p s b^p s = b^p b^{ps} s^2 = b^p b^{ps}\alpha_s.$$

Again, conjugacy implies equality since α_s is central, so we have

$$\alpha_s = b^p b^{ps}\alpha_s \text{ thus } (b^p)^{-1} = b^{ps} \text{ and so } b^{-1} = b^s.$$

We have shown that $b^s = b^{ps} = b^{-1}$ so we must have $b = 1$, i.e. $\varphi(ps) = ps$.

Similarly, squaring both sides of $\varphi(s) = cs$ we have

$$\alpha_s = \varphi(s^2) \sim (cs)^2 = cc^s s^2 = cc^s\alpha_s.$$

Conjugacy again implies equality so $\alpha_s = cc^s\alpha_s$ thus $c^s = c^{-1}$. We also have $\varphi(p \cdot s) \sim pcs = c^p ps$ and squaring both sides gives

$$\alpha_{ps} = \varphi((ps)^2) \sim (c^p ps)^2 = c^p (c^p)^{ps} psps = c^p c^s \alpha_{ps}.$$

Again we may assume we have equality so $\alpha_{ps} = c^p c^s \alpha_{ps}$ thus $(c^p)^{-1} = c^s$ and conjugating both sides by p gives $c^{-1} = c^{ps}$. We have shown that $c^s = c^{ps} = c^{-1}$ so $c = 1$, and thus $\varphi(s) = s$. □

The following proposition applies to groups G_{10}, G_{12}, G_{13}, and also the eighteen groups listed in Table 4.2. However, this result is not useful for the ten groups where $K = \langle x^2, y^2, z^2 \rangle$. It is only useful when $\langle x^2, y^2, z^2 \rangle \lneq K$, which is the case in the eleven groups $G_{12}, G_{63}, G_{64}, G_{65}$, $G_{66}, G_{67}, G_{68}, G_{69}, G_{72}, G_{73}$, and G_{74}.

Proposition 6.14. *Let G be a group with a normal abelian subgroup $A = \langle x_1, x_2, \ldots \rangle$.*

Suppose there exists $t \in F$ such that $t^2 = 1$ and $(at)^2 = 1$ for all $a \in A$. Let $f \in F$ and assume $ft \in F$. Let $\alpha_f = f^2$ and similarly $\alpha_{ft} = (ft)^2$. Assume $\alpha_f, \alpha_{ft} \in \mathbf{C}_2$. Let $\varphi \in \mathcal{W}(G)$ and assume $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$. Given $c \in A$, if we have $(c, f) \notin \langle x_1^2, x_2^2, \ldots \rangle$, then $\varphi(t) \neq ct$.

Proof. We will prove the contrapositive:

$$\text{If } \varphi(t) = ct \text{ for some } c \in A, \text{ then } (c, f) \in \langle x_1^2, x_2^2, \ldots \rangle.$$

Note that for $a \in A$ we have $a^{ft} = a^{tf}$, which is a consequence of the relation $a^t = a^{-1}$ for all $a \in A$. Also note that $a^{f^{-1}} = a^f$ and $a^{t^{-1}} = a^t$ since $f^2, t^2 \in A$. We will use these two facts throughout this proof.

Let $\varphi(f) = bf$ for some $b \in A$. Squaring both sides gives

$$\alpha_f = \varphi(\alpha_f) = \varphi(f \cdot f) \sim bfbf = bb^f f^2 = bb^f \alpha_f.$$

Since $\alpha_f^G = \{\alpha_f^{\pm 1}\}$, we see that $\alpha_f \sim bb^f \alpha_f$ implies that $bb^f = \alpha_f^i$ for $i \in \{-2, 0\}$. Conjugating by t and solving for b^{ft} we have $b^{ft} = b\alpha_f^{-i}$.

Recall that by assumption $\varphi(t) = ct$ for some $c \in A$, thus we have $\varphi(f \cdot t) \sim bfct$. Squaring both sides of this relation gives

$$\alpha_{ft} = \varphi(\alpha_{ft}) = \varphi(ft \cdot ft) \sim bfct\, bfct = bc^f b^{ft} c^t (ft)^2 = bc^f b^{ft} c^t \alpha_{ft}.$$

Since $\alpha_{ft}^G = \{\alpha_{ft}^{\pm 1}\}$ we have $bc^f b^{ft} c^t = \alpha_{ft}^j$ for $j \in \{0, -2\}$. Using $b^{ft} = b\alpha_f^{-i}$ and algebraically rearranging we have

$$c^f c^t = b^{-1}(b\alpha_f^{-i})^{-1}\alpha_{ft}^j = b^{-2}\alpha_f^i \alpha_{ft}^j.$$

Since i and j are either 0 or -2, this shows that $c^f c^t = (c, f)$ is the square of an element in A, i.e. $(c, f) \in \langle x_1^2,\, x_2^2,\, \ldots \rangle$. □

The following applies to $G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68}.

Corollary 6.15. *Let G be a group with a presentation of the form given in Eq. (4.4) (hence we write the presentation of G with generators x, y, z, p, r, and t), and assume that*

$\delta = 1, \alpha_r \in \langle y \rangle$, and $\alpha_{rt} \in \langle z \rangle$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $\varphi(Ar) = Ar$. Then $\varphi(t) \neq xt$.

Proof. We will use Proposition 6.14 which states that if $(x, r) \notin \langle x^2, y^2, z^2 \rangle$ then $\varphi(t) \neq xt$. To justify applying the proposition we note that by Proposition 6.3 we have $\mathbf{C}_2 = \langle x^2 y^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$, thus $\alpha_r, \alpha_{rt} \in \mathbf{C}_2$. We have $(x, r) = x^{-2} y$ which is not a square. Therefore, by the proposition, $\varphi(t) \neq xt$. □

The following applies to G_{72}, G_{73}, and G_{74}.

Corollary 6.16. *Let G be a group with a presentation of the form given in Eq. (4.5) (hence we write the presentation of G with generators x, y, z, p, r, and t), and assume that $\alpha_p \in \langle z \rangle, \alpha_{pt} \in \langle x^2 y^{-1} z^{-1} \rangle \cup \langle y \rangle$ and $\delta = 1$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $\varphi(Ap) = Ap$. Then $\varphi(t) \neq xt$.*

Proof. To prove this is a straightforward application of Proposition 6.14. By Proposition 6.3 we have $\mathbf{C}_2 = \langle x^2 y^{-1} z^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$. Thus we have $\alpha_p, \alpha_{pt} \in \mathbf{C}_2$. Then by the proposition, since

$$(x, p) = x^{-2} z \notin \langle x^2, y^2, z^2 \rangle$$

we conclude $\varphi(t) \neq xt$. □

Proposition 6.17. *Let G be a group with abelian normal subgroup A and let $|G/A| = n \in \mathbb{N}$. Let $\varphi \in \mathcal{W}(G)$ and assume $\varphi|_A = \mathrm{Id}$. Fix $f \in F$ such that $\alpha = f^2 \in A$. Let $\varphi(f) = bf$ for some $b \in A$. Then*

(i) $b^f = b^{-1}$.

Furthermore, suppose there exists $t \in F$ such that $a^t = a^{-1}$ for all $a \in A$ and $(ft)^2 \in A$. Assume we have $\varphi(t) = t$. Let $\alpha_{ft} = (ft)^2$. Then

(ii) $\alpha_{ft} \sim b^2 \alpha_{ft}$, in other words, $b^2 \alpha_{ft} \in \alpha_{ft}^G$.

From the above we immediately have these two statements:

(iii) If $\alpha_{ft} \in \mathbf{C}_2$ *(i.e.* $\alpha_{ft}^G = \{\alpha_{ft}, \alpha_{ft}^{-1}\}$*), then* $b \in \{1, \alpha_{ft}^{-1}\}$*;*

(iv) If ft *has order 2, then* $b = 1$*, i.e.* $\varphi(f) = f$*.*

Proof. For any $k \in \mathbb{Z}$ we have $\varphi(\alpha^k \cdot f) \sim \alpha^k bf$. Note that α commutes with f and thus also with bf. Then squaring both sides we have

$$\alpha^{2k+1} = \varphi(\alpha^{2k} f^2) \sim \alpha^{2k} bfbf = \alpha^{2k} b(\alpha f^{-1})bf = \alpha^{2k} b\alpha b^f = \alpha^{2k+1} bb^f. \tag{6.10}$$

Let $\gamma = bb^f$ and note that to prove $b^f = b^{-1}$ it suffices to show that $\gamma = 1$. Now Eq. (6.10) becomes $\alpha^{2k+1} \sim \alpha^{2k+1}\gamma$. This implies that for any $j \in \mathbb{Z}$,

$$\alpha^{(2k+1)j} \sim (\alpha^{2k+1}\gamma)^j = \alpha^{(2k+1)j}\gamma^j.$$

We note that α and γ are fixed, but the stated conjugacy must hold for any $j, k \in \mathbb{Z}$. Recall $n = |G/A|$ and put $(2k+1)j = 3^n$. (For each $j \in \{1, 3, 9, \ldots, 3^n\}$ there is a corresponding value of k so as to ensure $(2k+1)j = 3^n$.) Thus we have

$$\alpha^{3^n} \sim \alpha^{3^n}\gamma^j. \tag{6.11}$$

Eq. (6.11) thus yields the following $n+1$ statements:

$$\begin{aligned} \alpha^{3^n} &\sim \alpha^{3^n}\gamma^1; \\ \alpha^{3^n} &\sim \alpha^{3^n}\gamma^3; \\ \alpha^{3^n} &\sim \alpha^{3^n}\gamma^9; \\ &\vdots \\ \alpha^{3^n} &\sim \alpha^{3^n}\gamma^{3^n}. \end{aligned}$$

Now if $\gamma \neq 1$ then this implies that $|(\alpha^{3^n})^G| \geq n+1$. Since $\alpha^{3^n} \in A$ and $n = |G/A|$ this is a contradiction. We conclude that $\gamma = 1$ and so $b^f = b^{-1}$.

It follows that b commutes with ft. Now since $\varphi(t) = t$ we have $\varphi(f \cdot t) \sim bft$. Squaring both sides gives $(ft)^2 \sim (bft)^2 = b^2(ft)^2$, i.e. $\alpha_{ft} \sim b^2\alpha_{ft}$. □

Proposition 6.18. *Let* G *be a group. Let* $f_1, f_2, t \in G$ *and assume* $t^2 = 1$*. Let* $\alpha_1 = (f_1t)^2$ *and* $\alpha_2 = (f_2t)^2$*. Let* $\varphi \in \mathcal{W}(G.)$

(i) *For* $i \in \{1, 2\}$, *if* $\varphi(f_i) = \alpha_i^{-1} f_i$ *then* $(I_t \circ \iota \circ \varphi)(f_i) = f_i$.

(ii) *If* $f_i t$ *has order 2 then* $I_t \circ \iota$ *acts trivially on* f_i, *and also on* t.

(iii) *If* $\varphi(f_1 f_2) \sim f_1 f_2 \nsim \alpha_1^{-1} f_1 f_2$ *and* $\varphi(f_2) = f_2$ *then* $\varphi(f_1) \neq \alpha_1^{-1} f_1$.

Proof. A straightforward calculation proves (i):

$$\begin{aligned}(I_t \circ \iota \circ \varphi)(f_i) =& (I_t \circ \iota)(\alpha_i^{-1} f_i) \\ =& (I_t \circ \iota)((f_i t)^{-2} f_i) \\ =& (I_t \circ \iota)(t f_i^{-1} t f_i^{-1} f_i) \\ =& (I_t \circ \iota)((f_i^{-1})^t) \\ =& f_i.\end{aligned}$$

The first statement in (ii) follows from (i) with $\alpha_i = 1$. It is also clear that $I_t \circ \iota$ acts trivially on t since $t = t^{-1}$ and since $I_t(t) = t$.

To prove (iii) we assume that $\varphi(f_1 f_2) \sim f_1 f_2$ and $\varphi(f_2) = f_2$. Now suppose to the contrary that $\varphi(f_1) = \alpha_1^{-1} f_1$. Then

$$f_1 f_2 \sim \varphi(f_1 \cdot f_2) \sim \alpha_1^{-1} f_1 \cdot f_2,$$

which contradicts $f_1 f_2 \nsim \alpha_1^{-1} f_1 f_2$ and we are done. □

Proposition 6.19. *The following maps are automorphisms of the indicated groups. (One can show that these are outer automorphisms.)*

$$
\begin{aligned}
G_{10}, G_{13}: &\qquad \psi_x : (x, y, z, r, t) \mapsto (x, y, z, xr, xt),\\
G_{10}, G_{12}, G_{13}: &\qquad \psi_y : (x, y, z, r, t) \mapsto (x, y, z, r, yt),\\
G_{10}, G_{12}, G_{13}: &\qquad \psi_z : (x, y, z, r, t) \mapsto (x, y, z, zr, zt),\\
G_{16}, G_{17}: &\qquad \psi_x : (x, y, z, p, r) \mapsto (x, y, z, xp, xr),\\
G_{22}: &\qquad \psi_x : (x, y, z, p, r) \mapsto (x, y, z, xy^{-1}p, xr),\\
G_{16}, G_{17}, G_{21}: &\qquad \psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r),\\
G_{16}, G_{17}, G_{21}, G_{22}: &\qquad \psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr),\\
G_{25}, G_{26}, G_{27}, G_{38}, G_{39}: &\qquad \psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),\\
G_{25}, G_{26}, G_{27}: &\qquad \psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys),\\
G_{47}, G_{49}, G_{50}, G_{51}, G_{53}, G_{54}, G_{55}, G_{57}: &\qquad \psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),\\
\textit{All groups listed in Table 4.2 except } G_{69}: &\qquad \psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),\\
\textit{All groups listed in Table 4.2}: &\qquad \psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).
\end{aligned}
$$

Proof. This follows from the relations in the respective group presentations. □

6.5 Step five

Here we prove Theorem 6.21 which shows that step five is true for any n-dimensional crystallographic group. We begin with a lemma.

Lemma 6.20. *Let G be a group with a normal abelian subgroup A. Let $\varphi \in \mathcal{W}(G)$. Suppose that $\varphi|_A = \mathrm{Id}$ and $t \in G$ satisfies $\varphi(t) = t$. Let $a, b \in A$. If $\varphi(at) = bt$ then $a \sim b$.*

Proof. Given the hypotheses we have

$$a \sim a^t = \varphi(a^t) = \varphi(t^{-1} \cdot at) \sim \varphi(t^{-1}) \cdot \varphi(at) = t^{-1}bt \sim b. \qquad \square$$

Recall that F is a set of coset representatives for G/A. In the situation of Lemma 6.20, we will write $\varphi(at) = a^{r_a}t$, where $r_a \in F$.

Theorem 6.21. *Let G be a crystallographic group with translation subgroup $A \cong \mathbb{Z}^n$ for $n \in \mathbb{N}$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $t \in F$ satisfies $\varphi(t) = t$. Then there is an $f \in F$ such that $\varphi(at) = a^f t$ for all $a \in A$.*

Proof. From Proposition 1.1 (*vii*), we see that $\varphi(At) = At$. Now, for $a, b \in A$, we have

$$ab^{-1} = at(bt)^{-1} = \varphi(at \cdot (bt)^{-1}) \sim a^{r_a}t \cdot t^{-1}(b^{r_b})^{-1} = a^{r_a}(b^{r_b})^{-1}.$$

Thus, there is some $f \in F$ such that $ab^{-1} = (a^{r_a}(b^{r_b})^{-1})^f$, so that letting $\alpha = r_a f, \beta = r_b f$, this may be rewritten as $ab^{-1} = a^{\alpha}(b^{-1})^{\beta}$. Thus we have

$$a(a^{-1})^{\alpha} = b(b^{-1})^{\beta}. \tag{6.12}$$

Recall that every element of A corresponds to a translation in Euclidean $n-$space, and thus to a point on the lattice $\mathfrak{L}$. Let $\mathbf{v}_a$ denote the point on $\mathfrak{L}$ that corresponds to $a \in A$. For $a \in A$, let S_a denote the $(n-1)$-sphere in $\mathbb{E}^n$ that contains the origin and that is centered at $\mathbf{v}_a$, and let $T_a = \{\mathbf{v}_{a(a^{-1})^f} : f \in F\}$. Then, T_a consists of $|a^G|$ points that lie on S_a. Note that the origin is in T_a for all $a \in A$.

Lemma 6.22. *(i) If $|T_a \cap T_b| = 1$ then there is a $\delta \in F$ such that $a^{r_a} = a^{\delta}, b^{r_b} = b^{\delta}$.*

(ii) If the origin, $\mathbf{v}_a$, and $\mathbf{v}_b$ are collinear, then there is a $\delta \in F$ such that $a^{r_a} = a^{\delta}, b^{r_b} = b^{\delta}$.

Proof.

(i) If $|T_a \cap T_b| = 1$, then $T_a \cap T_b = \{\mathbf{0}\}$ and so from Eq. (6.12), we get $a(a^{-1})^{\alpha} = b(b^{-1})^{\beta} = 1$, so that $a = a^{\alpha}, b = b^{\beta}$. From this we obtain $a^{f^{-1}} = a^{r_a}, b^{f^{-1}} = b^{r_b}$, so that we can let $\delta = f^{-1}$.

(ii) We may assume that $a \neq b$. By hypothesis the origin, $\mathbf{v}_a$, and $\mathbf{v}_b$ are collinear, in other words, the centers of the $(n-1)$-spheres S_a, S_b are on the line through these points. Since $a \neq b$, we have $S_a \neq S_b$, and this together with collinearity tells us that the radius of S_a is not equal to the radius of S_b. Therefore, $S_a \neq S_b$ implies that $S_a \cap S_b$ consists of just the origin (remembering that the origin is common to S_a and S_b.) Thus we have $|T_a \cap T_b| = 1$, as in (i), which then gives the result. □

Lemma 6.23. *Let $b \in A$ satisfy $|b^G| = |G/A|$. Then, for all $a \in A$ there is a unique $f = f_{a,b} \in F$ such that $\varphi(at) = a^f t, \varphi(bt) = b^f t$.*

Proof. If the origin, $\mathbf{v}_a$, and $\mathbf{v}_b$ are collinear, then the existence of such a $\delta \in F$ follows from Lemma 6.22 (ii), while the uniqueness follows from $|b^G| = |F|$.

Now, assume that the origin, $\mathbf{v}_a$, and $\mathbf{v}_b$ are not collinear. If $|T_a \cap T_b| = 1$, then by Lemma 6.22 (i), there is a $\delta \in F$ such that $a^{r_a} = a^\delta, b^{r_b} = b^\delta$, and the fact that δ is unique follows from $|b^G| = |F|$. So, now assume that $|T_a \cap T_b| > 1$. Note that for $2 \leq k \in \mathbb{N}$, the origin, $\mathbf{v}_b$, and $\mathbf{v}_{b^k}$ are collinear. Then, by Lemma 6.22 (ii) applied to b and b^k, there is some $h \in F$ such that $b^{r_b} = b^h$ and $(b^k)^{r_{b^k}} = (b^k)^h$. Since $|b^G| = |F|$ this element h is unique. Since T_a is finite, there is some $1 < k \in \mathbb{N}$ such that $|T_a \cap T_{b^k}| = 1$; then by Lemma 6.22 (i) we have $h' \in F$ with $(b^k)^{r_{b^k}} = (b^k)^{h'}, a^{r_a} = a^{h'}$. Since $|b^G| = |F|$ we again see that h, h' are unique, so that $h = h'$. Thus we have $a^{r_a} = a^h$ and $b^{r_b} = b^h$, as required. □

Now let $a, b, c \in A$, where b satisfies $|b^G| = |F|$. Then, by Lemma 6.23 there are unique $f, h \in F$ such that $\varphi(at) = a^f t, \varphi(bt) = b^f t$ and $\varphi(bt) = b^h t, \varphi(ct) = c^h t$. Since f, h are unique and $\varphi(bt) = b^f t, \varphi(bt) = b^h t$ we must have $f = h$; it follows (by fixing a and varying c) that for all $d \in A$ we must have $\varphi(dt) = d^f t$ for this value of $f \in F$ that is completely determined by an element b such that $|b^G| = |F|$. This concludes the proof of Theorem 6.21. □

6.6 Step six

In this section we will prove results useful for proving step six. These results will be applied in Ch. 7 and Ch. 8 to the thirty-one space groups listed in Tables 4.1 and 4.2.

Lemma 6.24. *Let G be a group with a normal abelian subgroup A. Assume that G/A is abelian. Let $n = |G/A|$. Let $a \in A$ and $f \in F$. If $f \sim a^{2k} f$ for all $k \in \mathbb{Z}$ such that $0 \leq k \leq n$,* *then* $a^{2m} \in K_f$ *for some* $1 \leq m \leq n$.

Proof. By Proposition C.2 we have

$$f^G = \bigcup_{h \in F} K_f f^h = \bigcup_{h \in F} K_f (h, f^{-1}) f.$$

Thus $f \sim a^{2k} f$ implies that $a^{2k} \in K_f(h, f^{-1})$ for some $h \in F$. In other words, there exists an $h \in F$ for every $0 \leq k \leq n$ so that $a^{2k} \in K_f(h, f^{-1})$. Since there are at most n choices for h there must be some $h \in F$ and some $j \in \mathbb{Z}$ such that $a^{2j}, a^{2(j+m)} \in K_f(h, f^{-1})$ for some $1 \leq m \leq n$. It follows that $a^{2m} \in K_f$. □

Definition Let G be a space group and let F be a set of coset representatives for G/A. For $f \in F, f \neq 1$, we define the set

$$\mathcal{R}_f = \{h \in F : f \sim (h, \alpha) f \text{ for all } \alpha \in \mathbf{C}_2\}.$$

Recall that given a set $B \subseteq A$ we have the following definition of the subset $\mathrm{Inv}(f)$:

$$\mathrm{Inv}(B, f) = \{\beta \in B \,:\, \beta^f = \beta^{-1}\}.$$

The following proposition applies to the thirty-one groups listed in Tables 4.1 and 4.2.

Proposition 6.25. *Let* $j, n \in \mathbb{N}$. *Let* G *be a group with normal subgroup* $A \cong \mathbb{Z}^n$ *where* G/A *is abelian and finite. Suppose that there exists* $B = \{\beta_i\}_{i=1}^{j} \subseteq \mathbf{C}_2 \subseteq \langle B \rangle \cong \mathbb{Z}^j$.

Assume that the action of G/A *on* B *defined by* $\beta \cdot (Ag) = \beta^g$ *is well-defined and faithful. Let* $1 \neq f \in F$ *and assume that rank*$(K_f) = |\mathrm{Inv}(B, f)|$. *Then*

$$h \in \mathcal{R}_f \textit{ if and only if } \mathrm{Inv}(B, h) \subseteq \mathrm{Inv}(B, f).$$

Proof. ($\Longrightarrow$) We assume $h \in \mathcal{R}_f$. Note that if $h = 1$, then $\mathrm{Inv}(h) = \varnothing$ so $\mathrm{Inv}(h) \subseteq \mathrm{Inv}(f)$ is satisfied. Thus we may assume that $h \neq 1$. This implies that $\mathrm{Inv}(h)$ is not empty because G/A acts faithfully on B. We will show that $\beta \in \mathrm{Inv}(h)$ and $f \sim (h, \alpha) f$ for all $\alpha \in \mathbf{C}_2$ together imply that $\beta \in \mathrm{Inv}(f)$.

Suppose to the contrary that $\beta \notin \mathrm{Inv}(f)$. As $\beta \in \mathbf{C}_2$ its only conjugates are itself and its inverse. It follows that β commutes with f. Since $\beta \in \mathrm{Inv}(h)$ we have $(h, \beta) = \beta^2$.

Then for any $k \in \mathbb{Z}$ we have $(h, \beta^k) = \beta^{2k}$ and note that $\beta^k \in \mathbf{C}_2$. We are assuming $f \sim (h, \alpha)f$ for all $\alpha \in \mathbf{C}_2$, so in particular we have $f \sim (h, \beta^k)f = \beta^{2k}f$. By Lemma 6.24 we have $\beta^{2m} \in K_f$ for some $m \in \mathbb{N}$. Now $\beta_i \in \mathrm{Inv}(f)$ implies that $\beta_i^2 \in K_f$ and therefore $\{\beta_i^2 : \beta_i \in \mathrm{Inv}(f)\} \subseteq K_f$. However, recall that by assumption, β commutes with f; thus β^{2m} commutes with f and so $\beta^{2m} \notin \langle \beta_i^2 : \beta_i \in \mathrm{Inv}(f)\rangle$. The fact that $\mathrm{rank}(\langle B\rangle) = j$ implies that the subgroup generated by β^{2m} and $\{\beta_i^2 : \beta_i \in \mathrm{Inv}(f)\}$ would be a subgroup of K_f with rank $1 + |\mathrm{Inv}(f)|$, a contradiction.

($\Longleftarrow$) Assume that $\mathrm{Inv}(h) \subseteq \mathrm{Inv}(f)$. We need to show that $f \sim (h, \alpha)f$ for all $\alpha \in \mathbf{C}_2$. For $\alpha \in \mathbf{C}_2$ which commutes with h there is nothing to show so we may assume that $\alpha^h = \alpha^{-1}$. We have $\alpha \in \mathbf{C}_2 \subseteq \langle B\rangle$, therefore we may write $\alpha = \beta_1^{k_1}\beta_2^{k_2}\cdots\beta_j^{k_j}$ for some $k_1, k_2, \ldots, k_j \in \mathbb{Z}$. Notice that for each $\beta_i \notin \mathrm{Inv}(h)$ we must have $k_i = 0$, in order to satisfy $\alpha^h = \alpha^{-1}$. This is true because $\langle B\rangle$ is a free group of rank j. This shows that $\alpha \in \langle \mathrm{Inv}(h)\rangle$. By hypothesis $\mathrm{Inv}(h) \subseteq \mathrm{Inv}(f)$, so $\alpha \in \langle \mathrm{Inv}(f)\rangle$. We thus have $\alpha^f = \alpha^{-1}$ and so $(h, \alpha) = (f, \alpha)$. Then

$$f \sim f^{\alpha f} = (f^{-1}\alpha^{-1})f(\alpha f) = (f, a)f = (h, \alpha)f.$$

This shows $h \in \mathcal{R}_f$. □

Corollary 6.26. *Let $G \in \{G_{10}, G_{12}, G_{13}\}$. We write the presentation of G using generators x, y, z, r, t and we define $F = \{r, t, rt, 1\}$. For these groups we have*

$$\mathcal{R}_t = F; \qquad \mathcal{R}_r = \{1, r\}; \qquad \mathcal{R}_{rt} = \{1, rt\}.$$

Proof. For G_{10} and G_{13} we have $\mathbf{C}_2 = \langle x, z\rangle \cup \langle y\rangle$. Without loss of generality, let $B = \{x, y, z\}$. Then $\mathrm{Inv}(t) = B, \mathrm{Inv}(r) = \{x, z\}$, and $\mathrm{Inv}(rt) = \{y\}$. The result follows from Proposition 6.25.

For G_{12} we have $\mathbf{C}_2 = \langle x^2y^{-1}, z\rangle \cup \langle y\rangle$. Without loss of generality, let $B = \{x^2y^{-1}, y, z\}$. Then $\mathrm{Inv}(t) = B, \mathrm{Inv}(r) = \{x^2y^{-1}, z\}$, and $\mathrm{Inv}(rt) = \{y\}$. The result follows from Proposition 6.25. □

Corollary 6.27. *Let* $G \in \{G_{16}, G_{17}, G_{21}, G_{22}\}$. *These presentations use generators* x, y, z, p, r, *and we define* $F = \{p, r, pr, 1\}$. *For these groups we have*

$$\mathcal{R}_p = \{1, p\}; \qquad \mathcal{R}_r = \{1, r\}; \qquad \mathcal{R}_{pr} = \{1, pr\}.$$

Proof. For G_{16} and G_{17} we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x, y, z\}$. Then $\mathrm{Inv}(p) = \{x, y\}, \mathrm{Inv}(r) = \{x, z\}$, and $\mathrm{Inv}(pr) = \{y, z\}$. The result follows from Proposition 6.25.

For G_{21} we have $\mathbf{C}_2 = \langle x^2y^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x^2y^{-1}, y, z\}$. Then $\mathrm{Inv}(p) = \{x^2y^{-1}, y\}, \mathrm{Inv}(r) = \{x^2y^{-1}, z\}$, and $\mathrm{Inv}(pr) = \{y, z\}$. The result follows from Proposition 6.25.

For G_{22} we have $\mathbf{C}_2 = \langle x^2z^{-1} \rangle \cup \langle y^2z^{-1} \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x^2z^{-1}, y^2z^{-1}, z\}$. Then $\mathrm{Inv}(p) = \{x^2z^{-1}, y^2z^{-1}\}, \mathrm{Inv}(r) = \{x^2z^{-1}, z\}$, and $\mathrm{Inv}(pr) = \{y^2z^{-1}, z\}$. The result follows from Proposition 6.25. □

Corollary 6.28. *Let* $G \in \{G_{25}, G_{26}, G_{27}, G_{38}, G_{39}, G_{42}\}$. *We write the presentation of* G *using generators* x, y, z, p, s, *and we define* $F = \{p, s, ps, 1\}$. *For these groups we have*

$$\mathcal{R}_p = \{1, p, ps, s\}; \qquad \mathcal{R}_s = \{1, s\}; \qquad \mathcal{R}_{ps} = \{1, ps\}.$$

Proof. For G_{25}, G_{26}, and G_{27} we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle$. Without loss of generality, let $B = \{x, y\}$.

For G_{38} and G_{39} we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y^2z^{-1} \rangle$. Without loss of generality, let $B = \{x, y^2z^{-1}\}$.

For G_{42} we have $\mathbf{C}_2 = \langle x^2z^{-1} \rangle \cup \langle y^2z^{-1} \rangle$. Without loss of generality, let $B = \{x^2z^{-1}, y^2z^{-1}\}$.

In all cases, $\mathrm{Inv}(p) = B$. On the other hand, $\mathrm{Inv}(s)$ and $\mathrm{Inv}(ps)$ each contain exactly one element of B and $\mathrm{Inv}(s) \neq \mathrm{Inv}(ps.)$ The result follows from Proposition 6.25. □

Corollary 6.29. *Let* G *be a group with a presentation of the form given in Eqs. (4.4) or (4.5). These presentations use generators* x, y, z, p, r, t, *and we define* $F = \{p, r, pr, prt, rt, pt, t, 1\}$. *For these groups we have*

$\mathcal{R}_t = F;$

$\mathcal{R}_p = \{1, p, prt, rt\};$ $\mathcal{R}_{pt} = \{1, pt\};$

$\mathcal{R}_r = \{1, r, prt, pt\};$ $\mathcal{R}_{rt} = \{1, rt\};$

$\mathcal{R}_{pr} = \{1, pr, rt, pt\};$ $\mathcal{R}_{prt} = \{1, prt\}.$

Proof. For groups with a presentation of the form given in Eq. (4.4) with $\delta = 0$ we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x, y, z\}$.

For groups with a presentation of the form given in Eq. (4.4) with $\delta = 1$ we have $\mathbf{C}_2 = \langle x^2 y^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x^2 y^{-1}, y, z\}$.

For groups with a presentation of the form given in Eq. (4.5) with $\delta = 0$ we have $\mathbf{C}_2 = \langle x^2 z^{-1} \rangle \cup \langle y^2 z^{-1} \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x^2 z^{-1}, y^2 z^{-1}, z\}$.

For groups with a presentation of the form given in Eq. (4.5) with $\delta = 1$ we have $\mathbf{C}_2 = \langle x^2 y^{-1} z^{-1} \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x^2 y^{-1} z^{-1}, y, z\}$.

In all cases

- $\mathrm{Inv}(prt)$ is contained in $\mathrm{Inv}(p) \cap \mathrm{Inv}(r)$;
- $\mathrm{Inv}(rt)$ is contained in $\mathrm{Inv}(p) \cap \mathrm{Inv}(pr)$;
- $\mathrm{Inv}(pt)$ is contained in $\mathrm{Inv}(r) \cap \mathrm{Inv}(pr)$;
- for $f \in F$ we have $\mathrm{Inv}(f) \subseteq \mathrm{Inv}(t)$.

The result follows from Proposition 6.25. □

Here we make a comment that applies to the eight space groups with presentation of the form given in Eq. (4.4) with $\delta = 0$. For these groups we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. A consequence of this is that the definition of $\mathcal{R}_f$ is equivalent to

$$\{h \in F \,:\, f \sim (h, \alpha) f \text{ for all } \alpha \in A\},$$

as we now show.

Proof of the equivalence: Note that for any crystallographic group we have $\mathbf{C}_2 \subseteq A$. It follows that the set $\{h \in F : f \sim (h, \alpha)f \text{ for all } \alpha \in A\}$ is contained in $\mathcal{R}_f$. We will show that the reverse containment holds when G is a group with presentation of the form given in Eq. (4.4) with $\delta = 0$.

$$\begin{aligned} h \in \mathcal{R}_f &\implies \mathrm{Inv}(h) \subseteq \mathrm{Inv}(f) \quad \text{by Proposition 6.25} \\ &\implies K_h \leq K_f \ \text{ by Lemma 6.30,} \\ &\implies \text{for } a \in A, (h, a) \in K_f, \\ &\implies f \sim (h, a)f \text{ for } a \in A \quad \text{by Lemma 2.10.} \end{aligned}$$

Lemma 6.30. *Let G be a group with presentation of the form given in Eq. (4.4) with $\delta = 0$. Thus we have $A = \langle x, y, z\rangle$ and $\mathbf{C}_2 = \langle x\rangle \cup \langle y\rangle \cup \langle z\rangle$. Let $B = \{x, y, z\}$. Let $h, f \in F$. If $\mathrm{Inv}(B, h) \subseteq \mathrm{Inv}(B, f)$ then $K_h \leq K_f$.*

Proof. By definition we know that K_h is generated by commutators of the form (β, h) for $\beta \in B$. To show $K_h \leq K_f$ it suffices to show that $(\beta, h) \in K_f$. We have two cases to consider: either $\beta \in \mathrm{Inv}(h)$ or $\beta \notin \mathrm{Inv}(h)$. Note that for $g \in F$ we have $(\beta, g) \in \{\beta^{-2}, 1\}$ and $(\beta, g) = \beta^{-2}$ if and only if $\beta \in \mathrm{Inv}(g)$. Therefore for $\beta \in \mathrm{Inv}(h)$ we have $(\beta, h) = \beta^{-2} = (\beta, f) \in K_f$ since by assumption $\beta \in \mathrm{Inv}(h)$ implies $\beta \in \mathrm{Inv}(f)$. For $\beta \notin \mathrm{Inv}(h)$ we have $(\beta, h) = 1 \in K_f$. □

In general however, the set $\{h \in F : f \sim (h, \alpha)f \text{ for all } \alpha \in A\}$ will be a subset of $\mathcal{R}_f$.

Example: For $G \in \{G_{63}, G_{64}, G_{65}, G_{66}\}$, we have $\mathcal{R}_p = \{1, prt, rt, p\}$. On the other hand,

$$\{h \in F : p \sim (h, \alpha)p \text{ for all } \alpha \in A\}$$

does not include prt since $(prt, x) = x^2y^{-1}$ and $p \nsim x^2y^{-1}p$.

Lemma 6.31. *Let G be a crystallographic group and assume $\mathbf{C}_2 \neq \{1\}$. Let $\varphi \in \mathcal{W}(G)$ and assume that $\varphi|_A = \mathrm{Id}$. Suppose that for some $f \in F$ we have $\varphi(f) = f$. Then there exists some $h \in \mathcal{R}_f$ such that $\varphi(af) = a^h f$ for all $a \in A$.*

Proof. We know by Theorem 6.21 that there exists some $h \in F$ such that $\varphi(af) = a^h f$ for all $a \in A$. Then

$$f = \varphi(a^{-1} \cdot af) \sim a^{-1}(a)^h f = (a, h)f.$$

Since this must hold in particular for $a \in \mathbf{C}_2$ we must have $h \in \mathcal{R}_f$. $\square$

Definition For $f \in F, f \neq 1$, we define the set

$$\mathcal{S}_f = \{h \in F : af \sim a^h f \text{ for all } a \in A\}.$$

Lemma 6.32. *Let $f, h \in F$ and assume $f \neq 1$.*

(i) If $(f, h) \in K_f$, then $h \in \mathcal{S}_f$.

(ii) If $K_h \leq K_f$, then $h \in \mathcal{S}_f$.

(iii) If $h_1, h_2 \in \mathcal{S}_f$, then the element in F representing the coset $Ah_1^{-1}h_2$ is in $\mathcal{S}_f$.

(iv) $\mathcal{S}_f$ is a set of coset representatives for a subgroup of G/A.

Proof. Let $a \in A$. Assume $(f, h) \in K_f$. First we show that $af \sim (f, h)a^h f$:

$$af \sim fa \sim (fa)^h = f^h a^h \sim (f^h a^h)^f = f^{-1} f^h a^h f = (f, h)a^h f.$$

By Lemma 2.10, $(f, h) \in K_f$ implies $a^h f \sim (f, h)a^h f$. Thus by transitivity $af \sim a^h f$ and so $h \in \mathcal{S}_f$, proving (i).

Next, suppose that $K_h \leq K_f$; thus for $a \in A$, we have $(a, h) \in K_f$. Then by Lemma 2.10,

$$af \sim (a, h)af = a^{-1}a^h af = a^h f,$$

and so $h \in \mathcal{S}_f$, proving (ii).

To prove (iii), suppose that $h_1, h_2 \in \mathcal{S}_f$. We will show that there exists $c \in A$ such that $ch_1^{-1}h_2 \in \mathcal{S}_f$. By definition of $\mathcal{S}_f$ for $a \in A$, we have $af \sim a^{h_1} f$ and $af \sim a^{h_2} f$.

Taking $a = b^{h_1^{-1}}$ these two assertions become respectively

$$b^{h_1^{-1}} f \sim b^{h_1^{-1}h_1} f = bf \text{ and } b^{h_1^{-1}} f \sim b^{h_1^{-1}h_2} f.$$

Again using transitivity we have $bf \sim b^{h_1^{-1}h_2}f$, in other words, there exists some $h \in F$ such that $h = ch_1^{-1}h_2$ for some $c \in A$ and $bf \sim b^h f$ for all $b \in A$. This proves (iii). The fourth statement follows from (iii) and from the fact that $1 \in \mathcal{S}_f$. $\square$

Theorem 6.33. *Let G be a group with abelian normal subgroup A such that G/A abelian. Let $\varphi \in \mathcal{W}(G)$ and assume $\varphi|_A = \mathrm{Id}$. Let $f \in F$ and let $g \in G$ satisfy $fg \in F$ or $gf \in F$. Let $\gamma \in F$ be the coset representative for the Afg coset (i.e. $\gamma = fg$ or $\gamma = gf$). Suppose $\varphi(f) = f$, $\varphi(g) = g$, and $\varphi(\gamma) = \gamma$. (We also assume that $1 \notin \{f, g, \gamma\}$.)*

Then there is an $h \in \mathcal{R}_f \cap \mathcal{S}_\gamma$ such that $\varphi(af) = a^h f$ for all $a \in A$.

Proof. We have $\varphi(f) = f$, so by Lemma 6.31 we know there exists an $h \in \mathcal{R}_f$ such that for $a \in A$ we have $\varphi(af) = a^h f$. It remains to show that $h \in \mathcal{S}_\gamma$.

Case 1: $\gamma = fg$: Then for $a \in A$ we have

$$a\gamma = \varphi(a)\varphi(\gamma) \sim \varphi(a \cdot \gamma) = \varphi(a \cdot fg) = \varphi(af \cdot g) \sim a^h fg = a^h \gamma.$$

Case 2: $\gamma = gf$: (Here we will use the fact that G/A is abelian, thus $a^{gh} = a^{hg}$.) Then for $a \in A$,

$$a\gamma \sim \varphi(a \cdot \gamma) = \varphi(a \cdot gf) = \varphi(g \cdot a^g f) \sim g a^{gh} f = a^h gf = a^h \gamma.$$

In both cases we arrive at $a\gamma \sim a^h \gamma$ for all $a \in A$, which shows that $h \in \mathcal{S}_\gamma$. $\square$

Corollary 6.34. *Let G be a group with presentation of the form given in Eqs. (4.4) or (4.5). These presentations use generators x, y, z, p, r, t, and we define $F = \{p, r, pr, prt, rt, pt, t, 1\}$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $\varphi(t) = t$. Fix $f \in \{prt, rt, pt\}$ and suppose $\varphi(f) = f$ and $\varphi(ft) = ft$. Then $f \notin \mathcal{S}_{ft}$ implies that $\varphi|_{Af} = \mathrm{Id}$.*

Proof. Recall that $t^2 = 1$; thus for $f \in \{prt, rt, pt\}$ we have $ft \in F \setminus \{1\}$. Therefore we may apply Theorem 6.33 which asserts that for $a \in A$ we have $\varphi(af) = a^h f$ for some $h \in \mathcal{R}_f \cap \mathcal{S}_{ft}$. To show $\varphi|_{Af} = \mathrm{Id}$ it suffices to show this intersection is $\{1\}$. Now Corollary 6.29 indicates that for $f \in \{prt, rt, pt\}$ we have $\mathcal{R}_f = \{1, f\}$. Since $f \notin \mathcal{S}_{ft}$ by assumption, we see $\mathcal{R}_f \cap \mathcal{S}_{ft} = \{1\}$ so we are done. $\square$

Theorem 6.35. *Let G be a group with abelian normal subgroup A. Let $\varphi \in \mathcal{W}(G)$. Assume $\varphi|_A = \mathrm{Id}$ and let $\varphi(f) = f$ for some $f \in F \setminus \{1\}$.*

(i) Suppose that $\varphi|_{Ag'} = \mathrm{Id}$ for some $Ag' \in (G/A) \setminus \{Af^{-1}\}$. Let $g \in Ag'$ satisfy $fg \in F \setminus \{1\}$. Then there exists $h \in \mathcal{R}_f \cap \mathcal{R}_{fg}$ so that for $a \in A$ we have $\varphi(af) = a^h f$.

(ii) Suppose that for $j \in \mathbb{Z}$, there are cosets $Ag'_1, Ag'_2, \ldots, Ag'_j$ in G/A such that $\varphi|_{Ag'_i} = \mathrm{Id}$ for $1 \le i \le j$. Let $g_i \in Ag'_i$ satisfy $fg_i \in F \setminus \{1\}$ for $1 \le i \le j$. If $\mathcal{R}_f \cap \bigcap_{i=1}^{j} \mathcal{R}_{fg_i} = \{1\}$, then $\varphi|_{Af} = \mathrm{Id}$.

Proof. By Lemma 6.31 we know there exists an $h \in \mathcal{R}_f$ such that for all $a \in A$ we have $\varphi(af) = a^h f$. Then for all $\alpha \in \mathbf{C}_2$ we have $\varphi(g) = g$, since $g \in Ag'$, so

$$fg = \varphi(f)\varphi(g) \sim \varphi(\alpha^{-1}\alpha f \cdot g) = \varphi(\alpha^{-1} f \cdot \alpha^f g) \sim (\alpha^{-1})^h f \cdot \alpha^f g = (\alpha^{-1})^h \alpha fg = (h, \alpha) fg;$$

This shows $h \in \mathcal{R}_{fg}$, proving (i). The second statement follows from applying the first statement j times. □

The following applies to space groups G_{16}, G_{17}, G_{21}, and G_{22}.

Corollary 6.36. *Let G be a group with presentation of the form given in Eq. (4.2). These presentations use generators x, y, z, p, r, and we define $F = \{1, p, r, pr\}$. Let $\varphi \in \mathcal{W}(G)$ and assume $\varphi|_A = \mathrm{Id}$. Let $f \in F \setminus \{1\}$. Suppose that for some $g \in G$ such that $fg \in F \setminus \{1, f\}$ we have $\varphi|_{Ag} = \mathrm{Id}$. Then*

$$\varphi(f) = f \text{ implies that } \varphi|_{Af} = \mathrm{Id}.$$

Proof. We will apply Theorem 6.35 (i) and use the fact that by Corollary 6.27, $\mathcal{R}_f = \{1, f\}$ for all $f \in F$. Since $fg \in F \setminus \{1, f\}$ the cosets Af and Afg are distinct, thus $\mathcal{R}_f \cap \mathcal{R}_{fg} = \{1\}$. The result follows directly. □

The following applies to space groups $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42}.

Corollary 6.37. *Let G be a group with presentation of the form given in Eq. (4.3). These presentations use generators x, y, z, p, s, and we define $F = \{p, ps, s, 1\}$. Let $\varphi \in \mathcal{W}(G)$ and* *suppose that* $\varphi|_A = \mathrm{Id}$ *, and* $\varphi(f) = f$ *for all* $f \in F$*. Then*

$$\varphi|_{Aps} = \varphi|_{As} = \mathrm{Id} \textit{ implies that } \varphi = \mathrm{Id}.$$

Proof. Note that $|G/A| = 4$ and so it suffices to show that $\varphi|_{Ap} = \mathrm{Id}$. We assume that $\varphi|_{Aps} = \varphi|_{As} = \mathrm{Id}$ and apply Theorem 6.35 (ii). Then since $\varphi(p) = p$ and $\mathcal{R}_{ps} \cap \mathcal{R}_s = \{1\}$ by Corollary 6.28, the theorem implies $\varphi|_{Ap} = \mathrm{Id}$. □

Corollary 6.38. *Let* G *be a group with presentation of the form given in Eqs. (4.4) or (4.5). These presentations use generators* x, y, z, p, r, t*, and we define* $F = \{p, r, pr, prt, rt, pt, t, 1\}$*. Let* $\varphi \in \mathcal{W}(G)$ *and suppose that* $\varphi|_A = \mathrm{Id}$ *, and* $\varphi(f) = f$ *for all* $f \in F$*. Then*

(i) $\varphi|_{At} = \mathrm{Id}$ *implies that* $\varphi = \mathrm{Id}$*,*

(ii) $\varphi|_{Aprt} = \varphi|_{Art} = \varphi|_{Apt} = \mathrm{Id}$ *implies that* $\varphi = \mathrm{Id}$.

Proof. We will use the following results that follow from Corollary 6.29.

$$\text{For } f \in F \setminus \{1, t\}, \mathcal{R}_f \cap \mathcal{R}_{ft} = \{1\}. \tag{6.13}$$

$$\text{For } f_1, f_2 \in \{prt, rt, pt\}, \mathcal{R}_{f_1} \cap \mathcal{R}_{f_2} = \{1\}. \tag{6.14}$$

First we prove that $\varphi|_{At} = \mathrm{Id}$ implies that $\varphi = \mathrm{Id}$. It suffices to show that for $f \in \{p, r, pr, prt, rt, pt\}$, $\varphi(af) = a^h f$ implies that $h = 1$. We apply Theorem 6.35 (i), using $\varphi|_{At} = \mathrm{Id}$ and $\varphi(f) = f$. Then by the theorem we have $h \in \mathcal{R}_f \cap \mathcal{R}_{ft}$. By Eq. (6.13) this intersection is $\{1\}$, so we conclude $\varphi|_{Af} = \mathrm{Id}$.

Now assume that $\varphi|_{Aprt} = \varphi|_{Art} = \varphi|_{Apt} = \mathrm{Id}$. To prove this implies $\varphi = \mathrm{Id}$ it suffices to show that $\varphi|_{Af} = \mathrm{Id}$ for $f \in \{p, r, pr, t\}$. We proceed by first showing that this holds for $f \in \{p, pr\}$. We will apply Theorem 6.35 (ii), using $\varphi(p) = p$ and $\varphi|_{Art} = \varphi|_{Aprt} = \mathrm{Id}$. Since $\mathcal{R}_{prt} \cap \mathcal{R}_{rt} = \{1\}$ by Eq. (6.14), the theorem implies $\varphi|_{Ap} = \mathrm{Id}$. Similarly, by using $\varphi(pr) = pr$ with $\varphi|_{Apt} = \varphi|_{rt} = \mathrm{Id}$, and $\mathcal{R}_{pr} \cap \mathcal{R}_{rt} \cap \mathcal{R}_{pt} = \{1\}$ by Eq. (6.14), Theorem 6.35 (ii) gives $\varphi|_{Apr} = \mathrm{Id}$.

Now that we have $\varphi|_{Ap} = \varphi|_{Apr} = \mathrm{Id}$, we use this to apply the theorem a third time. Using $\varphi(t) = t$ and since Eq. (6.14) gives $\mathcal{R}_{pt} \cap \mathcal{R}_{prt} = \{1\}$, we have $\varphi|_{At} = \mathrm{Id}$. From (i), this implies $\varphi = \mathrm{Id}$. $\square$

Chapter 7. $\mathcal{W}(G)$ of space groups with point group $\frac{\mathbf{2}}{\mathbf{m}}$, **222**, or **mm2**

7.1 Groups 10 through 13

Lemma 7.1. *The following results will be useful as we determine the step 2 automorphisms which can be found in* G_{10}, G_{12}, *and* G_{13}.

(i) The group of automorphisms of $\mathbb{Z}^2$ *is* $\mathrm{GL}(2,\mathbb{Z})$. *It is generated by*

$$a = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix},\ b = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix},\ \textit{and } c = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(ii) The set of all matrices $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \in \mathrm{GL}(2,\mathbb{Z})$ *such that* $j \in 2\mathbb{Z}$ *is an index three subgroup of* $\mathrm{GL}(2,\mathbb{Z})$ *and it is generated by*

$$a^2 = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix},\ b = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix},\ \textit{and } c = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(iii) The set of all matrices $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \in \mathrm{GL}(2,\mathbb{Z})$ *such that* $k \in 2\mathbb{Z}$ *is an index three subgroup of* $\mathrm{GL}(2,\mathbb{Z})$ *and it is generated by*

$$(a^2)^T = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix},\ b^T = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix},\ \textit{and } c = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Proof. We know $\mathrm{SL}(2,\mathbb{Z})$ is an index two subgroup of $\mathrm{GL}(2,\mathbb{Z})$ and it is generated by a and b [N]. Since c has determinant -1, these three matrices generate $\mathrm{GL}(2,\mathbb{Z})$, thus we have (i).

Let H denote the subset of interest in (ii), i.e. the subset of matrices $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \in \mathrm{GL}(2,\mathbb{Z})$ such that j is even. We verify that this subset is a subgroup by checking that it contains inverses and is closed under multiplication. Let $\epsilon = i\ell - kj \in \{\pm 1\}$. Then

$$\begin{pmatrix} i & j \\ k & \ell \end{pmatrix}^{-1} = \epsilon \begin{pmatrix} \ell & -j \\ -k & i \end{pmatrix} \in H.$$

Also, for some $m, n, p \in \mathbb{Z}$,

$$\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \begin{pmatrix} i' & j' \\ k' & \ell' \end{pmatrix} = \begin{pmatrix} m & ij' + j\ell` \\ n & p \end{pmatrix} \in H.$$

It is apparent that $a^2, b, c \in H$, so $\langle a^2, b, c \rangle \leq H$. Using Reidemeister-Schreier's algorithm as implemented in Magma [BCP],[MKS], (see Appendix B), we verified that $\langle a^2, b, c \rangle$ is an index three subgroup of $\mathrm{GL}(2, \mathbb{Z})$. Since three is prime, evidently $\langle a^2, b, c \rangle$ is not a proper subgroup of H, proving (ii).

Statement (iii) follows from (ii) and from the fact that for matrices B, C we have

$$(B^{-1})^T = (B^T)^{-1} \text{ and } (BC)^T = C^T B^T. \qquad \square$$

We will now apply steps one through six to the group G_{10} to determine a set of generators of $\mathcal{W}(G_{10})$. Let $\varphi \in \mathcal{W}(G_{10})$. By Proposition 6.6 we have $\varphi(Af) = Af$ for all $f \in F$ and $\varphi(y) \in \{y, y^{-1}\}$. If we have $\varphi(y) = y^{-1}$ then we may compose with I_t and now we may assume that $\varphi(y) = y$. Since $\mathbf{C}_2 = \langle x, z \rangle \cup \langle y \rangle$, Proposition 6.5 (ii) gives $\varphi(\langle x, z \rangle) = \langle x, z \rangle$. Thus $\varphi|_{\langle x, z \rangle}$ is an automorphism of a free abelian group of rank 2. The set of all such maps is $\mathrm{GL}(2, \mathbb{Z})$. Let $\xi : \langle x, z \rangle \to \langle x, z \rangle$ be one such automorphism. Then

$$\psi_\xi : (x, y, z, r, t) \mapsto (\xi(x), y, \xi(z), r, t)$$

determines an automorphism of G_{10} as it satisfies all the relations in the presentation of G_{10}. By Lemma 7.1 we know $GL(2, \mathbb{Z})$ can be generated by three matrices, therefore there exist three corresponding automorphisms that generate all the automorphisms that are of the form described by ψ_ξ. These are:

$$\psi_1 : (x, y, z, r, t) \mapsto (x, y, xz, r, t);$$

$$\psi_2 : (x, y, z, r, t) \mapsto (xz^{-1}, y, z, r, t);$$

$$\psi_3 : (x, y, z, r, t) \mapsto (x^{-1}, y, z, r, t).$$

Composing with these three outer automorphisms, we can ensure that $\varphi|_{\langle x,z\rangle} = \mathrm{Id}$. Since we also have $\varphi(y) = y$ we now have $\varphi|_A = \mathrm{Id}$.

By Proposition 6.19 we may compose with outer automorphisms ψ_x, ψ_y, and ψ_z as necessary so as to have $\varphi(t) = t$. Since $r^2 = (rt)^2 = 1$, Proposition 6.17 gives $\varphi(r) = r$ and $\varphi(rt) = rt$; thus we have $\varphi(f) = f$ for all $f \in F$.

Applying Theorem 6.21 with Lemma 6.31 we have for all $a \in A, \varphi(art) = a^h rt$ for some $h \in \{1, rt\}$. If $h = 1$, then we are done. If $h = rt$ then we may compose with $I_t \circ \iota$. Since $(rt)^2 = (rt, t) = 1$,

$$(I_t \circ \iota)(a^{rt} rt) = I_t(rt(a^{-1})^{rt}) = rta^{rt} = art,$$

we now have $\varphi|_{Art} = \mathrm{Id}$.

Now by Lemma 6.31, for some $h \in \mathcal{R}_r = \{1, r\}, a \in A$, we have $\varphi(ar) = a^h r$. If $h = r$ we may compose with the non-trivial wct $\tau(r, \{Ar, At\})$ so that $\varphi|_{Ar} = \mathrm{Id}$. (Theorem 5.9 proves τ_r is non-trivial.) Note that Corollary 6.26 gives $\mathcal{R}_t \cap \mathcal{R}_{rt} \cap \mathcal{R}_r = \{1\}$. We use this to apply Theorem 6.35 (ii). We have $\varphi(t) = t$ and $\varphi|_{Art} = \varphi|_{Ar} = \mathrm{Id}$. Then by the theorem we have $\varphi|_{At} = \mathrm{Id}$; and therefore $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.2. *For crystallographic group G_{10}, the group $\mathcal{W}(G)$ is generated by the inverse* *map ι, the inner automorphisms,*

$$\psi_1 : (x, y, z, r, t) \mapsto (x, y, xz, r, t),$$

$$\psi_2 : (x, y, z, r, t) \mapsto (xz^{-1}, y, z, r, t),$$

$$\psi_3 : (x, y, z, r, t) \mapsto (x^{-1}, y, z, r, t),$$

$$\psi_x : (x, y, z, r, t) \mapsto (x, y, z, xr, xt),$$

$$\psi_y : (x, y, z, r, t) \mapsto (x, y, z, r, yt),$$

$$\psi_z : (x, y, z, r, t) \mapsto (x, y, z, zr, zt),$$

and the non-trivial wct τ_r. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_r \rangle$. □

Let $\varphi \in \mathcal{W}(G_{12})$. By Proposition 6.6 we have $\varphi(Af) = Af$ for all $f \in F$ and $\varphi(y) \in \{y, y^{-1}\}$. Composing with I_t if necessary we have $\varphi(y) = y$. By Proposition 6.5 (*ii*) we know that $\varphi(\langle x^2y^{-1}, z\rangle) = \langle x^2y^{-1}, z\rangle$. In other words, $\varphi|_{\langle x^2y^{-1},z\rangle}$ is an automorphism of a free abelian group of rank 2. We may write $\varphi(x^2y^{-1}) = (x^2y^{-1})^i z^j$ and $\varphi(z) = (x^2y^{-1})^k z^\ell$ for $i, j, k, \ell \in \mathbb{Z}$, and thus $\varphi|_A$ corresponds to the matrix $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \in \mathrm{GL}(2, \mathbb{Z})$, relative to the basis x^2y^{-1}, z. Now by Proposition A.1,

$$K_r = \langle x^2y^{-1}, z^2\rangle,\ K_t = \langle x^2, y^2, z^2\rangle \text{ and } K_{rt} = \langle y\rangle;$$

thus we have $K = \langle x^2, y, z^2\rangle$. By Lemma 2.11, $\varphi(K) = K$. Then since $x^2y^{-1} \in K$,

$$\varphi(x^2y^{-1}) = (x^2y^{-1})^i z^j \in K = \langle x^2, y, z^2\rangle,$$

so j is even.

Let $\xi : \langle x^2y^{-1}, z\rangle \to \langle x^2y^{-1}, z\rangle$ be the automorphism given by

$$\xi : (x^2y, z) \mapsto ((x^2y^{-1})^i z^j, (x^2y^{-1})^k z^\ell).$$

Thus ξ corresponds to a matrix $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix}$ in the subgroup of $\mathrm{GL}(2, \mathbb{Z})$ of matrices with j

even. The map

$$\begin{aligned}\psi_\xi : (x^2y^{-1}, y, z, r, t) &\mapsto (\xi(x^2y^{-1}), y, \xi(z), r, t)\\ = (x, y, z, r, t) &\mapsto (x^i y^{(1-i)/2} z^{j/2}, y, x^k z^\ell, r, t)\end{aligned}$$

determines an automorphism of G_{12} because it satisfies the relations in the presentation of G_{12}. By Lemma 7.1 (ii) we know that the set of matrices $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix}$ in $\mathrm{GL}(2,\mathbb{Z})$ with j even is a subgroup of $\mathrm{GL}(2,\mathbb{Z})$ and that it can be generated by three matrices. Therefore there exist three corresponding automorphisms that generate all the automorphisms that are of the form described by ψ_ξ. These are:

$$\psi_4 : (x, y, z, r, t) \mapsto (xz, y, z, r, t);$$

$$\psi_5 : (x, y, z, r, t) \mapsto (x, y, x^{-2}yz, r, t);$$

$$\psi_6 : (x, y, z, r, t) \mapsto (x^{-1}y, y, z, r, t).$$

Composing with these three outer automorphisms gives $\varphi|_{\langle x^2y^{-1}, z\rangle} = \mathrm{Id}$. Since we also have $\varphi(y) = y$ and $\langle y\rangle \times \langle x^2y^{-1}, z\rangle$ has finite index in A, we conclude that $\varphi|_A = \mathrm{Id}$.

By Proposition 6.19 we may compose with outer automorphisms if necessary so as to have $\varphi(t) \in \{t, x^i t\}$ for some $i \in \mathbb{Z}$. Composing with I_x can ensure $\varphi(t) \in \{t, xt\}$. However, Proposition 6.14 implies that since $\varphi(Ar) = Ar$ and $(x, r) = x^{-2}y \notin \langle x^2, y^2, z^2\rangle$, we cannot have $\varphi(t) = xt$. Thus we have $\varphi(t) = t$.

Since $r^2 = (rt)^2 = 1$, Proposition 6.17 gives $\varphi(r) = r$ and $\varphi(rt) = rt$; thus we have $\varphi(f) = f$ for all $f \in F$.

Applying Theorem 6.21 with Lemma 6.31 for all $a \in A$, we have $\varphi(art) = a^h rt$ for some $h \in \{1, rt\}$. If $h = rt$ then we may compose with $I_t \circ \iota$. Since

$$(I_t \circ \iota)(a^{rt} rt) = I_t(rt(a^{-1})^{rt}) = rta^{rt} = art,$$

we now have $\varphi|_{Art} = \mathrm{Id}$.

By Lemma 6.31, for all $a \in A$ we have $\varphi(ar) = a^h r$ for some $h \in \mathcal{R}_r$ where $\mathcal{R}_r = \{1, r\}$

by Corollary 6.26. Suppose that $h = r$. Then

$$x^2y^{-1}t \sim \varphi(x(xy^{-1}) \cdot t) = \varphi(xr \cdot x^{-1}rt) \sim \varphi(xr)\varphi(x^{-1}rt) = x^r r \cdot x^{-1}rt = x^r(x^{-1})^r t = t.$$

However, $x^2y^{-1}t \notin t^G = \langle x^2, y^2, z^2\rangle t$. This contradiction implies that $h \neq r$; thus $\varphi|_{Ar} = \mathrm{Id}$.

Now by Corollary 6.26 we have $\mathcal{R}_t \cap \mathcal{R}_{rt} \cap \mathcal{R}_r = \{1\}$. We use this to apply Theorem 6.35 (ii). Since $\varphi|_{Art} = \varphi|_{Ar} = \mathrm{Id}$ and $\varphi(t) = t$, by the theorem it follows that $\varphi|_{At} = \mathrm{Id}$ and therefore $\varphi = \mathrm{Id}$..

We have shown that

Theorem 7.3. *For crystallographic group G_{12}, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms and*

$$\psi_4 : (x, y, z, r, t) \mapsto (xz, y, z, r, t);$$

$$\psi_5 : (x, y, z, r, t) \mapsto (x, y, x^{-2}yz, r, t);$$

$$\psi_6 : (x, y, z, r, t) \mapsto (x^{-1}y, y, z, r, t);$$

$$\psi_y : (x, y, z, r, t) \mapsto (x, y, z, r, yt);$$

$$\psi_z : (x, y, z, r, t) \mapsto (x, y, z, zr, zt).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Let $\varphi \in \mathcal{W}(G_{13})$. By Proposition 6.6 we have $\varphi(Af) = Af$ for all $f \in F$ and $\varphi(y) \in \{y, y^{-1}\}$. If we have $\varphi(y) = y^{-1}$ then composing with I_t we may assume that $\varphi(y) = y$. Since $\mathbf{C}_2 = \langle x, z\rangle \cup \langle y\rangle$, by Proposition 6.5 (ii) we have $\varphi(\langle x, z\rangle) = \langle x, z\rangle$. In other words, $\varphi|_{\langle x,z\rangle}$ is an automorphism of a free abelian group of rank 2. We may write $\varphi(x) = x^i z^j$ and $\varphi(z) = x^k z^\ell$ for $i, j, k, \ell \in \mathbb{Z}$, and so $\varphi|_A$ corresponds to the matrix $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix} \in \mathrm{GL}(2, \mathbb{Z})$. Now for this group we have $G' = \langle x^2, y^2, z\rangle$ and by Lemma 2.11 $\varphi(G') = G'$. Then since $z \in G'$,

$$\varphi(z) = x^k z^\ell \in G' = \langle x^2, y^2, z\rangle$$

so k is even.

Let $\xi : \langle x, z\rangle \to \langle x, z\rangle$ be the automorphism determined by

$$\xi : (x, z) \mapsto (x^i z^j, x^k z^\ell).$$

Thus ξ corresponds to a matrix $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix}$ in the subgroup of $\mathrm{GL}(2,\mathbb{Z})$ of matrices with k even. For $a \in A$, the map

$$\psi_{\xi,a} : (x, y, z, r, t) \mapsto (\xi(x), y, \xi(z), ar, t)$$

determines an automorphism of G_{13} if it satisfies the relations in the presentation of G_{13}. (The pertinent relations here are $r^2 = 1$ and $(rt)^2 = z$.) Accordingly, we require $(ar)^2 = 1$ (which implies $a^r = a^{-1}$) and $(art)^2 = aa^{rt}z = \xi(z)$, i.e. $a^2 z = x^k z^\ell$. Equivalently, we require that $a = x^{k/2} z^{(\ell-1)/2}$. By Lemma 7.1 (*iii*) we know that the set of matrices $\begin{pmatrix} i & j \\ k & \ell \end{pmatrix}$ in $\mathrm{GL}(2,\mathbb{Z})$ with k even is a subgroup of $\mathrm{GL}(2,\mathbb{Z})$ and that it can be generated by three matrices. Therefore there exist three corresponding automorphisms that generate all the automorphisms that are of the form described by ψ_ξ. These are:

$$\psi_7 : (x, y, z, r, t) \mapsto (x, y, x^2 z, xr, t);$$

$$\psi_8 : (x, y, z, r, t) \mapsto (xz^{-1}, y, z, r, t);$$

$$\psi_9 : (x, y, z, r, t) \mapsto (x^{-1}, y, z, r, t).$$

Composing with these three outer automorphisms, we can ensure that $\varphi|_{\langle x,z\rangle} = \mathrm{Id}$. Since we also have $\varphi(y) = y$ we conclude that $\varphi|_A = \mathrm{Id}$.

By Proposition 6.19 we may compose with outer automorphisms ψ_x, ψ_y, and ψ_z if necessary so as to have $\varphi(t) = t$. Since $r^2 = 1$ and $(rt)^2 = z^{-1}$, Proposition 6.17 gives $\varphi(r) \in \{r, zr\}$ and $\varphi(rt) = rt$. If $\varphi(r) = zr$ then composing with $I_t \circ \iota$ we have $\varphi(r) = r$. (Notice that we still have $\varphi(rt) = rt$ as $(rt)^t = (rt)^{-1}$. Another way to see this is to realize that after composing with $I_t \circ \iota$ the hypotheses of Proposition 6.17 are still met; thus we still have $\varphi(rt) = rt$.) Thus we now have $\varphi(f) = f$ for all $f \in F$.

Let $i, j, k \in \mathbb{Z}$. For $G = G_{13}$ we have

$$(x^i y^j z^k r)^G = \langle x^2, z^2 \rangle x^i y^j z^k r \cup \langle x^2, z^2 \rangle x^i y^{-j} z^{k-1} r.$$

From this we see that $yzr \not\sim (yz)^t r = y^{-1} z^{-1} r$;, thus $t \notin \mathcal{S}_r$. By Lemma 6.32 (iv) we conclude $\mathcal{S}_r = \{1, r\}$. By Corollary 6.26 $\mathcal{R}_{rt} = \{1, rt\}$. We use this to apply Theorem 6.33 to the Art coset. Since $\mathcal{R}_{rt} \cap \mathcal{S}_r = \{1\}$ we must have $\varphi|_{Art} = \mathrm{Id}$.

Next we use a similar argument to show that $\varphi|_{Ar} = \mathrm{Id}$. We have

$$(x^i y^j z^k rt)^G = \langle y^2 \rangle x^i y^j z^k rt \cup \langle y^2 \rangle x^{-i} y^j z^{-k-1} rt.$$

Therefore $zrt \not\sim z^t rt = z^{-1} rt$ which shows that $t \notin \mathcal{S}_{rt}$; so by Lemma 6.32 (iv) we have $\mathcal{S}_{rt} = \{1, rt\}$. Corollary 6.26 gives $\mathcal{R}_r = \{1, r\}$, and so $\mathcal{R}_r \cap \mathcal{S}_{rt} = \{1\}$. By Theorem 6.33 we conclude $\varphi|_{Ar} = \mathrm{Id}$.

Note that we have $\mathcal{R}_r \cap \mathcal{R}_{rt} = \{1\}$ by Corollary 6.26. We use this to apply Theorem 6.35 (ii), using the fact that $\varphi|_{Ar} = \varphi|_{Art} = \mathrm{Id}$ and $\varphi(t) = t$. Then by the theorem we have $\varphi|_{At} = \mathrm{Id}$ and therefore $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.4. *For crystallographic group G_{13}, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_7 : (x, y, z, r, t) \mapsto (x, y, x^2 z, xr, t);$$

$$\psi_8 : (x, y, z, r, t) \mapsto (xz^{-1}, y, z, r, t);$$

$$\psi_9 : (x, y, z, r, t) \mapsto (x^{-1}, y, z, r, t);$$

$$\psi_x : (x, y, z, r, t) \mapsto (x, y, z, xr, xt);$$

$$\psi_y : (x, y, z, r, t) \mapsto (x, y, z, r, yt);$$

$$\psi_z : (x, y, z, r, t) \mapsto (x, y, z, zr, zt).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

7.2 Groups 16 through 22

Let $\varphi \in \mathcal{W}(G_{16})$. By Proposition 6.3 we have $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. By Proposition 6.5 (iv) for $\beta \in B = \{x, y, z\}$ we have $\varphi(\beta) \in \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. Composing φ with either

$$\psi_1 : (x, y, z, p, r) \mapsto (y, z, x, pr, p) \text{ or}$$

$$\psi_1^2 : (x, y, z, p, r) \mapsto (z, x, y, r, pr)$$

we may assume we have $\varphi(x) \in \{x^{\pm 1}\}$. Then composing φ with

$$\psi_2 : (x, y, z, p, r) \mapsto (x, z, y, r, p)$$

we have $\varphi(\beta) \in \beta^G$ for all $\beta \in \{x, y, z\}$. Composing with I_p and I_{pr} if necessary we have $\varphi(x) = x$ and $\varphi(y) = y$. To arrive at $\varphi(z) = z$ we may compose with I_p composed with

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r). \tag{7.1}$$

We may now assume that $\varphi|_A = \text{Id}$.

By Proposition 6.9 (ii) we have $\varphi(Af) = Af$ for all $f \in F$. Thus we have $\varphi(p) = ap$ for some $a \in A$. Squaring both sides we have $1 = \varphi(p^2) \sim (ap)^2 = aa^p$, thus $a^p = a^{-1}$. We may therefore assume $a \in \langle x, y \rangle$. By Proposition 6.19 the following are outer automorphisms:

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xp, xr) \text{ and}$$

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r).$$

Composing φ with these maps we may then assume that we have $\varphi(p) = p$.

Let $\varphi(r) = br$. Squaring both sides we have $1 = \varphi(r^2) \sim (br)^2 = bb^r$; thus $b^r = b^{-1}$. We also have $\varphi(p \cdot r) = pbr$, and squaring both sides we have

$$1 = \varphi((pr)^2) \sim (pbr)^2 = pbrpbr = b^p b^r = b^p b^{-1},$$

so that $b^p = b$, which implies $b \in \langle z \rangle$. Composing with

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr),$$

we have $\varphi(r) = r$.

We have by Lemma 6.31 and Corollary 6.27 that $\varphi(ap) = a^h p$ for some $h \in \{1, p\}$. Note that $(\psi_\iota \circ \iota)(ap) = \psi_\iota(pa^{-1}) = pa = a^p p$, thus if we have $h = p$, then composing with this anti-automorphism we have arranged to have $\varphi|Ap = \mathrm{Id}$. Since $\varphi(r) = r$, Corollary 6.36 gives $\varphi|_{Ar} = \mathrm{Id}$.

Let $\varphi(pr) = cpr$ for some $c \in A$. This gives $\varphi(pr \cdot p) \sim cr$ and $\varphi(pr \cdot r) \sim cp$. Squaring both sides of each of these equations gives the following:

$$1 \sim (cpr)^2 = cc^{pr} \text{ which implies } c^{pr} = c^{-1};$$

$$1 \sim (cr)^2 = cc^r \text{ which implies } c^r = c^{-1};$$

$$1 \sim (cp)^2 = cc^p \text{ which implies } c^p = c^{-1}.$$

This shows $c^{-1} = c^p = c^r = c^{pr}$, thus $c = 1$. We now have $\varphi(pr) = pr$ and therefore by Corollary 6.36 $\varphi|_{Apr} = \mathrm{Id}$, so that $\varphi = \mathrm{Id}$.

We have shown

Theorem 7.5. *For crystallographic group G_{16}, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_1 : (x, y, z, p, r) \mapsto (y, z, x, pr, p),$$

$$\psi_2 : (x, y, z, p, r) \mapsto (x, z, y, r, p),$$

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r),$$

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xp, xr),$$

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r),$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Let $\varphi \in \mathcal{W}(G_{17})$. Since Ar and Apr contain elements of order 2 but Ap does not, we must have $\varphi(Ap) = Ap$. If we have $\varphi(Ar) = Apr$ then we may compose φ with

$$\psi_3 : (x, y, z, p, r) \mapsto (y, x, z, p, p^{-1}r), \tag{7.2}$$

and now we have $\varphi(Af) = Af$ for all $f \in F$. By Proposition 6.9 (ii) we have $\varphi(\beta) \in \{\beta^{\pm 1}\}$ for all $\beta \in \{x, y, z\}$. Composing with I_p and I_{pr} if necessary we have $\varphi(x) = x$ and $\varphi(y) = y$. To arrive at $\varphi(z) = z$ we may compose with I_p composed with

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, r). \tag{7.3}$$

We may now assume that $\varphi|_A = \mathrm{Id}$.

Let $\varphi(r) = br$. Squaring both sides we have $1 = \varphi(r^2) \sim (br)^2 = bb^r$, so $b^r = b^{-1}$; thus we have $b \in \langle x, z\rangle$. By Proposition 6.19 the following maps are outer automorphisms:

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xp, xr) \text{ and}$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Composing φ with these maps as necessary we have $\varphi(r) = r$.

Let $\varphi(p) = ap$ for some $a \in A$. Then $\varphi(p \cdot r) \sim apr$, and squaring both sides we have $1 \sim aa^{pr}$. This implies that $a \in \langle y, z\rangle$. Squaring both sides of $\varphi(p) = ap$ we have $z = \varphi(p^2) \sim (ap)^2 = aa^p z$, thus $aa^p \in \{1, z^{-2}\}$. This gives $a \in \langle x, y\rangle \cup \langle x, y\rangle z^{-1}$. Since we also have $a \in \langle y, z\rangle$, we conclude that $a \in \langle y\rangle \cup \langle y\rangle z^{-1}$. Then composing φ with

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r), \tag{7.4}$$

we can arrange to have $\varphi(p) \in \{p, z^{-1}p\}$. Note $zp \sim (zp)^r = z^{-2}p$, thus $\varphi(zp) \sim \varphi(z^{-2}p)$. However, if we have $\varphi(p) = z^{-1}p$, then

$$\varphi(z \cdot p) \sim z \cdot z^{-1}p = p,$$

while

$$\varphi(z^{-2} \cdot p) \sim z^{-2} \cdot z^{-1}p = z^{-3}p.$$

Since $p^G = \langle x^2, y^2\rangle p \cup \langle x^2, y^2\rangle z^{-1}p$, we see $p \nsim z^{-3}p$ which is a contradiction. We therefore must have $\varphi(p) = p$.

We have by Lemma 6.31 and Corollary 6.27 that $\varphi(ap) = a^h p$ for some $h \in \{1, p\}$. Note that $(\psi_\iota \circ \iota)(ap) = \psi_\iota(p^{-1}a^{-1}) = pa = a^p p$, thus if we have $h = p$ then composing with this anti-automorphism we may assume we have $\varphi|_{Ap} = \mathrm{Id}$. We have $\varphi(r) = r$, thus by Corollary 6.36, $\varphi|_{Ar} = \mathrm{Id}$.

Let $\varphi(pr) = cpr$. Squaring both sides we have $1 \sim (cpr)^2 = cc^{pr}$ so $c^{pr} = c^{-1}$; thus $c \in \langle y, z\rangle$. We also have $r = \varphi(p^{-1} \cdot pr) \sim p^{-1}cpr = c^p r$. Squaring both sides this is $1 \sim (c^p r)^2 = (cc^r)^p$, which implies $c^r = c^{-1}$; thus $c \in \langle x, z\rangle$. Combining these results we have $c \in \langle z\rangle$. Now $\varphi(pr \cdot r) \sim cp$, and squaring both sides we have $z \sim cc^p z = c^2 z$, so $c^2 \in \{1, z^{-2}\}$. Thus we have $c \in \{1, z^{-1}\}$. Suppose that $c = z^{-1}$. Then using $\varphi|_A = \varphi|_{Ap} = \varphi|_{Ar} = \mathrm{Id}$ we have

$$xz^{-1}pr = \varphi(x \cdot pr) = \varphi(xp \cdot r) \sim xpr.$$

Proposition C.2 gives $(xpr)^G = \langle y^2, z^2\rangle xpr \cup \langle y^2, z^2\rangle x^{-1}zpr$ which implies $xpr \nsim xz^{-1}pr$. This is a contradiction. We therefore must have $c = 1$ i.e. $\varphi(pr) = pr$. Corollary 6.36 then gives $\varphi|_{Apr} = \mathrm{Id}$ and thus $\varphi = \mathrm{Id}$.

We have shown

Theorem 7.6. *For crystallographic group $G = G_{17}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_3 : (x, y, z, p, r) \mapsto (y, x, z, p, p^{-1}r);$$

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, r);$$

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xp, xr);$$

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r);$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Let $\varphi \in \mathcal{W}(G_{21})$. Proposition 6.3 gives $\mathbf{C}_2 = \langle x^2y^{-1}\rangle \cup \langle y\rangle \cup \langle z\rangle$. By Corollary 6.7 we have $\varphi(z) \in z^G$. By Lemma 6.4 it follows that $\varphi(Ap) = Ap$. Composing φ with

$$\psi_4 : (x, y, z, p, r) \mapsto (x, x^2y^{-1}, z, p, pr)$$

we may assume we have $\varphi(\beta) \in \beta^G$ for all $\beta \in B = \{x^2y^{-1}, y, z\}$. Composing φ with I_p and I_{pr} if necessary we have $\varphi(x^2y^{-1}) = x^2y^{-1}$ and $\varphi(y) = y$. To arrive at $\varphi(z) = z$ we may compose with I_p composed with

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r).$$

We now have $\varphi(\beta) = \beta$ for $\beta \in B$, and since $\langle B \rangle = \langle \mathbf{C}_2 \rangle$ and $\varphi|_A$ is a homomorphism, we have $\varphi|_{\langle \mathbf{C}_2 \rangle} = \mathrm{Id}$. Since $\langle \mathbf{C}_2 \rangle$ has finite index in A and we conclude that $\varphi|_A = \mathrm{Id}$. Now by Proposition 6.9 (ii) we have $\varphi(Af) = Af$ for all $f \in F$.

Let $\varphi(pr) = cpr$ for some $c \in A$. Squaring both sides gives $1 \sim cc^{pr}$ i.e. $c^{pr} = c^{-1}$ thus $c \in \langle y, z \rangle$. By Proposition 6.19 the maps below define outer automorphisms.

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r) \text{ and}$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Composing φ with these automorphisms we may assume we have $\varphi(pr) = pr$. We have by Lemma 6.31 and Corollary 6.27 that $\varphi(apr) = a^h pr$ for some $h \in \{1, pr\}$. Note that $(\psi_\iota \circ \iota)(apr) = \psi_\iota(pra^{-1}) = pra = a^{pr}pr$, thus if we have $h = pr$ then composing φ with this anti-automorphism we may assume we have $\varphi|_{Apr} = \mathrm{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Squaring both sides we have $1 \sim aa^p$ so $a^p = a^{-1}$ thus $a \in \langle x, y \rangle$. Squaring both sides of $\varphi(p \cdot pr) \sim ap \cdot pr$ gives $1 \sim aa^r$, so $a^r = a^{-1}$, thus $a \in \langle x^2y^{-1}, z \rangle$. Therefore we have $a \in \langle x^2y^{-1} \rangle$. Composing φ with the inner automorphism

$$I_x : (x, y, z, p, r) \mapsto (x, y, z, x^{-2}p, x^{-2}yr)$$

we may assume that we have $\varphi(p) = p$ and by Corollary 6.36 $\varphi|_{Ap} = \mathrm{Id}$.

Let $\varphi(r) = br$ for some $b \in A$. This gives $\varphi(r \cdot p) \sim bpr$ and $\varphi(r \cdot pr) \sim bp$. Squaring both sides of each of these equations gives the following:

$$1 \sim (br)^2 = bb^r \text{ which implies } b^r = b^{-1};$$

$$1 \sim (bpr)^2 = bb^{pr} \text{ which implies } b^{pr} = b^{-1};$$

$$1 \sim (bp)^2 = bb^p \text{ which implies } b^p = b^{-1}.$$

This shows $b^{-1} = b^p = b^r = b^{pr}$ and so we must have $b = 1$. We now have $\varphi(r) = r$ and therefore by Corollary 6.36, $\varphi|_{Ar} = \mathrm{Id}$ and thus $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.7. *For crystallographic group $G = G_{21}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_4 : (x, y, z, p, r) \mapsto (x, x^2y^{-1}, z, p, pr);$$

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r);$$

$$\psi_y : (x, y, z, p, r) \mapsto (x, y, z, yp, r);$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Let $\varphi \in \mathcal{W}(G_{22})$. We have $\varphi(Ap) \in \{Ap, Ar, Apr\}$. Note that the following automorphisms permute these three cosets:

$$\psi_5 : (x, y, z, p, r) \mapsto (xy^{-1}, x, x^2z^{-1}, pr, p);$$

$$\psi_6 : (x, y, z, p, r) \mapsto (y, x, z, p, pr).$$

Thus by composing φ with these maps we can assume we have $\varphi(Af) = Af$ for all $f \in F$. Note that by Proposition 6.3 we have $\mathbf{C}_2 = \langle x^2z^{-1}\rangle \cup \langle y^2z^{-1}\rangle \cup \langle z\rangle$. Then by Proposition 6.9 (ii) we have $\varphi(\beta) \in \beta^G$ for all $b \in B = \{x^2z^{-1}, y^2z^{-1}, z\}$. Composing φ with I_p and I_r as necessary we have $\varphi(x^2z^{-1}) = x^2z^{-1}$ and $\varphi(y^2z^{-1}) = y^2z^{-1}$. Now we have the automorphism

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r)$$

and note that

$$I_p \circ \psi_\iota : (x^2z^{-1}, y^2z^{-1}, z) \mapsto (x^2z^{-1}, y^2z^{-1}, z^{-1}).$$

If we have $\varphi(z) = z^{-1}$ then composing with $I_p \circ \psi_\iota$ we have we have $\varphi(\beta) = \beta$ for all $\beta \in B$. Using the fact that $\varphi|_A$ is a homomorphism gives $\varphi|_{\langle \mathbf{C}_2 \rangle} = \mathrm{Id}$ and since and $\langle \mathbf{C}_2 \rangle$ has finite index in A, it also gives $\varphi|_A = \mathrm{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Squaring both sides we have $1 \sim aa^p$ thus $a^p = a^{-1}$. This implies $a \in \langle xy^{-1}, xyz^{-1} \rangle = \langle xy^{-1}, y^2z^{-1} \rangle$. By Proposition 6.19 the map below defines an outer automorphism:

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xy^{-1}p, xr). \tag{7.5}$$

Composing φ with ψ_x and with

$$I_y^{-1} : (x, y, z, p, r) \mapsto (x, y, z, y^2z^{-1}p, zr), \tag{7.6}$$

we may assume that $\varphi(p) = p$. Now by Lemma 6.31 and Corollary 6.27 that $\varphi(ap) = a^hp$ for some $h \in \{1, p\}$. If we have $h = p$ then we may compose φ with

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r)$$

and then with ι. Since $(\psi_\iota \circ \iota)(ap) = \psi_\iota(pa^{-1}) = pa = a^pp$, composing φ with this anti-automorphism we now have $\varphi|_{Ap} = \mathrm{Id}$.

Let $\varphi(r) = br$ for some $b \in A$. Squaring both sides gives $1 \sim bb^r$, thus $b \in \langle x, z \rangle$. We also have $\varphi(p \cdot r) \sim pbr = b^ppr$ and squaring both sides of this relation gives $1 \sim (b^ppr)^2 = b^pb^r$. This implies $b \in \langle y, z \rangle$, thus we must have $\beta \in \langle z \rangle$. Composing φ with the automorphism

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr)$$

we now have $\varphi(r) = r$ and so by Corollary 6.36 $\varphi|_{Ar} = \mathrm{Id}$.

Let $\varphi(pr) = cpr$ for some $c \in A$. This gives $\varphi(pr \cdot p) \sim cr$ and $\varphi(pr \cdot r) \sim cp$. Squaring both sides of each of these relations gives the following:

$$1 \sim (cpr)^2 = cc^{pr} \text{ which implies } c^{pr} = c^{-1};$$

$$1 \sim (cr)^2 = cc^{r} \text{ which implies } c^{r} = c^{-1};$$

$$1 \sim (cp)^2 = cc^{p} \text{ which implies } c^{p} = c^{-1}.$$

This shows $c^{-1} = c^p = c^r = c^{pr}$, thus $c = 1$. We now have $\varphi(pr) = pr$ and therefore by Corollary 6.36, $\varphi|_{Apr} = \text{Id}$ and thus $\varphi = \text{Id}$.

We have shown that

Theorem 7.8. *For crystallographic group $G = G_{22}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_5 : (x, y, z, p, r) \mapsto (xy^{-1}, x, x^2z^{-1}, pr, p);$$

$$\psi_6 : (x, y, z, p, r) \mapsto (y, x, z, p, pr);$$

$$\psi_\iota : (x, y, z, p, r) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, r);$$

$$\psi_x : (x, y, z, p, r) \mapsto (x, y, z, xy^{-1}p, xr);$$

$$\psi_z : (x, y, z, p, r) \mapsto (x, y, z, p, zr).$$

Thus we have $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

7.3 Groups 25 through 42

Let $\varphi \in \mathcal{W}(G_{25})$. By Lemma 6.8 (vi) composing φ with ψ_ι if necessary we may assume $\varphi(z) = z$. By Corollary 6.10 (i) we have $\varphi(Ap) = Ap$. If $\varphi(As) = Aps$ we may compose φ with

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

and now we have $\varphi(Af) = Af$ for all $f \in F$. Then by Corollary 6.10 (ii), by composing φ with inner automorphisms as necessary we have $\varphi|_A = \text{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Note p has order 2 thus ap must have order 2 which implies $a \in \langle x, y\rangle$. By Proposition 6.19 the maps below determine outer automorphisms:

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s) \text{ and}$$

$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys).$$

Composing φ with these maps we can ensure that $\varphi(p) = p$. Then by Proposition 6.13 we have $\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. Suppose we have $h = s$, thus $\varphi(as) = a^s s = sa$. Now composing φ with

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1})$$

and then composing again with ι, we now have $\varphi|_{A\cup As} = \mathrm{Id}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing φ with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we now have $\varphi|_{Aps} = \mathrm{Id}$. (Theorem 5.9 proves τ_{ps} is non-trivial.)

By Corollary 6.37, since $\varphi|_{As\cup Aps} = \mathrm{Id}$ we conclude $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.9. *For crystallographic group $G = G_{25}$, $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, s),$$

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),$$

$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys),$$

and the non-trivial wct τ_{ps}. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{ps}\rangle$. □

Let $\varphi \in \mathcal{W}(G_{26})$. By Lemma 6.8$(vi)$, composing φ with ψ_ι if necessary we have $\varphi(z) = z$. By Corollary 6.10 (i) we have $\varphi(Ap) = Ap$. Next we note that the As coset contains no involutions but there are involutions in Aps. Thus we see that $\varphi(As) \neq Aps$. Therefore we have $\varphi(Af) = Af$ for all $f \in F$. By Corollary 6.10 (ii), by composing φ with inner automorphisms as necessary we have $\varphi|_A = \mathrm{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Squaring both sides gives (since $z \in Z(G)$) we have $z = (ap)^2 = aa^p z$, thus $a^p = a^{-1}$. This implies $a \in \langle x, y \rangle$. By Proposition 6.19 the following maps define outer automorphisms:

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s) \text{ and}$$
$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys).$$

By composing with these maps we can ensure that $\varphi(p) = p$. Then by Proposition 6.13 we have $\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. Suppose we have $h = s$, thus $\varphi(as) = a^s s = sa$. composing φ with

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1}),$$

and then with ι, we now have $\varphi|_{A \cup As} = \mathrm{Id}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing φ with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we now have $\varphi|_{Aps} = \mathrm{Id}$. (Theorem 5.9 proves τ_{ps} is non-trivial.) By Corollary 6.37, since $\varphi|_{As \cup Aps} = \mathrm{Id}$ we conclude $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.10. *For crystallographic group $G = G_{26}$ $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1}),$$
$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),$$
$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys),$$

and the non-trivial wct τ_{ps}. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{ps} \rangle$. □

Let $\varphi \in \mathcal{W}(G_{27})$. By Lemma 6.8 (vi) composing φ with ψ_ι if necessary we may assume $\varphi(z) = z$. By Corollary 6.10 (i) we have $\varphi(Ap) = Ap$. If $\varphi(As) = Aps$ we may compose φ with

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

and now we have $\varphi(Af) = Af$ for all $f \in F$. Then by Corollary 6.10 (ii), by composing φ with inner automorphisms as necessary we have $\varphi|_A = \text{Id}$. Let $\varphi(p) = ap$ for some $a \in A$. Note p has order 2 thus ap must have order 2 which implies $a \in \langle x, y\rangle$. By Proposition 6.19 the maps below determine outer automorphisms:

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s) \text{ and}$$
$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys).$$

By composing φ with these maps we can assume that $\varphi(p) = p$. Then by Proposition 6.13 we have $\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. Suppose we have $h = s$, thus $\varphi(as) = a^s s = sa$. composing with ι composed with

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1})$$

we now have $\varphi|_{A\cup As} = \text{Id}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing φ with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we now have $\varphi|_{Aps} = \text{Id}$. (Theorem 5.9 proves τ_{ps} is non-trivial.)

We have shown that

Theorem 7.11. *For crystallographic group $G = G_{27}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, the inner automorphisms,

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, s^{-1}),$$

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),$$

$$\psi_y : (x, y, z, p, s) \mapsto (x, y, z, yp, ys),$$

and the non-trivial wct τ_{ps}. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{ps} \rangle$. □

Let $\varphi \in \mathcal{W}(G_{38})$. By Lemma 6.8 (vi), composing φ with ψ_ι if necessary we have $\varphi(z) = z$. By Proposition 6.3, $\mathbf{C}_2 = \langle x \rangle \cup \langle y^2 z^{-1} \rangle$, thus by Proposition 6.5 (iv) we have $\varphi(y^2 z^{-1}) \in \{x^{\pm 1}\}, (y^2 z^{-1})^{\pm 1}\}$. Now consider that

$$\varphi(y)^2 = \varphi(y^2) = \varphi(y^2 z^{-1} \cdot z) = \varphi(y^2 z^{-1})\varphi(z) = \varphi(y^2 z^{-1})z.$$

The left hand side is a square but if $\varphi(y^2 z^{-1}) \in \{x, x^{-1}\}$ then the right hand side would not be a square. We conclude $\varphi(y^2 z^{-1}) \in (y^2 z^{-1})^G$. Then by Proposition 6.9 (ii) we have $\varphi(Af) = Af$ for all $f \in F$ and by Corollary 6.10 (ii), composing with inner automorphisms if necessary, we have $\varphi|_A = \mathrm{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Note p has order 2 thus ap must have order 2 which implies $a \in \langle x, y^2 z^{-1} \rangle$. By composing φ with the automorphisms below we can ensure that $\varphi(p) = p$.

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s) \text{ and}$$

$$I_y : (x, y, z, p, s) \mapsto (x, y, z, y^{-2}zp, y^{-2}zs).$$

(Note ψ_x is an outer autmorphism by Proposition 6.19.) Then by Proposition 6.13 we have $\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. Suppose we have $h = s$, thus

$\varphi(as) = a^s s = sa$. composing with ι composed with

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, s)$$

we now have $\varphi|_{A \cup As} = \mathrm{Id}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing φ with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we now have $\varphi|_{Aps} = \mathrm{Id}$. (Theorem 5.9 proves τ_{ps} is non-trivial.) By Corollary 6.37, since $\varphi|_{As \cup Aps} = \mathrm{Id}$ we conclude $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.12. *For crystallographic group $G = G_{38}$, $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, s),$$

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),$$

and the non-trivial wct τ_{ps}. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{ps} \rangle$. □

Let $\varphi \in \mathcal{W}(G_{39})$. By Lemma 6.8 (vi), composing φ with ψ_ι if necessary we have $\varphi(z) = z$. By Corollary 6.10 (i) we have $\varphi(Ap) = Ap$. Since As contains involutions but Aps does not, $\varphi(As) = Aps$ is not possible thus we have $\varphi(Af) = Af$ for all $f \in F$. Then by Corollary 6.10 (ii), composing with inner automorphisms if necessary, we have $\varphi|_A = \mathrm{Id}$.

Let $\varphi(p) = ap$ for some $a \in A$. Squaring both sides of this equation we have

$$z = \varphi(z) = \varphi(p^2) \sim (ap)^2 = aa^p p^2 = aa^p z.$$

Since $z \in Z(G)$ we have equality, i.e. $z = aa^p z$ thus $a^p = a^{-1}$. This tells us $a \in \langle x, y^2 z^{-1} \rangle$. By composing with the maps below we can ensure that $\varphi(p) = p$.

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s) \text{ and}$$

$$I_y : (x, y, z, p, s) \mapsto (x, y, z, y^{-2} zp, y^{-2} zs).$$

(By Proposition 6.19 ψ_x is an outer autmorphism.) Then by Proposition 6.13 we have$\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. If $h = s$ then we may compose with the non-trivial wct $\tau(s, \{Ap, As\})$ and now we have $\varphi|_{As} = \mathrm{Id}$.

By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing if necessary with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we may assume that $\varphi|_{Aps} = \mathrm{Id}$. (Theorem 5.9 proves τ_s and τ_{ps} are non-trivial.) We note that $\tau_{ps} = \iota \circ \psi_\iota \circ \tau_s$, therefore τ_{ps} will not be listed as a generator of $\mathcal{W}(G)$. By Corollary 6.37, since $\varphi|_{As \cup Aps} = \mathrm{Id}$ and $\mathcal{R}_{ps} \cap \int = 1$, we conclude $\varphi|Ap = \mathrm{Id}$.

We have shown that

Theorem 7.13. *For crystallographic group 39, $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s),$$

$$\psi_x : (x, y, z, p, s) \mapsto (x, y, z, xp, s),$$

and the non-trivial wct τ_s. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_s \rangle$. □

Let $\varphi \in \mathcal{W}(G_{42})$. By Lemma 6.8 (vi), composing φ with ψ_ι if necessary we may assume $\varphi(z) = z$. By Corollary 6.10 (i) we have $\varphi(Ap) = Ap$. If $\varphi(As) = Aps$ we may compose φ with the outer automorphism

$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

and now we have $\varphi(Af) = Af$ for all $f \in F$. Then by Corollary 6.10 (ii), by composing with inner automorphisms as necessary we have $\varphi|_A = \mathrm{Id}$.

Let $\varphi(p) = bp$ for some $b \in A$. Note p has order 2 thus bp also has order 2 which implies $b \in \langle xy^{-1}, xyz^{-1} \rangle$. Note that $\langle xy^{-1}, xyz^{-1} \rangle$ has index 2 in $\langle x^2z^{-1}, y^2z^{-1} \rangle$, thus by composing

φ with the inner automorphisms

$$I_x : (x, y, z, p, s) \mapsto (x, y, z, x^{-2}zp, s)$$
$$\text{and } I_y : (x, y, z, p, s) \mapsto (x, y, z, y^{-2}zp, y^{-2}zs),$$

we may assume that $\varphi(p) \in \{p, xy^{-1}p\}$. Suppose that $\varphi(p) = xy^{-1}p$ and let $\varphi(s) = as$ for some $a \in A$. Then

$$\varphi(p \cdot s) \sim xy^{-1}pas = xy^{-1}a^p ps.$$

Since s and ps have order 2, as and $xy^{-1}a^p ps$ also have order 2. We have $|as| = 2$ which implies $a \in \langle y^2z^{-1}\rangle$ and so we have $a^p = a^{-1}$. Also, $xy^{-1}a^p ps$ has order 2, which implies it is contained in the subgroup $\langle x^2z^{-1}\rangle$. Thus we conclude that $xy^{-1}a^p = xy^{-1}a^{-1} \in \langle x^2z^{-1}\rangle$. This indicates that $a \in \langle y^2z^{-1}\rangle \cap \langle x^2z^{-1}\rangle xy^{-1}$ which is empty. This is a contradiction thus $\varphi(p) = xy^{-1}p$ is not possible. We may assume therefore that $\varphi(p) = p$, and now by Proposition 6.13 we have $\varphi(f) = f$ for all $f \in F$.

Now by Corollary 6.28 we have $\mathcal{R}_f = \{1, f\}$ for $f \in \{s, ps\}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(as) = a^h s$ for some $h \in \mathcal{R}_s = \{1, s\}$. Suppose we have $h = s$, thus $\varphi(as) = a^s s = sa$. composing φ with ι and then with the automorphism

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p^{-1}, s^{-1})$$

we now have $\varphi|_{A\cup As} = \mathrm{Id}$. By Lemma 6.31, for all $a \in A$ we have $\varphi(aps) = a^h ps$ for some $h \in \mathcal{R}_{ps} = \{1, ps\}$. Composing φ with the non-trivial wct $\tau(ps, \{Ap, Aps\})$ we now have $\varphi|_{Aps} = \mathrm{Id}$. (Theorem 5.9 proves τ_{ps} is non-trivial.) By Corollary 6.37, since $\varphi|_{As\cup Aps} = \mathrm{Id}$ we conclude $\varphi = \mathrm{Id}$.

We have shown that

Theorem 7.14. *For crystallographic group $G = G_{42}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_\iota : (x, y, z, p, s) \mapsto (x^{-1}, y^{-1}, z^{-1}, p, s),$$
$$\psi_1 : (x, y, z, p, s) \mapsto (y, x, z, p, ps),$$

and the non-trivial wct τ_{ps}. *Thus we have* $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{ps} \rangle$. $\square$

Chapter 8. The wct groups of space groups having point group $\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}\frac{\mathbf{2}}{\mathbf{m}}$

8.1 Groups 47 through 57

Let $\varphi \in \mathcal{W}(G_{47})$. By Proposition 6.3 $\mathbf{C}_2 = \langle x\rangle \cup \langle y\rangle \cup \langle z\rangle$. Without loss of generality, let $B = \{x, y, z\}$. By Proposition 6.5 (iv) we have $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. If $\varphi(x) \in \{y^{\pm 1}\}$ then we may compose φ with the automorphism

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t)$$

so that $\varphi(x) \in x^G$. Alternatively, if $\varphi(x) \in \{z^{\pm 1}\}$ then we may compose φ with the automorphism

$$\psi_2 : (x, y, z, p, r, t) \mapsto (z, y, x, pr, r, t)$$

so that $\varphi(x) \in x^G$. If $\varphi(y) \in \{z^{\pm 1}\}$ then we may compose φ with the automorphism

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, z, y, r, p, t),$$

so that we may now assume that $\varphi(\beta) \in \beta^G$ for all $\beta \in B$. Applying Proposition 6.9 (iv) we may compose with inner automorphisms so that $\varphi|_A = \mathrm{Id}$ and by (ii) we also have $\varphi(Af) = Af$ for all $f \in F$. By Proposition 6.19 we may compose with automorphisms ψ_x, ψ_y, and ψ_z in order to arrange that $\varphi(t) = t$. Then by Proposition 6.17, since every element of F has order 2 we have $\varphi(f) = f$ for all $f \in F$.

Now by Lemma 6.31 for $a \in A$ we have $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t$. We have $\mathcal{R}_t = F$ by Corollary 6.29. Since $\langle Aprt, Art, Apt\rangle = G/A$, we see that composing with the non-trivial wcts $\tau(prt, \{Aprt, At, Ap, Ar\})$, $\tau(rt, \{Art, At, Apr, Ap\})$, and $\tau(pt, \{Apt, At, Ar, Apr\})$, we can assume that we have $\varphi|_{At} = \mathrm{Id}$. (Theorem 5.9 proves these three functions are non-trivial wcts.) We note that $\tau_{rt} = \psi_1 \circ \psi_2 \circ \tau_{prt} \circ \psi_2 \circ \psi_1$ and $\tau_{pt} = \psi_1 \circ \psi_3 \circ \tau_{prt} \circ \psi_3 \circ \psi_1$ so we will only include τ_{prt} when we list the generators of the wct group. Applying Corollary 6.38 we have $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.1. *For crystallographic group $G = G_{47}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t),$$

$$\psi_2 : (x, y, z, p, r, t) \mapsto (z, y, x, pr, r, t),$$

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, z, y, r, p, t),$$

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt),$$

and that $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{prt} \rangle$. □

Proposition 8.2. *For group 49 we have*

$$\mathcal{S}_p = \mathcal{S}_r = \mathcal{S}_{pr} = \mathcal{S}_t = F; \qquad \mathcal{S}_{prt} = \{1, prt, rt, p\};$$

$$\mathcal{S}_{rt} = \{1, prt, rt, p\}; \qquad \mathcal{S}_{pt} = \{1, pt, p, t\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.4. □

Let $\varphi \in \mathcal{W}(G_{49})$. By Proposition 6.3 $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x, y, z\}$. By Proposition 6.5 (iv) we have $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. By Proposition C.4 we have $G' = \langle x^2, y^2, z \rangle$, thus by applying Lemma 2.11 we conclude $\varphi(z) \in \{z^{\pm 1}\}$. If $\varphi(x) \in \{y^{\pm 1}\}$ then we may compose φ with the automorphism $\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t)$ and now $\varphi(x) \in x^G$ and $\varphi(y) \in y^G$. Applying Proposition 6.9 (iv) we may compose φ with inner automorphisms so that $\varphi|_A = \mathrm{Id}$ and by (ii) we have $\varphi(Af) = Af$ for all $f \in F$. By Proposition 6.19 we may compose φ with ψ_x, ψ_y, and ψ_z so that we may have $\varphi(t) = t$.

The elements of F that have order 2 (besides t) are p, r, pr, and pt. By Proposition 6.17 we must have $\varphi(pt) = pt, \varphi(rt) = rt, \varphi(prt) = prt$, and $\varphi(p) = p$. Recall that $(prt)^2 = (rt)^2 =$

z^{-1}, so by Proposition 6.17 $\varphi(pr) \in \{pr, zpr\}$ and $\varphi(r) \in \{r, zr\}$. If we have $\varphi(r) = zr$ then by Proposition 6.18 (i) we may compose φ with $I_t \circ \iota$ so as to have $\varphi(r) = r$. Now by (ii) we have $\varphi(f) = f$ for all $f \in F - \{pr\}$. Note that $\varphi(pr \cdot r) = \varphi(p) = p$ and we also have $p \not\sim zp$ by Proposition C.4. Therefore by Proposition 6.18 (iii) $\varphi(r) = r$ implies $\varphi(pr) \neq zpr$ thus $\varphi(pr) = pr$. Thus we have $\varphi(f) = f$ for all $f \in F$.

We now apply Theorem 6.33 three times. We will use the following facts from Proposition 8.2: $prt \notin \mathcal{S}_{pt}; rt \notin \mathcal{S}_{pt}$, and $pt \notin \mathcal{S}_{rt}$. Also recall that by Corollary 6.29 $\mathcal{R}_f = \{1, f\}$ for $f \in \{prt, rt, pt\}$. Now since p commutes with r we have $r \cdot prt = pt$. Then since $\mathcal{R}_{prt} \cap \mathcal{S}_{pt} = 1$ Theorem 6.33 implies $\varphi|_{Aprt} = \mathrm{Id}$. Since $r^2 = 1$ we have $pr \cdot rt = pt$ and $\mathcal{R}_{rt} \cap \mathcal{S}_{pt} = 1$ so the theorem implies $\varphi|_{Art} = \mathrm{Id}$. Since p commutes with r we have $pr \cdot pt = rt$ so since $\mathcal{R}_{pt} \cap \mathcal{S}_{rt} = 1$ we have $\varphi|_{Apt} = \mathrm{Id}$. It follows by Corollary 6.38 that $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.3. *For crystallographic group $G = G_{49}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms and*

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t),$$

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt),$$

and that $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.4. *For group 50 we have*

$$\mathcal{S}_p = \mathcal{S}_r = \mathcal{S}_{pr} = \mathcal{S}_t = F; \qquad \mathcal{S}_{prt} = \{1, prt\};$$

$$\mathcal{S}_{rt} = \{1, rt\}; \qquad \mathcal{S}_{pt} = \{1, pt\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.5. □

Let $\varphi \in \mathcal{W}(G_{50})$. By Proposition 6.3, $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. We apply Proposition 6.5 (iv), with $B = \{x, y, z\}$ and we conclude $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. Proposition

C.5 gives $G' = \langle x, y, z^2 \rangle$ so by Lemma 2.11 we have $\varphi(z) \in \{z^{\pm 1}\}$. If $\varphi(x) \in \{y^{\pm 1}\}$ then we may compose with the automorphism

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t)$$

and now $\varphi(x) \in x^G$ and $\varphi(y) \in y^G$. By Proposition 6.9 (iv) we may now compose with inner automorphisms so that $\varphi|_A = \mathrm{Id}$ and by (ii) $\varphi(Af) = Af$ for all $f \in F$. By Proposition 6.19 we may compose with ψ_x, ψ_y, and ψ_z in order to ensure $\varphi(t) = t$.

We have $(rt)^2 = x^{-1}$, thus by Proposition 6.17 we conclude that $\varphi(r) \in \{r, xr\}$. If we have $\varphi(r) = xr$ we consider the map I_t which maps r to xr. Then composing with $I_t \circ \iota$ we may assume that we have $\varphi(r) = r$.

Since p, r, and pr are involutions, we may conclude by Proposition 6.17 that $\varphi(pt) = pt, \varphi(rt) = rt$, and $\varphi(prt) = prt$.

Now let $\varphi(p) = bp$ for some $b \in A$. We have $(pt)^2 = x^{-1}y^{-1}$ thus applying the Proposition again we see that $b^2x^{-1}y^{-1} \in \{xy, xy^{-1}, x^{-1}y, x^{-1}y^{-1}\}$ which gives $b^2 \in \{x^2y^2, x^2, y^2, 1\}$ thus $b \in \{1, x, y, xy\}$. However we also have $bp = \varphi(pt \cdot t) \sim pt \cdot t = p$. Since $p^G = \langle xy, xy^{-1} \rangle p$ we see $b \in \{x, y\}$ would give a contradiction, thus we have $b \in \{1, xy\}$.

Let $\varphi(pr) = cpr$. We again apply Proposition 6.17. Since $(prt)^2 = y^{-1}$ we see that $c \in \{1, y\}$. Now $p \sim bp = \varphi(pr \cdot r) \sim cp$ but $yp \nsim p$, therefore we must have $\varphi(pr) = pr$. Lastly, $pr = \varphi(p \cdot r) \sim bpr$ and $(pr)^G = \langle y, z^2 \rangle pr$ so $b = xy$ gives a contradiction thus $\varphi(p) = p$. We have shown that we can assume $\varphi(f) = f$ for all $f \in F$.

We will now apply Theorem 6.33 twice to the At coset. By the theorem, $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t \cap \mathcal{S}_{rt}$ and also $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t \cap \mathcal{S}_{pt}$. Combining these we have $h \in \mathcal{R}_t \cap \mathcal{S}_{rt} \cap \mathcal{S}_{pt}$. Proposition 8.4 states that $\mathcal{S}_{rt} = \{1, rt\}$ and $\mathcal{S}_{pt} = \{1, pt\}$. We conclude that $h = 1$, i.e. $\varphi|_{At} = \mathrm{Id}$. We apply Corollary 6.38 and now we have $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.5. *For crystallographic group $G = G_{50}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, the inner automorphisms and

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t),$$

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Thus, $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.6. *For group 51 we have*

$$\mathcal{S}_r = \mathcal{S}_{rt} = \mathcal{S}_t = F;$$

$$\mathcal{S}_p = \mathcal{S}_{prt} = \{1, p, rt, prt\};$$

$$\mathcal{S}_{pr} = \mathcal{S}_{pt} = \{1, pr, rt, pt\};$$

Proof. This follows from Lemma 6.32 and Proposition C.6. □

Let $\varphi \in \mathcal{W}(G_{51})$. Note that by Lemma 6.12, Apr and Apt are the only cosets that do not contain elements of order 2. This together with Corollary 6.11 gives $\varphi(Apr) = Apr$, $\varphi(Apt) = Apt$, and $\varphi(At) = At$. Note that $\langle Apr, Apt, At\rangle = G/A$. Since G/A is abelian $\overline{\varphi}$ is a homomorphism we conclude that $\varphi(Af) = Af$ for all $f \in F$. Then by Proposition 6.9 (*ii*) and (*iv*), we may now compose φ with inner automorphisms so that $\varphi|_A = \text{Id}$. By Proposition 6.19 we may compose with ψ_x, ψ_y, and ψ_z so as to have $\varphi(t) = t$.

We now consider that p, r, prt, and rt all have order 2 thus by Proposition 6.17 we have $\varphi(f) = f$ for all $f \in \{pt, rt, pr, r\}$. Applying the proposition again, since $(pt)^2 = (pr)^2 = x^{-1}$ we have $\varphi(p) \in \{p, xp\}$ and $\varphi(prt) \in \{prt, xprt\}$. If we have $\varphi(prt) = xprt$ then by Proposition 6.18 (*i*),composing with $I_t \circ \iota$ we have $\varphi(prt) = prt$. By (*ii*) we have $\varphi(f) = f$ for all $f \in F - \{p\}$. Now by Proposition C.6 we have $(rt)^G = \langle y^2\rangle rt$ thus $rt \nsim xrt$. We use this as we apply Proposition 6.18 (*iii*). Since $\varphi(p \cdot prt) = p \cdot prt \nsim xrt$, it follows by (*iii*) that $\varphi(prt) = prt$ implies $\varphi(p) \neq xp$ therefore we conclude $\varphi(p) = p$. Thus we now have $\varphi(f) = f$ for all $f \in F$.

Since $pt \notin \mathcal{S}_p$ and $prt \notin \mathcal{S}_{pr}$, we may apply Corollary 6.34 with $f \in \{pt, prt\}$ which gives $\varphi|_{Apt \cup Aprt} = \mathrm{Id}$. Now Lemma 6.31 gives $\varphi(art) = a^h rt$ for some $h \in \mathcal{R}_{rt} = \{1, rt\}$. If $h = rt$ we may compose with $\tau(rt, \{Art, At, Apr, Ap\})$ so as to have $\varphi|_{Art} = \mathrm{Id}$. (Theorem 5.9 proves τ_{rt} is a non-trivial wct.) We now have $\varphi(g) = g$ for all $g \in Aprt \cup Art \cup Apt$, thus by Corollary 6.38 that $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.7. *For crystallographic group $G = G_{51}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt),$$

and $\tau_r t$. Thus $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{rt} \rangle$. □

Proposition 8.8. *For group 53 we have*

$$\mathcal{S}_{pr} = \mathcal{S}_t = F; \qquad \mathcal{S}_p = \{1, p, prt, rt\};$$

$$\mathcal{S}_r = \{1, r, prt, pt\}; \qquad \mathcal{S}_{prt} = \{1, pr, prt, t\};$$

$$\mathcal{S}_{rt} = \{1, rt\}; \qquad \mathcal{S}_{pt} = \{1, pt\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.7. □

Let $\varphi \in \mathcal{W}(G_{53})$. Corollary 6.11 tells us $\varphi(At) = At$ and $\varphi(Ap) \in \{Ap, Ar, Apr\}$. However by Lemma 6.12, Ap contains no elements of order 2 and Ar and Apr do, thus we have $\varphi(Ap) = Ap$. Similarly $Aprt$ contains elements of order 2 but Apt and Art do not thus by Corollary 6.11 $\varphi(Aprt) = Aprt$. We know $\overline{\varphi}$ is a homomorphism as G/A is abelian. Since $\langle Ap, At, Aprt \rangle = G/A$, we conclude $\varphi(Af) = Af$ for all $f \in F$. Now by Proposition 6.9 (ii) and (iv), we may compose with inner automorphisms so that $\varphi|_A = \mathrm{Id}$. By Proposition 6.19 we may compose φ with ψ_x, ψ_y, and ψ_z as necessary so we may now assume $\varphi(t) = t$.

We now apply Proposition 6.17 with $f = p$ using the fact that $(pt)^2 = x^{-1}$ to deduce that $\varphi(p) \in \{p, xp\}$. If we have $\varphi(p) = xp$ then we may compose φ with $I_t \circ \iota$ and now we have $\varphi(p) = p$.

Again applying the proposition we see that since r, pr, and prt have order 2, we must have $\varphi(rt) = rt, \varphi(prt) = prt$, and $\varphi(pr) = pr$, and since $p^2 = z$ we must have $\varphi(pt) \in \{pt, z^{-1}pt\}$. However if $\varphi(pt) = z^{-1}pt$ then

$$t = \varphi(p^{-1} \cdot pt) \sim p^{-1}z^{-1}pt = z^{-1}t.$$

However, $t^G = \langle xz, x^{-1}z, y^2 \rangle t$ which does not contain $z^{-1}t$, thus we have a contradiction. We conclude that $\varphi(pt) = pt$.

Using Proposition 6.17 with $f = r$ and thus $\delta = (rt)^2 = x^{-1}z^{-1}$ we see that $\varphi(r) = br$ implies that $b \in \{1, x, z, xz\}$. However $\varphi(r)$ must also satisfy

$$t = \varphi(r \cdot rt) \sim br \cdot rt = bt,$$

yet $t^G = \langle xz, x^{-1}z, y^2 \rangle t$ does not contain xt nor zt. We also have

$$pr = \varphi(p \cdot r) = pbr = b^p pr,$$

but $(pr)^G = \langle y^2, z \rangle pr$ which does not contain $(xz)^p pr = x^{-1}zpr$. Thus we must have $\varphi(r) = r$. We now have $\varphi(f) = f$ for all $f \in F$.

We now apply Theorem 6.33 twice to the At coset. By the theorem, $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t \cap \mathcal{S}_{rt}$ and also $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t \cap \mathcal{S}_{pt}$. We conclude $h \in \mathcal{R}_t \cap \mathcal{S}_{rt} \cap \mathcal{S}_{pt}$. Proposition 8.8 states that $\mathcal{S}_{rt} = \{1, rt\}$ and $\mathcal{S}_{pt} = \{1, pt\}$. We conclude that $h = 1$, i.e. $\varphi|_{At} = \mathrm{Id}$. We apply Corollary 6.38 and now we have $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.9. *For crystallographic group $G = G_{53}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, the inner automorphisms and

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Thus $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.10. *For group 54 we have*

$$\mathcal{S}_{pt} = \{1, pt\}; \qquad \mathcal{S}_p = \mathcal{S}_{prt} = \mathcal{S}_{rt} = \{1, p, prt, rt\};$$

$$\mathcal{S}_r = \{1, r, prt, pt\}; \qquad \mathcal{S}_{pr} = \{1, pr, rt, pt\};$$

$$\mathcal{S}_t = F.$$

Proof. This follows from Lemma 6.32 and Proposition C.8. □

Let $\varphi \in \mathcal{W}(G_{54})$. By Proposition 6.3 $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. We apply Proposition 6.5 (*iv*), with $B = \{x, y, z\}$ and we conclude $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. Now by Corollary 6.11 we have $\varphi(At) = At$ and $\varphi(Apr) \in \{Ap, Ar, Apr\}$. However, as Ap and Ar each contain elements of order 2 but by Lemma 6.12, Apr does not, we know $\varphi(Apr) = Apr$. Since G/A is abelian, $\overline{\varphi}$ is a homomorphism thus $\varphi(Aprt) = Aprt$. By Lemma 6.4 this implies that $\varphi(x) \in \{x^{\pm 1}\}$ (because y and z commute with every element in $Aprt$.) Now Proposition C.8 gives $G' = \langle x, y^2, z \rangle$ so by Lemma 2.11 we have $\varphi(z) \in \{z^{\pm 1}\}$ thus we have $\varphi(\beta) \in \beta^G$ for all $\beta \in B$. By Proposition 6.9 (*ii*) and (*iv*) we have $\varphi(Af) = Af$ for all $f \in F$ and by composing with inner automorphisms we have $\varphi|_A = \mathrm{Id}$. Now by Proposition 6.19 we may compose with ψ_x, ψ_y, and ψ_z so that we may assume $\varphi(t) = t$.

We now apply Proposition 6.17 with $f = p$ using the fact that $(pt)^2 = x^{-1}$ to deduce that $\varphi(p) \in \{p, xp\}$. If we have $\varphi(p) = xp$ then we may compose with $I_t \circ \iota$ and now we have $\varphi(p) = p$.

Again applying the proposition we see that since p and r have order 2, we must have $\varphi(pt) = pt$ and $\varphi(rt) = rt$. Since $(pr)^2 = x^{-1}$ we must have $\varphi(prt) \in \{prt, xprt\}$. However if

$\varphi(prt) = xprt$ then

$$xprt = \varphi(p \cdot rt) \sim p \cdot rt,$$

which contradicts $(prt)^G = \langle x^2 \rangle prt \cup \langle x^2 \rangle xzprt$. Therefore $\varphi(prt) = prt$.

Since $(prt)^2 = (rt)^2 = z^{-1}$ Proposition 6.17 indicates we must have $\varphi(pr) \in \{pr, zpr\}$ and $\varphi(r) \in \{r, zr\}$. Suppose that $\varphi(pr) = zpr$. Then

$$prt = \varphi(pr \cdot t) \sim zpr \cdot t$$

which is a contradiction since $zprt \notin (prt)^G$. We conclude that $\varphi(pr) = pr$. Lastly, suppose that $\varphi(r) = zr$. Then

$$p = \varphi(p) = \varphi(pr \cdot r) \sim pr \cdot zr = z^{-1}p.$$

This contradicts $(p)^G = \langle x^2, y^2 \rangle p \cup \langle x^2, y^2 \rangle xp$ thus $\varphi(r) = r$. We now have $\varphi(f) = f$ for all $f \in F$.

Note that according to Proposition 8.10 $prt \notin \mathcal{S}_{pr}, rt \notin \mathcal{S}_r$, and $pt \notin \mathcal{S}_p$. We therefore may apply Corollary 6.34 with $f \in \{prt, rt, pt\}$ which gives $\varphi|_{Aprt \cup Art \cup Apt} = \mathrm{Id}$. Then by Corollary 6.38 we see that φ is the identity map on all of G.

We have shown that

Theorem 8.11. *For crystallographic group $G = G_{54}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xr, xt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.12. *For group 55 we have*

$$\mathcal{S}_p = \mathcal{S}_{pt} = \mathcal{S}_t = F;$$

$$\mathcal{S}_r = \mathcal{S}_{prt} = \{1, r, prt, pt\};$$

$$\mathcal{S}_{pr} = \mathcal{S}_{rt} = \{1, pr, rt, pt\};$$

Proof. This follows from Lemma 6.32 and Proposition C.9. □

Let $\varphi \in \mathcal{W}(G_{55})$. By Corollary 6.11 we have $\varphi(Apt) \in \{Apt, Art, Aprt\}$. Now by Lemma 6.12, Apt contains elements of order 2 and Art and $Aprt$ do not, thus we know $\varphi(Apt) = Apt$. By Proposition 6.3 $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. Without loss of generality, let $B = \{x, y, z\}$. By Proposition 6.5 (iv) we have $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. Now we apply Lemma 6.4 using $\varphi(Apt) \in Apt$. This implies that $\varphi(z) \in z^G$ (because z is inverted by every element in Apt but x and y commute with every element in Apt.) If $\varphi(x) \in y^G$ we may compose φ with the outer automorphism

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t)$$

and now we have $\varphi(\beta) = \beta$ for all $\beta \in \{x, y, z\}$. By Proposition 6.9 (ii) $\varphi(Af) = Af$ for all $f \in F$ and by (iv) we may compose φ with inner automorphisms so that we have $\varphi|_A = \mathrm{Id}$. By Proposition 6.19 there exist automorphisms ψ_x, ψ_y, and ψ_z and composing φ with these maps we have $\varphi(t) = t$.

The squares of the elements in F are $p^2 = (pt)^2 = 1$, $r^2 = y$, $(pr)^2 = x$, $(rt)^2 = x^{-1}$, and $(prt)^2 = y^{-1}$. Applying these facts to Proposition 6.17 we have $\varphi(p) = p$, $\varphi(pt) = pt$, $\varphi(r) \in \{r, xr\}$, $\varphi(pr) \in \{pr, ypr\}$, $\varphi(prt) \in \{prt, x^{-1}prt\}$, and $\varphi(rt) \in \{rt, y^{-1}rt\}$. If we have $\varphi(rt) = y^{-1}rt$, then by Proposition 6.18 (i)we may compose φ with $I_t \circ \iota$ so as to ensure that $\varphi(rt) = rt$. Then by (ii) we have $\varphi(f) = f$ for all $f \in F - \{r, pr, prt\}$. We will now Proposition 6.18 (iii) to show that this implies $\varphi(f) = f$ for all $f \in \{r, pr, prt\}$. Accordingly, we note that by Proposition C.9,

$$yt \nsim xyt \text{ since } (xyt)^G = \langle xy, xy^{-1}, z^2 \rangle t;$$
$$y^{-1}pt \nsim pt \text{ since } (pt)^G = \langle z^2 \rangle pt;$$
$$xp \nsim p \text{ since } (p)^G = \langle xy, xy^{-1} \rangle p.$$

Therefore we have

$$\varphi(r \cdot rt) = \varphi(y \cdot t) \sim yt \nsim xyt;$$

thus by Proposition 6.18 (iii) , $\varphi(r) \neq xr$ and so we have $\varphi(r) = r$. Similarly we have

$$\varphi(pr \cdot rt) = \varphi(pyt) = \varphi(y^{-1} \cdot pt) \sim y^{-1}pt \nsim pt;$$

thus by the proposition, $\varphi(pr) \neq ypr$ so $\varphi(pr) = pr$. Lastly, we have

$$\varphi(prt \cdot rt) = \varphi(px^{-1}) = \varphi(x \cdot p) \sim xp \nsim p;$$

thus by the proposition, $\varphi(prt) \neq x^{-1}prt$ i.e. $\varphi(prt) = prt$ and so we now have $\varphi(f) = f$ for all $f \in F$.

Note that $prt \notin \mathcal{S}_{pr}$ and $rt \notin \mathcal{S}_r$. Thus we may apply Corollary 6.34 to get $\varphi|_{Aprt \cup Art} = \mathrm{Id}$. Now by Lemma 6.31, for all $a \in A$ we have $\varphi(apt) = a^h pt$ for some $h \in \{1, pt\}$. If $h = pt$ then we may compose with the non-trivial wct $\tau(pt, \{At, Apt, Ar, Apr\})$ to get $\varphi|_{Apt} = \mathrm{Id}$. (Theorem 5.9 shows τ_{pt} is a non-trivial wct.) By Corollary 6.38 we now have $\varphi = \mathrm{Id}$ on all of G.

We have shown that

Theorem 8.13. *For crystallographic group $G = G_{55}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_1 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t),$$
$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xrxt),$$
$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, ryt),$$
$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zrzt),$$

and τ_{pt}. *Therefore* $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{pt} \rangle$. $\square$

Proposition 8.14. *For group 57 we have*

$$\mathcal{S}_p = \{1, p, prt, rt\}; \qquad \mathcal{S}_r = \mathcal{S}_{prt} = \mathcal{S}_{pt} = \{1, r, prt, pt\};$$

$$\mathcal{S}_{pr} = \{1, pr, rt, pt\}; \qquad \mathcal{S}_{rt} = \{1, rt\};$$

$$\mathcal{S}_t = F.$$

Proof. This follows from Lemma 6.32 and Proposition C.10. $\square$

Let $\varphi \in \mathcal{W}(G_{57})$. By Proposition 6.3 $\mathbf{C}_2 = \langle x \rangle \cup \langle y \rangle \cup \langle z \rangle$. We apply Proposition 6.5 (iv), with $B = \{x, y, z\}$ and we conclude $\{\varphi(x), \varphi(y), \varphi(z)\} \subseteq \{x^{\pm 1}, y^{\pm 1}, z^{\pm 1}\}$. Proposition C.10 gives $G' = \langle x^2, y, z \rangle$ so by Lemma 2.11 we have $\varphi(x) \in x^G$. By Corollary 6.11 we have $\varphi(Apt) \in \{Aprt, Art, Apt\}$. Since Apt contains elements of order 2 but by Lemma 6.12 $Aprt$ and Art do not, we have $\varphi(Apt) = Apt$. Applying Lemma 6.4 to the relation $z^{pt} = z^{-1}$ we see that $\varphi(z) \in y^G$ gives a contradiction. We conclude that $\varphi(z) \in z^G$ and so $\varphi(y^G) = y^G$ as well. By Proposition 6.9 (ii) and (iv) $\varphi(Af) = Af$ for all $f \in F$. and we may compose φ with inner automorphisms so that $\varphi|_A = \mathrm{Id}$. By Proposition 6.19 we may compose with automorphisms ψ_x, ψ_y, and ψ_z as necessary so as to have $\varphi(t) = t$.

We now apply Proposition 6.17 with $f = r$ using the fact that $(rt)^2 = z^{-1}$ to deduce that $\varphi(r) \in \{r, zr\}$. If we have $\varphi(r) = zr$ then we may compose with $I_t \circ \iota$ and now we have $\varphi(r) = r$.

Again applying the proposition we see that since pr and pt have order 2, we must have $\varphi(prt) = prt$ and $\varphi(p) = p$. Since $(prt)^2 = y^{-1}$ we have $\varphi(pr) \in \{pr, ypr\}$; also, $r^2 = y$ gives $\varphi(rt) \in \{rt, y^{-1}rt\}$. However if $\varphi(pr) = ypr$ then

$$r = \varphi(p^{-1} \cdot pr) \sim p^{-1} \cdot ypr = y^{-1}r,$$

and if $\varphi(rt) = y^{-1}rt$ then

$$r = \varphi(rt \cdot t) \sim y^{-1}rt \cdot t = y^{-1}r.$$

In both cases we arrive at $r \sim y^{-1}r$ which is a contradiction since $r^G = \langle x^2, z^2\rangle r \cup \langle x^2, z^2\rangle y^{-1}zr$. Therefore we have $\varphi(pr) = pr$ and $\varphi(rt) = rt$.

Lastly, since $p^2 = z$ the proposition gives $\varphi(pt) \in \{pt, z^{-1}pt\}$. If $\varphi(pt) = z^{-1}pt$ then

$$yz^{-1} \cdot prt \sim \varphi(yz^{-1} \cdot prt) = \varphi(r \cdot pt) \sim rz^{-1}pt = yprt,$$

which contradicts $(yprt)^G = \langle x^2\rangle y^u prt, u \in \{0, 1\}$, thus $\varphi(pt) = pt$.

We now have $\varphi(f) = f$ for all $f \in F$.

Note that $prt \notin \mathcal{S}_{pr}, rt \notin \mathcal{S}_r$, and $pt \notin \mathcal{S}_p$, thus by Corollary 6.34 we have $\varphi|_{Aprt \cup Art \cup Apt} = \mathrm{Id}$ and so by Corollary 6.38 we now have $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.15. *For crystallographic group $G = G_{57}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms and*

$$\psi_x : (x, y, z, p, r, t) \mapsto (x, y, z, xp, xrxt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, ryt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zrzt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

8.2 Groups 63 through 68

The following applies to $G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68}.

Proposition 8.16. *Let $\varphi \in \mathcal{W}(G)$ where $G \in \{G_{63}, G_{64}, G_{65}, G_{66}, G_{67}, G_{68}\}$.*

(i) $\varphi(z) \in \{z, z^{-1}\}$. Also, for $\alpha \in \{x^2y^{-1}, y\}$ we have $\varphi(\alpha) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$.

(ii) For $Af \in \{At, Ap, Apt\}$ we have $\varphi(Af) = Af$.

(iii) For $Af \in \{Ar, Apr\}$ we have $\varphi(Af) \in \{Ar, Apr\}$. Also, for $f \in \{prt, rt\}$ we have $\varphi(Af) \in \{Aprt, Art\}$. Finally, $\varphi(Ar) = Apr$ if and only if $\varphi(Art) = Aprt$.

Proof. Statement (i) comes directly from Corollary 6.7.

We prove $\varphi(Apt) = Apt$ by using Corollary 6.11. We have $\varphi(Apt) \in \{Aprt, Art, Apt\}$. Applying Lemma 6.4 to the relation $z^{pt} = z^{-1}$ we have $\varphi(z)^{\varphi(pt)} = \varphi(z)^{-1}$. Since both prt and rt commute with z we cannot have $\varphi(pt) \in Aprt \cup Art$.

By Corollary 6.11 we have $\varphi(At) = At$. Since G/A is abelian $\overline{\varphi}$ is a homomorphism, thus $\varphi(Ap) = \varphi(Apt \cdot At) = Apt \cdot At = Ap$, proving (ii). Statement (iii) follows by Corollary 6.11 and the fact that $\overline{\varphi}$ is a bijective homomorphism. □

The following applies to $G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68}.

Proposition 8.17. *Let G be a group with presentation of the form given in Eq. (4.4) with $\delta = 1$. Let $\varphi \in \mathcal{W}(G)$ and suppose that $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$ for all $f \in F$. Then there exists an automorphism ψ such that $\psi \circ \varphi$ satisfies $(\psi \circ \varphi)(t) = t$.*

Proof. Let $\varphi(t) = ct$ for some $c \in A$. By Proposition 6.19 there exist outer automorphisms

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$
$$\text{and } \psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Composing with these maps as well as with I_x, we may assume $c \in \{1, x\}$. By Corollary 6.15 $c = x$ is not possible so we are done. □

Proposition 8.18. *For group 63 we have*

$$\mathcal{S}_t = \mathcal{S}_{pr} = \mathcal{S}_{prt} = F;$$
$$\mathcal{S}_p = \mathcal{S}_{rt}\ \{1, p, prt, rt\};$$
$$\mathcal{S}_r = \mathcal{S}_{pt} = \{1, r, prt, pt\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.11. □

Let $\varphi \in \mathcal{W}(G_{63})$. Here the $Aprt$ coset contains involutions but by Lemma 6.12 the Art coset does not, therefore we cannot have $\varphi(Aprt) = Art$. As G/A is abelian, $\overline{\varphi}$ is a homomorphism and this together with Proposition 8.16 (ii) and (iii) gives $\varphi(Af) = Af$ for all $f \in F$. Then by Proposition 6.9 (iv) we may compose with inner automorphisms so that $\varphi|_A = \mathrm{Id}$. By Proposition 8.17 we may compose with an automorphism so that $\varphi(t) = t$.

Five of the seven nontrivial elements in F have order 2, thus by Proposition 6.17 we have $\varphi(f) = f$ for $f \in \{p, pr, prt, rt\}$. The proposition also gives $\varphi(r) \in \{r, zr\}$ and $\varphi(pt) \in \{pt, z^{-1}pt\}$. If we have $\varphi(pt) = z^{-1}pt$ then by Proposition 6.18 (i) we may compose with $I_t \circ \iota$ and now we have $\varphi(pt) = pt$. Then by (ii) we have $\varphi(f) = f$ for $f \in F - \{r\}$. We will use this with Proposition 6.18 (iii) to show that $\varphi(r) = r$ as well. One can check that $rpt = z^{-1}prt$ thus $zrpt = prt$. By Proposition C.11, $(prt)^G = \langle x^2y^{-1}\rangle prt$, so we have $prt \nsim z^{-1}prt$. Thus we have

$$\varphi(r \cdot pt) = \varphi(z^{-1} \cdot prt) \sim z^{-1} \cdot prt \nsim prt = zrpt.$$

By Proposition 6.18 (iii) this implies $\varphi(r) = r$ and therefore we now we have $\varphi(f) = f$ for all $f \in F$.

Notice that $pt \notin \mathcal{S}_p$, thus by Corollary 6.34 we have $\varphi|_{Apt} = \mathrm{Id}$.

By Proposition 8.18 $\mathcal{S}_{pt} = \{1, r, pt, prt\}$ and by Corollary 6.29 $\mathcal{R}_p = \{1, p, rt, prt\}$. Applying Theorem 6.33 to the Ap coset we see that since $\mathcal{R}_p \cap \mathcal{S}_{pt} = \{1, prt\}$ we have $\varphi(ap) = a^h p$ for all $a \in A$ where $h \in \{1, prt\}$. However if $h = prt$ then

$$p = \varphi(x^{-1} \cdot xp) \sim x^{-1}x^{prt}p = x^{-2}yp.$$

Since Proposition C.11 gives $p^G = \langle x^2, y^2\rangle p \cup \langle x^2, y^2\rangle z^{-1}p$ we see that this is a contradiction. Thus we conclude $\varphi|_{Ap} = \mathrm{Id}$.

Next we apply Theorem 6.35 (ii), using $\varphi(t) = t$ and $\varphi|_{Ap} = \varphi|_{Apt} = \mathrm{Id}$. Since $\mathcal{R}_t \cap \mathcal{R}_{pt} \cap \mathcal{R}_p = \{1\}$ by Corollary 6.29 then by the theorem it follows that $\varphi|_{At} = \mathrm{Id}$. By Corollary 6.38 $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.19. *For crystallographic group $G = G_{63}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι*, the inner automorphisms, and*

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt), .$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.20. *For group 64 we have*

$$\mathcal{S}_t = \mathcal{S}_{pr} = F;$$

$$\mathcal{S}_p = \mathcal{S}_{rt} \ \{1, p, prt, rt\};$$

$$\mathcal{S}_r = \mathcal{S}_{prt} = \mathcal{S}_{pt} = \{1, r, prt, pt\};$$

Proof. This follows from Lemma 6.32 and Proposition C.12. □

Let $\varphi \in \mathcal{W}(G_{64})$. The $Aprt$ coset contains involutions but by Lemma 6.12 the Art coset does not, therefore we cannot have $\varphi(Aprt) = Art$. As G/A is abelian, $\overline{\varphi}$ is a homomorphism and this together with Proposition 8.16 (ii) and (iii) gives $\varphi(Af) = Af$ for all $f \in F$. Then by Proposition 6.9 (iv) we may compose φ with inner automorphisms so that $\varphi|_A = \text{Id}$. By Proposition 8.17 we may compose φ with an automorphism so that $\varphi(t) = t$.

Recall that $p^2 = z$, $r^2 = y$, $(pr)^2 = 1$, $(rt)^2 = z^{-1}$, $(pt)^2 = y^{-1}$, and $(prt)^2 = y^{-2}$. Applying this information to Proposition 6.17 we have $\varphi(prt) = prt$ as well as

$$\varphi(p) \in \{p, yp\},\ \varphi(r) \in \{r, zr\},\ \varphi(pr) \in \{pr, y^2pr\},\ \varphi(rt) \in \{rt, y^{-1}rt\},\ \varphi(pt) \in \{pt, z^{-1}pt\}.$$

By Proposition 6.18 (i), we may compose φ with $I_t \circ \iota$ and now we may assume $\varphi(rt) = rt$. Thus by (ii) we now have $\varphi(f) = f$ for $f \in \{prt, rt, t\}$. We will use Proposition 6.18 (iii) to show that this implies that $\varphi(f) = f$ for $f \in \{p, r, pr, pt\}$. To show the hypotheses of the proposition are met we note that by Proposition C.12 we have

$$\begin{aligned}
yt &\nsim yzt && \text{since } (yt)^G = \langle x^2, yz, yz^{-1}\rangle yt; \\
prt &\nsim yprt && \text{since } (prt)^G = \langle x^2y^{-1}\rangle prt \cup \langle x^2y^{-1}\rangle y^2prt; \\
y^{-1}t &\nsim y^{-1}z^{-1}t && \text{since } (y^{-1}t)^G = \langle x^2, yz, yz^{-1}\rangle y^{-1}t; \\
y^{-1}pt &\nsim ypt && \text{since } (ypt)^G = \langle z^2\rangle ypt \cup \langle z^2\rangle zpt.
\end{aligned}$$

Now we have

$$\varphi(r \cdot rt) = \varphi(y \cdot t) \sim yt \nsim yzt = z(r \cdot rt) \text{ and } \varphi(rt) = rt,$$

thus Proposition 6.18 (iii) implies $\varphi(r) \neq zr$ and so $\varphi(r) = r$. Similarly, as we have

$$\varphi(p \cdot rt) = prt \nsim yp \cdot rt \text{ and } \varphi(rt) = rt,$$

by the proposition we have $\varphi(p) \neq yp$ thus $\varphi(p) = p$. Now we have (since $ptp = (pt)^2t = y^{-1}t$),

$$\varphi(pt \cdot p) = \varphi(y^{-1} \cdot t) \sim y^{-1}t \nsim z^{-1}y^{-1}t = z^{-1}pt \cdot p \text{ and } \varphi(p) = p.$$

By the proposition it follows that $\varphi(pt) \neq z^{-1}pt$ thus $\varphi(pt) = pt$. Lastly, we have

$$\varphi(pr \cdot rt) = \varphi(y^{-1} \cdot pt) \sim y^{-1}pt \nsim ypt = y^2(y^{-1}pt) = y^2pr \cdot rt \text{ and } \varphi(rt) = rt,$$

and so the proposition gives $\varphi(pr) = pr$. We now have $\varphi(f) = f$ for all $f \in F$.

By Proposition 8.20, $pt \notin \mathcal{S}_p$, so Corollary 6.34 gives $\varphi|_{Apt} = \text{Id}$.

Applying Theorem 6.33 to the Ap coset we have $\varphi(ap) = a^hp$ for some $h \in \mathcal{R}_p \cap \mathcal{S}_{pt}$. By Corollary 6.29 and Proposition 8.20 this intersection is $\{1, prt\}$. However if $h = prt$ then

$$p = \varphi(x^{-1} \cdot xp) \sim x^{-1}x^{prt}p = x^{-2}yp.$$

Since $p^G = \langle x^2, y^2\rangle p \cup \langle x^2, y^2\rangle yz^{-1}p$ this is a contradiction, thus $\varphi|_{Ap} = \text{Id}$.

Next we apply Theorem 6.35 (ii), using $\varphi(t) = t$ and $\varphi|_{Ap} = \varphi|_{Apt} = \text{Id}$. Since we have $\mathcal{R}_{pt} \cap \mathcal{R}_p = \{1\}$ by Corollary 6.29 the theorem gives $\varphi|_{At} = \text{Id}$. Then by Corollary 6.38 $\varphi = \text{Id}$.

We have shown that

Theorem 8.21. *For crystallographic group $G = G_{64}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.22. *For group 65 we have $\mathcal{S}_f = F$ for all $f \in F - \{1\}$.*

Proof. Here F is an abelian subgroup of G. It follows that for $f \in F - \{1\}, h \in F, a \in A$,

$$af \sim (af)^h = a^h f^h = a^h f.$$ □

Let $\varphi \in \mathcal{W}(G_{65})$. Proposition 8.16 ($i$) we have $\varphi(y) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$. If $\varphi(y) \notin y^G = \{y^{\pm 1}\}$ then we may compose with the outer automorphism

$$\psi_1 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, pr, t),$$

and now we have $\varphi(\beta) \in \beta^G$ for all $\beta \in \{x^2y^{-1}, y, z\}$. By Proposition 6.9 ($iv$) we can compose with inner automorphisms to get $\varphi|_A = \text{Id}$ and $\varphi(Af) = Af$ for all $Af \in G/A$. By Proposition 8.17 we may compose with an automorphism so that $\varphi(t) = t$.

Now for $f \in F$ we have $ft \in F$ and $(ft)^2 = 1$. Therefore by Proposition 6.17 we have $\varphi(f) = f$ for all $f \in F$.

By Lemma 6.31, for $a \in A$ we have $\varphi(art) = a^h rt$ for some $h \in \mathcal{R}_{rt} = \{1, rt\}$. If we have $\varphi(art) = a^{rt} rt$ then composing with $I_t \circ \iota$ we have

$$(I_t \circ \iota \circ \varphi)(art) = (I_t \circ \iota)(a^{rt} rt) = ((a^{rt} rt)^{-1})^t = (tr(a^{-1})^{rt})^t = (a^{-1} rt)^t = art.$$

Thus now we may assume we have $\varphi|_{Art} = \text{Id}$.

By Lemma 6.31, for $a \in A$ we have $\varphi(apt) = a^h pt$ for some $h \in \mathcal{R}_{pt} = \{1, pt\}$. If we have $\varphi(apt) = a^{pt} pt$ then composing with the non-trivial wct $\tau(pt, \{Apt, At, Ar, Apr\})$, we can assume we have $\varphi|_{Art \cup Apt} = \text{Id}$. (Theorem 5.9 shows that τ_{pt} is a non-trivial wct.) We apply

Theorem 6.35 (i) twice using $\varphi(t) = t$ and $\varphi|_{Art} = \varphi|_{Apt} = \mathrm{Id}$. Since $\mathcal{R}_t \cap \mathcal{R}_r \cap \mathcal{R}_p = \{1, prt\}$ by Corollary 6.29, the theorem indicates that for $a \in A, \varphi(at) = a^h t$ for some $h \in \{1, prt\}$. However, if $h = prt$ then

$$t = \varphi(x^{-1} \cdot xt) \sim x^{-1}x^{prt}t = x^{-2}yt,$$

which is a contradiction since Proposition C.13 gives $t^G = \langle x^2, y^2, z^2 \rangle t$, thus $x^{-2}yt \nsim t$. It follows that $h = 1$, in other words, $\varphi(at) = at$ for all $a \in A$. By Corollary 6.38 we have $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.23. *For crystallographic group $G = G_{65}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms,*

$$\psi_1 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, pr, t),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt),$$

and the non-trivial wct τ_{pt}. Thus we have $\mathcal{W}(G) = \langle \mathcal{W}_0(G), \tau_{pt} \rangle$. □

Proposition 8.24. *For group 66 we have*

$$\mathcal{S}_p = \mathcal{S}_r = \mathcal{S}_{pr} = F;$$

$$\mathcal{S}_{prt} = \mathcal{S}_{rt} = \{1, p, prt, rt\};$$

$$\mathcal{S}_t = \mathcal{S}_{pt} = \{1, p, pt, t\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.14. □

Let $\varphi \in \mathcal{W}(G_{66})$. By Proposition 8.16$(i)$ we have $\varphi(y) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$. If $\varphi(y) \notin y^G = \{y^{\pm 1}\}$ then we compose with the outer automorphism

$$\psi_1 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, pr, t),$$

and now we have $\varphi(\beta) \in \beta^G$ for all $\beta \in \{x^2y^{-1}, y, z\}$. By Proposition 6.9 (iv) we may compose φ with inner automorphisms to get $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$ for all $Af \in G/A$. By Proposition 8.17, composing φ with an automorphism gives $\varphi(t) = t$.

Now for $f \in \{p, prt, rt, pt\}$ we have $ft \in F$ and $(ft)^2 = 1$. Therefore by Proposition 6.17 we have $\varphi(f) = f$ for all $f \in \{p, prt, rt, pt\}$. The proposition also gives $\varphi(pr) \in \{pr, zpr\}$ and $\varphi(r) \in \{r, zr\}$. Composing φ with $I_t \circ \iota$ if necessary we can arrange to have $\varphi(r) = r$, by Proposition 6.18 (i). By (ii) we now have $\varphi(f) = f$ for $f \in F - \{pr\}$. We will show that $\varphi(pr) = pr$ as well by applying (iii). Now Proposition C.14 gives $p^G = \langle x^2, y^2\rangle p$, so $p \not\sim zp$. Thus we have

$$\varphi(pr \cdot r) = \varphi(p) = p \not\sim zp = zpr \cdot r \text{ and } \varphi(r) = r.$$

It follows by Proposition 6.18 (iii) that $\varphi(pr) = pr$ and we now have $\varphi(f) = f$ for all $f \in F$.

We now apply Theorem 6.33 three times. We will use the following facts from Proposition 8.24: $prt \notin \mathcal{S}_t, rt \notin \mathcal{S}_{pt}$; and $pt \notin \mathcal{S}_{rt}$. Also recall that by Corollary 6.29 $\mathcal{R}_f = \{1, f\}$ for $f \in \{prt, rt, pt\}$. First we will apply the theorem to the $Aprt$ coset. Since $(pr)^2 = 1$ we have $pr \cdot prt = t$. Then as $\mathcal{R}_{prt} \cap \mathcal{S}_t = 1$ Theorem 6.33 implies $\varphi|_{Aprt} = \mathrm{Id}$. Next we consider the Art coset. Since $r^2 = 1$ we have $pr \cdot rt = pt$. We also have $\mathcal{R}_{rt} \cap \mathcal{S}_{pt} = 1$ so the theorem implies $\varphi|_{Art} = \mathrm{Id}$. Lastly we apply the theorem to the Apt coset. Since p commutes with r we have $pr \cdot pt = rt$. We also have $\mathcal{R}_{pt} \cap \mathcal{S}_{rt} = 1$. By the theorem we conclude that $\varphi|_{Apt} = \mathrm{Id}$. Now it follows by Corollary 6.38 that $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.25. *For crystallographic group $G = G_{66}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, the inner automorphisms, and

$$\psi_1 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, pr, t),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.26. *For group 67 we have*

$$\mathcal{S}_t = \mathcal{S}_{pr} = \mathcal{S}_{rt} = F;$$

$$\mathcal{S}_p = \{1, p, prt, rt\};$$

$$\mathcal{S}_r = \mathcal{S}_{pt} = \mathcal{S}_{prt}\ \{1, r, prt, pt\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.15. □

Let $\varphi \in \mathcal{W}(G_{67})$. By Proposition 8.16 (i) we have $\varphi(y) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$. If $\varphi(y) \notin y^G = \{y^{\pm 1}\}$ then we compose φ with the outer automorphism

$$\psi_2 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, xpr, xy^{-1}t),$$

and now we have $\varphi(\beta) \in \beta^G$ for all $\beta \in \{x^2y^{-1}, y, z\}$. By Proposition 6.9 (iv) we may compose with inner automorphisms to get $\varphi|_A = \mathrm{Id}$ and by (ii) we have $\varphi(Af) = Af$ for all $Af \in G/A$. We may now compose φ with an automorphism so that $\varphi(t) = t$, according to Proposition 8.17.

Recall that p, pr and rt have order 2, thus by Proposition 6.17 we have $\varphi(f) = f$ for $f \in \{r, prt, pt\}$. The proposition also gives $\varphi(p) \in \{p, yp\}, \varphi(pr) \in \{pr, y^2pr\}$ and $\varphi(rt) \in \{rt, y^{-1}rt\}$. By Proposition 6.18 (i), composing with $I_t \circ \iota$ if necessary we may assume $\varphi(pr) = pr$. We now have $\varphi(f) = f$ for $f \in F - \{p, rt\}$, by (ii). Note that Proposition C.15 gives

$$r^G = \langle x^2y^{-1}, z^2\rangle r \cup \langle x^2y^{-1}, z^2\rangle y^{-1}r \text{ and } (ypt)^G = \langle z^2\rangle pt \cup \langle z^2\rangle ypt,$$

therefore $r \nsim yr$ and $ypt \nsim y^2pt$. So we have

$$\varphi(p \cdot pr) = \varphi(r) = r \nsim yr = yp \cdot pr \text{ and } \varphi(pr) = pr,$$

thus by Proposition 6.18 (iii) we have $\varphi(p) \neq yp$ so $\varphi(p) = p$. Similarly we have

$$\varphi(rt \cdot pr) = \varphi(y^2 \cdot pt) \sim y^2pt \nsim ypt = y^{-1}(y^2pt) = y^{-1}rt \cdot pr \text{ and } \varphi(pr) = pr.$$

Then by Proposition 6.18 (iii) we have $\varphi(rt) \neq y^{-1}rt$ thus $\varphi(rt) = rt$. We now have $\varphi(f) = f$ for all $f \in F$.

We apply Theorem 6.33 to the Ap coset, noting that since p has order 2, $p \cdot pr = r$, and thus for $a \in A$ we have $\varphi(ap) = a^h p$ for some $h \in \mathcal{R}_p \cap \mathcal{S}_r$. By Corollary 6.29 and Proposition 8.26 we see this intersection is $\{1, prt\}$. However, if $h = prt$ then

$$zp \sim \varphi(z \cdot p) = \varphi(x^{-1}z \cdot xp) \sim x^{-1}z \cdot x^{prt}p = x^{-1}z \cdot x^{-1}yp = x^{-2}yzp.$$

This is a contradiction since according to Proposition C.15 $(zp)^G = \langle x^2, y^2 \rangle zp \cup \langle x^2, y^2 \rangle yz^{-1}p$. We conclude that $\varphi_{Ap} = \text{Id}$.

Proposition 8.26 indicates $pt \notin \mathcal{S}_p$ thus by Corollary 6.34 $\varphi|_{Apt} = \text{Id}$. We therefore may apply Theorem 6.35 (ii) using $\varphi(t) = t, \varphi|_{Ap} = \varphi|_{Apt} = \text{Id}$. Since Corollary 6.29 indicates $\mathcal{R}_{pt} \cap \mathcal{R}_p = \{1\}$ the theorem implies that $\varphi|_{At} = \text{Id}$. Then by Corollary 6.38 $\varphi = \text{Id}$.

We have shown that

Theorem 8.27. *For crystallographic group $G = G_{67}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_2 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, xpr, xy^{-1}t),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Thus $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.28. *For group 68 we have*

$$\mathcal{S}_p = \mathcal{S}_{prt} = \mathcal{S}_{rt} = \{1, p, prt, rt\}; \qquad \mathcal{S}_{pr} = \{1, pr, rt, pt\};$$
$$\mathcal{S}_t = \{1, p, pt, t\}; \qquad \mathcal{S}_{pt} = \{1, pt\};$$
$$\mathcal{S}_r = F.$$

Proof. This follows from Lemma 6.32 and Proposition C.16. □

Let $\varphi \in \mathcal{W}(G_{68})$. By Proposition 8.16 (i) we have $\varphi(y) \in \{(x^2y^{-1})^{\pm 1}, y^{\pm 1}\}$. If $\varphi(y) \notin y^G = \{y^{\pm 1}\}$ then we compose φ with the outer automorphism

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}, z, p, xpr, xt),$$

and now we have $\varphi(\beta) \in \beta^G$ for all $\beta \in \{x^2y^{-1}, y, z\}$. By Proposition 6.9 (ii) and (iv) we may compose with inner automorphisms to get $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$ for all $Af \in G/A$. By Proposition 8.17 we may compose with an automorphism so that $\varphi(t) = t$.

From the presentation of G we see that p and r have order 2, thus by Proposition 6.17 we have $\varphi(pt) = pt$ and $\varphi(rt) = rt$. The proposition also gives

$$\varphi(p) \in \{p, x^2y^{-1}p\} \text{ and } \varphi(prt) \in \{prt, x^2y^{-1}prt\}.$$

By Proposition 6.18 (i) if $\varphi(prt) = x^2y^{-1}prt$ then composing with $I_t \circ \iota$ we have $\varphi(prt) = prt$, and now by (ii) we have $\varphi(f) = f$ for all $f \in \{prt, rt, pt, t\}$. Note that by Proposition C.16 we have

$$(rt)^G = \langle y \rangle rt \cup \langle y \rangle zrt;$$

therefore $rt \not\sim x^2y^{-1}rt$. Then

$$\varphi(p \cdot prt) = \varphi(rt) = rt \not\sim x^2y^{-1}rt = x^2y^{-1}p \cdot prt \text{ and } \varphi(prt) = prt,$$

and so by Proposition 6.18 (iii) we have $\varphi(p) = p$.

Now we have $\varphi(pt) = pt$ and $\varphi(p) = p$ so Corollary 6.34 may be applied to the Apt coset. Since $pt \notin \mathcal{S}_p$ the Corollary gives $\varphi|_{Apt} = \mathrm{Id}$. Next we apply Theorem 6.33 to the Ap coset. By Corollary 6.29 and Proposition 8.28 we have $\mathcal{R}_p \cap \mathcal{S}_{pt} = \{1\}$. The theorem therefore gives

$\varphi|_{Ap} = \mathrm{Id}$. Using this we may apply Theorem 6.35 (i) using $\varphi(prt) = prt$ and $\varphi|_{Ap} = \mathrm{Id}$. Since $\mathcal{R}_{prt} \cap \mathcal{R}_{rt} = 1$ by Corollary 6.29, then according to the theorem $\varphi|_{Aprt} = \mathrm{Id}$.

Now by Proposition 6.17 we have $\varphi(r) \in \{r, zr\}$. We will use $\varphi|_{Aprt} = \mathrm{Id}$ with Proposition 6.18 (iii) to show $\varphi(r) \neq zr$. By Proposition C.16 we have

$$(ypt)^G = \langle z^2 \rangle ypt \cup \langle z^2 \rangle y^{-1} zpt \cup \langle z^2 \rangle x^2 y^{-2} pt \cup \langle z^2 \rangle x^2 zpt,$$

so $ypt \nsim yzpt$. Thus we have

$$\varphi(r \cdot x^2 prt) = \varphi(y \cdot pt) \sim ypt \nsim yzpt = z(ypt) = zr \cdot x^2 prt \text{ and } \varphi(x^2 prt) = x^2 prt.$$

By statement (iii) of the proposition we have $\varphi(r) = r$.

Now by Proposition 6.17 $\varphi(pr) \in \{pr, zpr\}$. We will again apply Proposition 6.18 (iii) to show $\varphi(pr) \neq zpr$. Proposition C.16 gives

$$p^G = \langle x^2, y^2 \rangle p \cup \langle x^2, y^2 \rangle yp,$$

therefore $p \nsim zp$. Thus we have

$$\varphi(pr \cdot r) = \varphi(p) = p \nsim zp = zpr \cdot r \text{ and } \varphi(r) = r,$$

therefore by (iii) we have $\varphi(pr) = pr$. We now have $\varphi(f) = f$ for all $f \in F$.

Now that we have $\varphi(r) = r$ we may apply Theorem 6.33 to the Art coset. Since $\mathcal{R}_{rt} \cap \mathcal{S}_t = \{1\}$, we conclude that $\varphi|_{Art} = \mathrm{Id}$. We have shown that $\varphi|_{Aprt \cup Art \cup Apt} = \mathrm{Id}$, thus by Corollary 6.38 $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.29. *For crystallographic group $G = G_{68}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, x^2 y^{-1}, z, p, xpr, x^{-1} yt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Thus $\mathcal{W}(G) = \mathcal{W}_0(G)$. $\square$

8.3 Groups 69 through 74

Proposition 8.30. *For group* G_{69} *we have* $\mathcal{S}_f = F$ *for all* $f \in F$.

Proof. Fix $f \in F$. For any $h \in F$ we have $af \sim (af)^h = a^h f$ since F is an abelian subgroup of G. $\square$

Let $\varphi \in \mathcal{W}(G_{69})$. By Proposition 6.3 we have $\mathbf{C}_2 = \langle x^2z^{-1}\rangle \cup \langle y^2z^{-1}\rangle \cup \langle z\rangle$. We apply Proposition 6.5 (iv) with $B = \{x^2z^{-1}, y^2z^{-1}, z\}$ which gives $\{\varphi(x^2z^{-1}), \varphi(y^2z^{-1}), \varphi(z)\} \subseteq \{(x^2z^{-1})^{\pm 1}, (y^2z^{-1})^{\pm 1}, z^{\pm 1}\}$. Now

$$\psi_1 : (x, y, z, p, r, t) \mapsto (xy^{-1}, x, x^2z^{-1}pr, p, t) \text{ and}$$

$$\psi_2 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t)$$

determine automorphisms of G_{69} and note that

$$\begin{aligned} \psi_1 : x^2z^{-1} &\mapsto y^{-2}z & \qquad \psi_2 : x^2z^{-1} &\mapsto y^2z^{-1} \\ \psi_1 : y^2z^{-1} &\mapsto z & \qquad \psi_2 : y^2z^{-1} &\mapsto x^2z^{-1} \\ \psi_1 : z &\mapsto x^2z^{-1} & \qquad \psi_2 : z &\mapsto z. \end{aligned}$$

In other words, these two automorphisms permute the elements of B. Thus composing with ψ_1 and ψ_2 as needed we have $\varphi(\beta) \in \{\beta^{\pm 1}\}$ for all $\beta \in B$. Then by Proposition 6.9 (iv) we may compose with inner automorphisms to have $\varphi|_A = \text{Id}$ and by (ii) we have $\varphi(Af) = Af$ for all $f \in F$.

Let $\varphi(t) = ct$ for some $c \in A$. By Proposition 6.19 the following defines an automorphism:

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zrzt).$$

Composing φ with this map and also with I_x and I_y, as necessary we may assume that $c \in \{1, x, y, xy\}$.

We will use Proposition 6.14 to show that $\varphi(t) \notin \{xt, yt, xyt\}$. To justify using the proposition we note that $\alpha_p = \alpha_{pt} = \alpha_r = \alpha_{rt} = 1$ thus they clearly are contained in $\mathbf{C}_2$. Note also that we have $\varphi(Ar) = Ar$ and $\varphi(Ap) = Ap$. Then by the proposition,

$$(x,p) = x^{-2}z \notin \langle x^2, y^2, z^2\rangle \text{ therefore } \varphi(t) \neq xt;$$

$$(y,r) = z^{-1} \notin \langle x^2, y^2, z^2\rangle \text{ therefore } \varphi(t) \neq yt;$$

$$(xy,r) = x^{-2}z^{-1} \notin \langle x^2, y^2, z^2\rangle \text{ therefore } \varphi(t) \neq xyt.$$

We conclude that $\varphi(t) = t$. It follows by Proposition 6.17 that since every nontrivial element of F has order 2, $\varphi(f) = f$ for all $f \in F$.

Now by Lemma 6.31 for $a \in A$ we have $\varphi(at) = a^h t$ for some $h \in \mathcal{R}_t = F$. We will assume $h \in \{p, pr, prt, pt\}$ and show this leads to a contradiction. Note that $x^h \in \{(xz^{-1})^{\pm 1}\}$. This gives

$$x^2z^{-1}t \sim \varphi(x^2z^{-1} \cdot t) = \varphi(xz^{-1} \cdot xt) \sim xz^{-1} \cdot x^h t = xz^{-1}(xz^{-1})^{\pm 1}t.$$

Since $t^G = \langle x^2, y^2, z^2\rangle t$ we see $xz^{-1}(xz^{-1})^{\pm 1}t \sim t$ but $x^2z^{-1}t \nsim t$. This contradiction leads us to conclude that $\varphi(at) = a^h t$ for some $h \in \{1, r, rt, t\}$. We will give a similar argument to show that $h \notin \{r, rt\}$. Assuming $h \in \{r, rt\}$ we have $y^h \in \{(yz^{-1})^{\pm 1}\}$ thus

$$y^2z^{-1}t \sim \varphi(y^2z^{-1} \cdot t) = \varphi(yz^{-1} \cdot yt) \sim yz^{-1} \cdot y^h t = yz^{-1}(yz^{-1})^{\pm 1}t \sim t,$$

a contradiction. Therefore we have $\varphi(at) = a^h t$ for some $h \in \{1, t\}$. If $h = t$ then we have $\varphi(at) = a^t t = (at)^t$. Note that since every element $at \in At$ has order 2, composing with $I_t \circ \iota$ we now $\varphi|_{At} = \mathrm{Id}$ and so by Corollary 6.38, $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.31. *For crystallographic group $G = G_{69}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, the inner automorphisms, and

$$\psi_1 : (x, y, z, p, r, t) \mapsto (xy^{-1}, x, x^2z^{-1}pr, p, t),$$

$$\psi_2 : (x, y, z, p, r, t) \mapsto (y, x, z, p, pr, t),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zrzt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.32. *For group 72 we have*

$$\mathcal{S}_t = \mathcal{S}_p = \mathcal{S}_{pt} = F;$$

$$\mathcal{S}_r = \mathcal{S}_{prt} = \{1, r, prt, pt\};$$

$$\mathcal{S}_{pr} = \mathcal{S}_{rt} = \{1, pr, rt, pt\}.$$

Proof. This follows from Lemma 6.32 and Proposition C.18. □

Let $\varphi \in \mathcal{W}(G_{72})$. We have $\mathbf{C}_2 = \langle x^{-2}yz\rangle \cup \langle y\rangle \cup \langle z\rangle$ by Proposition 6.3. We apply Proposition 6.5 (*iv*) with $B = \{x^{-2}yz, y, z\}$ and conclude that for $\beta \in B$ we have $\varphi(\beta) \in \{(x^{-2}yz)^{\pm 1}, (y)^{\pm 1}, z^{\pm 1}\}$.

Lemma 6.12 indicates that the Apt coset is unlike Art and $Aprt$ in that Apt contains elements of order 2. This fact together with Corollary 6.11 gives $\varphi(Apt) = Apt$ and $\varphi(At) = At$. Since G/A is abelian $\overline{\varphi}$ is a homomorphism thus $\varphi(Ap) = Ap$. By Lemma 6.4 $\varphi(x^{-2}yz)$ and $\varphi(y)$ are inverted by the action of p therefore $\{\varphi(x^{-2}yz), \varphi(y)\} \subseteq \{(x^{-1}yz)^{\pm 1}, y^{\pm 1}\}$ and so $\varphi(z) \in \{z^{\pm 1}\}$. If we have $\varphi(x^{-2}yz) \in \{y^{\pm 1}\}$ then we may compose φ with

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}z^{-1}, z, p, pr, t),$$

and now we have $\varphi(x^{-2}yz) \in \{(x^{-2}yz)^{\pm 1}\}$ and $\varphi(y) \in \{y^{\pm 1}\}$. Then by Proposition 6.9 (*ii*) and (*iv*), composing φ with inner automorphisms if necessary we have $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$ for all $f \in F$.

Let $\varphi(t) = ct$ for some $c \in A$. By Proposition 6.19 the maps

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt)$$

$$\text{and} \psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt)$$

determine outer automorphisms. Composing φ with these maps and with I_x we may assume $c \in \{1, x\}$. By Corollary 6.16 $c = x$ is not possible so we have $\varphi(t) = t$.

It follows by Proposition 6.17 that since p and pt have order 2, $\varphi(p) = p$ and $\varphi(pt) = pt$. The proposition also gives

$$\varphi(pr) \in \{pr, ypr\};\ \varphi(r) \in \{r, x^2y^{-1}z^{-1}r\};\ \varphi(rt) \in \{rt, y^{-1}rt\};\ \varphi(prt) \in \{prt, x^{-2}yzprt\}.$$

By Proposition 6.18 (i), if $\varphi(prt) = x^{-2}yzprt$ then we may compose with $I_t \circ \iota$ and now $\varphi(prt) = prt$. It follows by (ii) that we now have $\varphi(f) = f$ for all $f \in \{p, prt, pt, t\}$. Now we will use Proposition 6.18 (iii) three times to show that this implies $\varphi(f) = f$ for $f \in \{r, pr, rt\}$ as well. The following facts from Proposition C.18 will be needed to satisfy the requisite hypotheses:

$p \nsim yp$ and $p \nsim y^{-1}p$	since $p^G = \langle x^2z^{-1}, y^2\rangle p$;
$t \nsim x^2y^{-1}z^{-1}t$	since $t^G = \langle x^2, y^2, z\rangle t$.

Now we have

$$\varphi(rt \cdot (prt)^{-1}) = \varphi(p) = p \nsim y^{-1}p = y^{-1}rt \cdot (prt)^{-1} \text{ and } \varphi(prt)^{-1} = (prt)^{-1},$$

therefore Proposition 6.18 (iii) implies $\varphi(rt) = rt$.

Next we consider that

$$\varphi(r^{-1} \cdot rt) = \varphi(t) = t \nsim x^2y^{-1}z^{-1}t = (x^2y^{-1}z^{-1}r)^{-1} \cdot rt \text{ and } \varphi(rt) = rt.$$

By the proposition we have $\varphi(r^{-1}) = r^{-1}$ thus $\varphi(r) = r$. Lastly we have

$$\varphi(pr \cdot r^{-1}) = \varphi(p) = p \nsim yp = ypr \cdot r^{-1} \text{ and } \varphi(r^{-1}) = r^{-1},$$

therefore $\varphi(pr) = pr$ by the proposition. We now have $\varphi(f) = f$ for all $f \in F$.

Now $rt \notin \mathcal{S}_r$ and $prt \notin \mathcal{S}_{pr}$ thus by Corollary 6.34, $\varphi|_{Art \cup Aprt} = \text{Id}$. Now by Lemma 6.31

and Corollary 6.29 we know that for all $a \in A, \varphi(apt) = a^h pt$ for some $h \in \{1, pt\}$. Suppose $h = pt$. Let $\gamma = x^2y^{-2}z^{-1}$ and note that $ptprt = \gamma r$. Then for $a, b \in A$ we have

$$ab^{pt}\gamma r \sim \varphi(ab^{pt}\gamma \cdot r) = \varphi(ab^{pt}ptprt) = \varphi(apt \cdot bprt) \sim a^{pt}pt \cdot bprt = (ab)^{pt}ptprt = (ab)^{pt}\gamma r.$$

Now if we let $a = b = x^{-1}y$, the left hand side becomes

$$ab^{pt}\gamma r = x^{-1}y(x^{-1}y)^{pt}\gamma r = x^{-1}y(x^{-1}yz)x^2y^{-2}z^{-1}r = r,$$

while the right hand side becomes

$$(ab)^{pt}\gamma r = (x^{-2}y^2)^{pt}\gamma r = x^{-2}y^2z^2x^2y^{-2}z^{-1}r = zr.$$

By Proposition C.18, $r^G = \langle x^2y^{-1}, z^2\rangle r \cup \langle x^2y^{-1}, z^2\rangle y^{-1}zr$ therefore $r \nsim zr$. This contradiction indicates that $\varphi(apt) = a^h pt$ is only possible if $h = 1$. In other words, $\varphi|_{Apt} = \mathrm{Id}$, and now by Corollary 6.38 $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.33. *For crystallographic group $G = G_{72}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_3 : (x, y, z, p, r, t) \mapsto (x, x^2y^{-1}z^{-1}, z, p, pr, t),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Thus $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.34. *For group 73 we have*

$$\mathcal{S}_{rt} = \{1, p, prt, rt\}; \qquad \mathcal{S}_{prt} = \{1, r, prt, pt\};$$

$$\mathcal{S}_{pt} = \{1, pr, rt, pt\}; \qquad \mathcal{S}_p = \{1, p\};$$

$$\mathcal{S}_r = \{1, r\}; \qquad \mathcal{S}_{pr} = \{1, pr\};$$

$$\mathcal{S}_t = F.$$

Proof. This follows from Lemma 6.32 and Proposition C.19. □

Let $\varphi \in \mathcal{W}(G_{73})$. We have $\mathbf{C}_2 = \langle x^{-2}yz\rangle \cup \langle y\rangle \cup \langle z\rangle$ by Proposition 6.3. We apply Proposition 6.5 (iv) with $B = \{x^{-2}yz, y, z\}$: thus for $\beta \in B$ we have $\varphi(\beta) \in \{(x^{-2}yz)^{\pm 1}, (y)^{\pm 1}, z^{\pm 1}\}$.

The following maps determine automorphisms of G_{73} :

$$\psi_4 : (x, y, z, p, r, t) \mapsto (xy^{-1}, z, x^2y^{-1}z^{-1}, x^2z^{-1}pr, p, t), \text{ and}$$

$$\psi_5 : (x, y, z, p, r, t) \mapsto (x, z, y, x^{-2}yzr, p, x^{-1}yt).$$

These two automorphisms permute the elements of B and so composing φ with ψ_4 and ψ_5 we can arrange to have $\varphi(\beta) \in \{\beta^{\pm 1} \ : \ \beta \in B\}$. Then by Proposition 6.9 (iv) we can compose φ with inner automorphisms to have $\varphi|_A = \mathrm{Id}$ and by (ii) we have $\varphi(Af) = Af$ for all $f \in F$.

Let $\varphi(t) = ct$ for some $c \in A$. By Proposition 6.19 the maps

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\text{and} \psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt)$$

determine outer automorphisms. Composing φ with these maps and with I_x we may assume $c \in \{1, x\}$. By Corollary 6.16 $c = x$ is not possible so we have $\varphi(t) = t$.

Now by Proposition 6.17 we have

$$\varphi(p) \in \{p, x^2y^{-1}z^{-1}p\}; \qquad \varphi(r) \in \{r, zr\}; \qquad \varphi(pr) \in \{pr, ypr\};$$

$$\varphi(prt) \in \{prt, x^2y^{-1}z^{-1}prt\}; \qquad \varphi(rt) \in \{rt, y^{-1}rt\}; \qquad \varphi(pt) \in \{pt, z^{-1}pt\}.$$

By Proposition 6.18 (i), composing with $I_t \circ \iota$ if necessary we may assume that we have $\varphi(p) = p$. We will now use Proposition 6.18 (iii) to show that $\varphi(p) = p$ implies $\varphi(prt) = prt$. Note that

$$(rt)^G = \langle y\rangle rt \cup \langle y\rangle zrt.$$

This gives two pertinent facts. The first is that $rt \sim y^{-1}rt$ therefore (since $\varphi(rt) \in \{rt, y^{-1}rt\}$), we have $\varphi(rt) \sim rt$. Secondly, we have $rt \nsim x^{-2}yzrt$. We are now ready to apply the proposition. We have

$$\varphi(prt \cdot p^{-1}) = \varphi((rt)^{p^{-1}}) \sim \varphi(rt) \sim rt \nsim x^{-2}yzrt = (x^2y^{-1}z^{-1})^p rt \sim x^2y^{-1}z^{-1}prt \cdot p^{-1}.$$

The above, together with $\varphi(p^{-1}) = p^{-1}$, implies that $\varphi(prt) = prt$, by Proposition 6.18 (*iii*).

Next we show that $\varphi(r) = r$ if and only if $\varphi(pt) = pt$. Suppose to the contrary that $\varphi(r) = r$ and $\varphi(pt) = z^{-1}pt$. Then (using $rpt = x^2z^{-2}prt$)

$$x^2z^{-2} \cdot prt \sim \varphi(x^2z^{-2} \cdot prt) = \varphi(r \cdot pt) \sim r \cdot z^{-1}pt = zrpt = x^2z^{-1}prt.$$

Since $x^2z^{-1}prt \in (prt)^G = \langle x^2y^{-1}z^{-1}\rangle prt \cup \langle x^2y^{-1}z^{-1}\rangle yprt$ by Proposition C.19, this gives a contradiction. Now to prove the converse suppose we have $\varphi(r) = zr$ and $\varphi(pt) = pt$. Then

$$x^2z^{-2} \cdot prt \sim \varphi(x^2z^{-2} \cdot prt) = \varphi(r \cdot pt) \sim zr \cdot pt = x^2z^{-1}prt.$$

We arrive at the same contradiction which proves the biconditional.

We will use this result to show that $\varphi|_{Aprt} = \mathrm{Id}$. To begin, we recall that by Lemma 6.31 and Corollary 6.29 that $\varphi(aprt) = a^hprt$ for some $h \in \{1, prt\}$. Suppose that $h = prt$. Then (using $prtr = z^{-1}pt$) we have

$$xz^{-1} \cdot \varphi(pt) \sim \varphi(xz^{-1} \cdot pt) = \varphi(xprt \cdot r) \sim x^{prt}prt \cdot \varphi(r) = x^{-1}yzprt \cdot \varphi(r).$$

We have two cases to consider. If $\varphi(pt) = pt$ thus $\varphi(r) = r$, the above is

$$xz^{-1}pt \sim x^{-1}yzprt \cdot r = x^{-1}ypt.$$

Alternatively, if $\varphi(pt) = z^{-1}pt$ thus $\varphi(r) = zr$, this becomes

$$xz^{-2}pt \sim x^{-1}yzprt \cdot zr = x^{-1}yzpt.$$

As $xz^{-1}pt, xz^{-2}pt \in (xpt)^G = \langle z\rangle xpt \cup \langle z\rangle xy^{-1}pt$ we see that in both cases we have a contradiction. Thus $h \neq prt$ and so $\varphi|_{Aprt} = \mathrm{Id}$.

We will use this result to show that $\varphi(rt) = rt$. Suppose to the contrary that $\varphi(rt) = y^{-1}rt$. Then since φ respects inverses, Then

$$xp \sim \varphi(x \cdot p) = \varphi(xprt \cdot (rt)^{-1}) \sim xprt(rt)^{-1}y = xy^{-1}p.$$

However $(xp)^G = \langle x^2z^{-1}, y^2\rangle xp \cup \langle x^2z^{-1}, y^2\rangle xyz^{-2}p$ thus $xp \nsim xy^{-1}p$, a contradiction. We conclude that $\varphi(rt) = rt$.

Now suppose that $\varphi(pr) = ypr$. This gives

$$y^{-1}\varphi(pt) \sim \varphi(y^{-1} \cdot pt) = \varphi(pr \cdot rt) \sim ypr \cdot rt = pt.$$

The left hand side is either $y^{-1}pt$ or $y^{-1}z^{-1}pt$, neither of which is contained in $(pt)^G = \langle z \rangle pt \cup \langle z \rangle x^2y^{-1}pt$. This shows that we must have $\varphi(pr) = pr$.

Next we apply Theorem 6.33 to the Art coset. (Recall that we have $\varphi(rt) = rt, \varphi(p) = p$ and $\varphi(prt) = prt$.) Since $\mathcal{R}_{rt} \cap \mathcal{S}_{prt} = \{1\}$ by Corollary 6.29 and Proposition 8.34, the theorem implies that $\varphi|_{Art} = \mathrm{Id}$.

We use this result to show that $\varphi(pt) = pt$. Suppose to the contrary that $\varphi(pt) = z^{-1}pt$. Then (using $ptrt = yzpr$) we have

$$x^{-1}{\cdot}pr \sim \varphi(x^{-1}{\cdot}pr) = \varphi(x^{-1}y^{-1}z^{-1}ptrt) = \varphi(pt{\cdot}x^{-1}y^{-1}z^2rt) \sim z^{-1}pt{\cdot}x^{-1}y^{-1}z^2rt = x^{-1}z^{-1}pr.$$

This is a contradiction because according to Proposition C.19, $(x^{-1}pr)^G = \langle yz, yz^{-1} \rangle x^{-1}pr \cup \langle yz, yz^{-1} \rangle x^3zpr$, so now we have $\varphi(pt) = pt$. We have already shown that this implies $\varphi(r) = r$, so now we have $\varphi(f) = f$ for all $f \in F$.

Notice that $pt \notin \mathcal{S}_p$, thus by Corollary 6.34 $\varphi|_{Apt} = \mathrm{Id}$. Then by Corollary 6.38 $\varphi = \mathrm{Id}$.

We have shown that

Theorem 8.35. *For crystallographic group $G = G_{73}$, the group $\mathcal{W}(G)$ is generated by the inverse map ι, the inner automorphisms, and*

$$\psi_4 : (x, y, z, p, r, t) \mapsto (xy^{-1}, z, x^2y^{-1}z^{-1}, x^2z^{-1}pr, p, t),$$

$$\psi_5 : (x, y, z, p, r, t) \mapsto (x, z, y, x^{-2}yzr, p, x^{-1}yt),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Proposition 8.36. *For group 74 we have*

$$\mathcal{S}_{pr} = \mathcal{S}_t = \{1, t, pr, prt\}; \qquad \mathcal{S}_p = \{1, p, prt, rt\};$$

$$\mathcal{S}_r = \mathcal{S}_{prt} = \mathcal{S}_{pt} = \{1, r, prt, pt\}; \qquad \mathcal{S}_{rt} = F.$$

Proof. This follows from Lemma 6.32 and Proposition C.20. □

Let $\varphi \in \mathcal{W}(G_{74})$. We have $\mathbf{C}_2 = \langle x^{-2}yz\rangle \cup \langle y\rangle \cup \langle z\rangle$ by Proposition 6.3. We apply Proposition 6.5 (iv) with $B = \{x^{-2}yz, y, z\}$, which tells us that for $\beta \in B$ we have $\varphi(\beta) \in \{(x^{-2}yz)^{\pm 1}, (y)^{\pm 1}, z^{\pm 1}\}$.

It is clear that the Art coset contains elements of order 2 (since rt has order 2). By Lemma 6.12 we find that the $Aprt$ coset also contains elements of order 2 but Apt does not. This fact together with Corollary 6.11 gives $\varphi(Apt) = Apt$ and $\varphi(At) = At$. Since G/A is abelian $\overline{\varphi}$ is a homomorphism and so $\varphi(Ap) = Ap$. By Lemma 6.4 $\varphi(x^{-2}yz)$ and $\varphi(y)$ are inverted by the action of p. It follows that $\{\varphi(x^{-2}yz), \varphi(y)\} \subseteq \{(x^{-1}yz)^{\pm 1}, y^{\pm 1}\}$ and thus $\varphi(z) \in \{z^{\pm 1}\}$. If we have $\varphi(x^{-2}yz) \in \{y^{\pm 1}\}$ then we may compose φ with the automorphism

$$\psi_6 : (x, y, z, p, r, t) \mapsto (x^{-1}z, x^{-2}yz, z, p, x^{-1}ypr, x^{-1}t),$$

and now we have $\varphi(x^{-2}yz) \in \{(x^{-2}yz)^{\pm 1}\}$ and $\varphi(y) \in \{y^{\pm 1}\}$. Then by Proposition 6.9 (ii) and (iv), composing with inner automorphisms if necessary we have $\varphi|_A = \mathrm{Id}$ and $\varphi(Af) = Af$ for $f \in F$.

Let $\varphi(t) = ct$ for some $c \in A$. By Proposition 6.19 the maps

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\text{and } \psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt)$$

determine outer automorphisms. Composing with these functions and with I_x we may assume $c \in \{1, x\}$. By Corollary 6.16 $c = x$ is not possible so we have $\varphi(t) = t$.

It follows by Proposition 6.17 that since p, pr and rt are involutions, $\varphi(pt) = pt, \varphi(prt) = prt$, and $\varphi(r) = r$. The proposition also gives

$$\varphi(p) \in \{p, yp\}; \ \varphi(pr) \in \{pr, y^2pr\}; \ \varphi(rt) \in \{rt, y^{-1}rt\}.$$

By Proposition 6.18 (i), we may compose φ with $I_t \circ \iota$ if necessary so as to have $\varphi(rt) = rt$. Then by (ii) we now have $\varphi(f) = f$ for all $f \in F - \{p, pr\}$. We will apply Proposition 6.18 (iii) twice in order to show that this implies that $\varphi(p) = p$ and $\varphi(pr) = pr$ as well. To justify this we will use the following facts from Proposition C.20:

$$yprt \notin (prt)^G = \langle x^2y^{-1}z^{-1}\rangle prt \cup \langle x^2y^{-1}z^{-1}\rangle y^2prt;$$
$$yr \notin r^G = \langle x^2y^{-1}, z^2\rangle r \cup \langle x^2y^{-1}, z^2\rangle y^{-1}r.$$

We have

$$\varphi(p \cdot rt) = prt \nsim yprt = (yp)(rt) \text{ and } \varphi(rt) = rt,$$

thus by the proposition we conclude $\varphi(p) \neq yp$ i.e. $\varphi(p) = p$.

Similarly, since we have $\varphi(p) = p$ and

$$\varphi(pr \cdot p) = \varphi(r^p) \sim \varphi(r) = r \sim r^p \nsim yr = (y^2pr)(p),$$

the proposition gives $\varphi(pr) = pr$. ; We now have $\varphi(f) = f$ for all $f \in F$.

Since $pt \notin \mathcal{S}_p$ and $rt \notin \mathcal{S}_r$, Corollary 6.34 gives $\varphi|_{Apt \cup Art} = \text{Id}$. We now apply Theorem 6.35 (i) using $\varphi(p) = p$ and $\varphi|_{Art} = \text{Id}$. Since Corollary 6.29 gives $\mathcal{R}_p \cap \mathcal{R}_{prt} = \{1, prt\}$ we have $\varphi(ap) = a^hp$ for some $h \in \{1, prt\}$. However if $h = prt$ then

$$zp \sim \varphi(z \cdot p) = \varphi(x^{-1}z \cdot xp) = x^{-1}z \cdot x^{prt}p = x^{-1}zx^{-1}yzp = x^{-2}yz^2p,$$

which is a contradiction since Proposition C.20 indicates that $x^{-2}yz^2p \sim yzp \notin (zp)^G = \langle x^2z^{-1}, y^2\rangle zp \cup \langle x^2z^{-1}, y^2\rangle yz^{-1}$. We conclude that $h = 1$ i.e. $\varphi|_{Ap} = \text{Id}$.

Again we apply Theorem 6.35, this time using $\varphi(prt) = prt$ and $\varphi|_{Ap} = \text{Id}$. We also use $\mathcal{R}_{prt} \cap \mathcal{R}_{rt} = 1$ as given by Corollary 6.29. It follows by the theorem that we have $\varphi|_{Aprt} = \text{Id}$. Then by Corollary 6.38 $\varphi = \text{Id}$.

We have shown that

Theorem 8.37. *For crystallographic group $G = G_{74}$, the group $\mathcal{W}(G)$ is generated by the*

inverse map ι, *the inner automorphisms, and*

$$\psi_6 : (x, y, z, p, r, t) \mapsto (x^{-1}z, x^{-2}yz, z, p, x^{-1}ypr, x^{-1}t),$$

$$\psi_y : (x, y, z, p, r, t) \mapsto (x, y, z, yp, r, yt),$$

$$\psi_z : (x, y, z, p, r, t) \mapsto (x, y, z, p, zr, zt).$$

Therefore $\mathcal{W}(G) = \mathcal{W}_0(G)$. □

Bibliography

[BCP] Bosma, Wieb; Cannon, John; Playoust, Catherine, *The Magma algebra system. I. The user language,* J. Symbolic Comput., **24** (1997), 235-265.

[CFHT] Conway, John H.; Friedrichs, Olaf Delgado; Huson, Daniel H.; Thurston, William P. *On Three-Dimensional Space Groups*, Beitrage Algebra Geom. **42** (2001), 475-507.

[E] Engel, Peter, *Geometric Crystallography*, D. Reidel Publishing Company, Dordrecht, Holland, (1986). 249 pp.

[Hu] Humphries, Stephen P., *Weak Cayley table groups*, J. Algebra **216** (1999), 135-158.

[HN] Humphries, Stephen P., Nguyen Long, *Weak Cayley table groups: Alternating and Coxeter groups*, Comm. Algebra 43 (2015), 4763-4782.

[HN2] ———, *Weak Cayley Table groups III:* $PSL(2, q)$, Comm. Algebra. 45 (2017), 3110-3136.

[HP] Humphries, Stephen P., Paulsen, Rebeca A., *Weak Cayley table groups of some crystallographic groups*, Glasgow Mathematical Journal 60 (2018), 635-660.

[I] *International Tables for Crystallography* (1995). Vol. A, *Space-group Symmetry*, 4th ed., edited by Theo Hahn. Dordrecht/Boston/London: Kluwer Academic Publishers.

[Ja] Janssen, T., *Crystallographic Groups*, American Elsevier Publishing Company, New York, (1973), 272 pp.

[JS] Johnson, K. W.; Smith, J. D. H., *On the category of weak Cayley table morphisms between groups.* Selecta Math. **13** (2007), no. 1, 57-67.

[JMS] Johnson, Kenneth W.; Mattarei, Sandro; Sehgal, Surinder K., *Weak Cayley tables*, J. London Math. Soc., **61** (2000), 395–411.

[L] Lyndon, Roger C., *Groups and geometry*, Cambridge University Press, Cambridge-New York-Melbourne, (1985). viii+217 pp.

[MKS] Magnus, W, Karrass, Solitar, *Combinatorial group theory*, Dover, (1976), xii+444 pp.

[F] Fedorov, E. *"Simmetrija na ploskosti" [Symmetry in the plane]*, Zapiski Imperatorskogo Sant-Petersburgskogo Mineralogicheskogo Obshchestva [Proceedings of the Imperial St. Petersburg Mineralogical Society], (2) **28**, (1891), 245-291 (in Russian).

[N] Newman, Morris *Integral Matrices*, Academic Press, 1972

George Pólya (1924) "Über die Analogie der Kristallsymmetrie in der Ebene," Zeitschrift für Kristallographie, vol. 60, pp. 278–282.

[SHC] Stokes, H. T.; Hatch, D. M.; Campbell, B. J., *ISO-IR, ISOTROPY Software Suite*, iso.byu.edu.

[SCC] Stokes, H. T.; Campbell, B. J.; Cordes, R., *Tabulation of Irreducible Representations of the Crystallographic Space Groups and Their Superspace Extensions.* Acta Cryst. A. **69** 388-395.

Appendix A. K_f subgroups

Proposition A.1. *Recall that for each $f \in F$ we define the subgroup K_f to be*

$$K_f = \langle (x, f), (y, f), (z, f) \rangle.$$

Below we have the K_f subgroups for groups that have a presentation of the form given in Eqs. (4.1), (4.2), (4.3), (4.4), or (4.5).

Table A.1: K_f subgroups for thirty-one groups

Group number(s)	K_p	K_r	K_{pr}	K_{ps} or K_{prt}	K_s or K_{rt}	K_{pt}
10, 13		$\langle x^2, z^2 \rangle$			$\langle y^2 \rangle$	
12		$\langle x^2y^{-1}, z^2 \rangle$			$\langle y \rangle$	
16, 17	$\langle x^2, y^2 \rangle$	$\langle x^2, z^2 \rangle$	$\langle y^2, z^2 \rangle$			
21	$\langle x^2, y^2 \rangle$	$\langle x^2y^{-1}, z^2 \rangle$	$\langle y, z^2 \rangle$			
22	$\langle x^2z^{-1}, y^2z^{-1} \rangle$	$\langle x^2, z \rangle$	$\langle y^2, z \rangle$			
25, 26, 27	$\langle x^2, y^2 \rangle$			$\langle x^2 \rangle$	$\langle y^2 \rangle$	
38, 39	$\langle x^2, y^2z^{-1} \rangle$			$\langle x^2 \rangle$	$\langle y^2z^{-1} \rangle$	
42	$\langle x^2z^{-1}, y^2z^{-1} \rangle$			$\langle x^2z^{-1} \rangle$	$\langle y^2z^{-1} \rangle$	
47-57	$\langle x^2, y^2 \rangle$	$\langle x^2, z^2 \rangle$	$\langle y^2, z^2 \rangle$	$\langle x^2 \rangle$	$\langle y^2 \rangle$	$\langle z^2 \rangle$
63-68	$\langle x^2, y^2 \rangle$	$\langle x^2y^{-1}, z^2 \rangle$	$\langle y, z^2 \rangle$	$\langle x^2y^{-1} \rangle$	$\langle y \rangle$	$\langle z^2 \rangle$
69	$\langle x^2z^{-1}, y^2z^{-1} \rangle$	$\langle x^2, z \rangle$	$\langle y^2, z \rangle$	$\langle x^2z^{-1} \rangle$	$\langle y^2z^{-1} \rangle$	$\langle z \rangle$
72, 73, 74	$\langle x^2z^{-1}, y^2 \rangle$	$\langle x^2y^{-1}, z^2 \rangle$	$\langle yz, yz^{-1} \rangle$	$\langle x^2y^{-1}z^{-1} \rangle$	$\langle y \rangle$	$\langle z \rangle$

Additionally, for groups having $t \in F$ we have $K_t = \langle x^2, y^2, z^2 \rangle$. (For brevity we write "47-57" to represent groups $G_{47}, G_{49}, G_{50}, G_{51}, G_{53}, G_{54}, G_{55}$, and G_{57} and we write "63-68" to represent $G_{63}, G_{64}, G_{65}, G_{66}, G_{67}$, and G_{68}.)

Note that G_{10}, G_{12} and G_{13} do not contain an element p (nor pr, ps, prt, pt) therefore we have nothing to write in the cell of the table that corresponds to those K_f subgroups. The next two rows in the table have blank cells in three places for a similar reason; G_{16}, G_{17}, G_{21} and G_{22} do not contain an element s nor t, (nor ps, prt, rt, pt); $G_{25}, G_{26}, G_{27}, G_{38}, G_{39}$, and G_{42} do not contain an element r, pr nor pt.

Proof. This follows from the relations found in the presentation of the respective groups. □

Appendix B. Proof of Lemma 7.1 (Magma)

Below is the code (with its output) that we used to prove that $H = \langle a^2, b, c\rangle$.

```
F⟨a, b, c⟩ := FreeGroup(3);

G := quo < F|{c^2, a * b * a * (b * a * b)^(−1), (a * b * a)^4, (a * c)^2, (b * c)^2,

(c * a)^2, (c * b)^2} >;

Index(G, sub < G|a, b >);

2

Index(G, sub < G|a^2, b, c >);

3
```

Appendix C. Commutators and conjugacy classes for eighteen space groups

Here we list the conjugacy classes for the eighteen groups listed in Table 4.2. We do not include the conjugacy classes for the elements in A, as those conjugacy classes are not needed as we determine $\mathcal{W}(G)$. Before we list these conjugacy classes, we give some results that were used to determine them.

The following lemma is applicable to the eighteen groups listed in Table 4.2. This lemma will be useful when determining certain commutators which are used when determining the conjugacy classes.

Lemma C.1. *Let G be a group with an abelian normal subgroup A such that G/A is abelian. Let $p, r, t \in G$ and suppose that $t^2 = 1$ and that $a^t = a^{-1}$ for $a \in A$.*

Let $U = (p, r),\ V = (p, t),$ and $W = (r, t)$. Then we have

$$(p, pr) = U; \qquad (p, prt) = (p, rt) = U^{-1}V;$$

$$(p, pt) = (t, pt) = V; \qquad (rt, pt) = U^{-1}VW^{-1};$$

$$(r, rt) = (t, rt) = W; \qquad (rt, prt) = (U^{-1}V)^r;$$

$$(r, pt) = UW; \qquad (pr, rt) = (U^{-1}V)^r W;$$

$$(pr, r) = U^r; \qquad (pr, t) = (pr, prt) = (t, prt) = V^r W;$$

$$(r, prt) = U^r W; \qquad (pr, pt) = UV^r W;$$

$$(pt, prt) = UV^r W \cdot V^{-1}.$$

Proof. Note that G/A abelian implies that every commutator is in A. We apply Eqs. (2.1), (2.3) and (2.5) and these results follow. $\square$

Proposition C.2. *Suppose G/A is abelian. Let $a \in A$ and $f \in F$. Then*

$$(af)^G = \bigcup_{\overline{\lambda} \in (G/A)/\langle \overline{f} \rangle} K_f a^{\lambda} (f, \lambda) f,$$

where $\overline{f} \in G/A$ *is the image of* f *in the quotient so we are taking the union over* $\lambda \in G$ *such that* $\overline{\lambda}$ *is a coset representative of the cosets in* G/A *after taking a quotient over* $\langle \overline{f} \rangle$*.*

Proof. Let $b \in A$. Using 2.3 we have

$$(af)^{-1}(af)^b = (af, b) = (f, b) \in K_f,$$

thus $K_f(af) = K_f(af)^b$. From this we see that

$$(af)^G = \bigcup_{\lambda \in F} K_f(af)^\lambda = \bigcup_{\lambda \in F} K_f a^\lambda f^\lambda f^{-1} f = \bigcup_{\lambda \in F} K_f a^\lambda (\lambda, f^{-1}) f.$$

Next we show that $K_f(\lambda, f^{-1}) = K_f(f, \lambda)$. Let $a = (f^{-1}, \lambda)$. Clearly $(a, f) \in K_f$. Then

$$\begin{aligned}(a, f) =& ((f^{-1}, \lambda), f) \\ =& (\lambda, f^{-1}) f^{-1} (f^{-1}, \lambda) f \\ =& \lambda^{-1} f \lambda f^{-1} (f^{-1} f) \lambda^{-1} f^{-1} \lambda f \\ =& (\lambda, f^{-1})(\lambda, f) \\ =& (\lambda, f^{-1})(f, \lambda)^{-1} \in K_f,\end{aligned}$$

so that $K_f(\lambda, f^{-1}) = K_f(f, \lambda)$.

Lastly we show that it suffices to take the union over $\lambda \in G$ where $\overline{\lambda}$ is a coset representative of the quotient $(G/A)/\langle \overline{f} \rangle$. In other words, we show that if $\lambda_1 f = \lambda_2$ then $K_f a^{\lambda_1}(\lambda_1, f^{-1}) = K_f a^{\lambda_2}(\lambda_2, f^{-1})$. Using the Witt-Hall Identities we have

$$\begin{aligned}a^{\lambda_1}(\lambda_1, f^{-1}) \cdot (a^{\lambda_2}(\lambda_2, f^{-1}))^{-1} =& a^{\lambda_1}(\lambda_1, f^{-1}) \cdot (a^{\lambda_1 f}(\lambda_1 f, f^{-1}))^{-1} \\ =& a^{\lambda_1}(\lambda_1, f^{-1}) \cdot (f^{-1}, \lambda_1 f)(a^{\lambda_1 f})^{-1} \\ =& a^{\lambda_1}(a^{-1})^{f\lambda_1}(\lambda_1, f^{-1}) \cdot (f^{-1}, \lambda_1 f) \\ =& (a(a^{-1})^f)^{\lambda_1}(\lambda_1, f^{-1}) \cdot (f^{-1}, f)(f^{-1}, \lambda_1)((f^{-1}, \lambda_1), f) \\ =& (a^{-1}, f)^{\lambda_1}((f^{-1}, \lambda_1), f).\end{aligned}$$

Since G/A is abelian, K_f is normal and $(f^{-1}, \lambda) \in A$. Thus $(a(a^{-1})^f)^{\lambda_1}((f^{-1}, \lambda), f)$ is the product of two elements of K_f. This shows that the K_f cosets corresponding to $\overline{\lambda_1}\langle \overline{f} \rangle$ and $\overline{\lambda_2}\langle \overline{f} \rangle$ are the same. □

Proposition C.3. *The conjugacy classes in G_{47} are as follows:*

For $i, j, k \in \mathbb{Z}$,

$$(x^i y^j z^k p)^G = \langle x^2, y^2 \rangle x^i y^j z^{\pm k} p;$$

$$(x^i y^j z^k r)^G = \langle x^2, z^2 \rangle x^i y^{\pm j} z^k r;$$

$$(x^i y^j z^k pr)^G = \langle y^2, z^2 \rangle x^{\pm i} y^j z^k pr;$$

$$(x^i y^j z^k prt)^G = \langle x^2 \rangle x^i y^{\pm j} z^{\pm k} prt$$

$$(x^i y^j z^k rt)^G = \langle y^2 \rangle x^{\pm i} y^j z^{\pm k} rt$$

$$(x^i y^j z^k pt)^G = \langle z^2 \rangle x^{\pm i} y^{\pm j} z^k pt$$

$$(x^i y^j z^k t)^G = \langle x^2, y^2, z^2 \rangle x^i y^j z^k t.$$

We also have $G' = K = \langle x^2, y^2, z^2 \rangle$.

Proof. This follows from Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{47}. The presentation of G_{47} is of the form given in Eq. (4.4), with $\alpha_p = \alpha_r = \alpha_{pr} = \alpha_{pt} = \alpha_{rt} = 1$ and $\delta = 0$. □

Proposition C.4. *For G_{49} we have the following commutators:*

$$(p, r) = (p, t) = (p, rt) = 1;$$

$$(t, r) = (pt, r) = (t, pr) = (pt, pr) = (prt, r) = (rt, pt) = z.$$

Thus $G' = \langle x^2, y^2, z \rangle$.

The conjugacy classes in G_{49} are as follows:

For $i, j, k \in \mathbb{Z}$,

$$(x^i y^j z^k p)^G = \langle x^2, y^2 \rangle x^i y^j z^{\pm k} p;$$

$$(x^i y^j z^k r)^G = \langle x^2, z \rangle x^i y^{\pm j} r;$$

$$(x^i y^j z^k pr)^G = \langle y^2, z \rangle x^{\pm i} y^j pr;$$

$$(x^i y^j z^k prt)^G = \langle x^2 \rangle x^i y^{\pm j} z^k prt \, \cup \, \langle x^2 \rangle x^i y^{\pm j} z^{1-k} prt;$$

$$(x^i y^j z^k rt)^G = \langle y^2 \rangle x^{\pm i} y^j z^k rt \, \cup \, \langle y^2 \rangle x^{\pm i} y^j z^{1-k} rt;$$

$$(x^i y^j z^k pt)^G = \langle z^2 \rangle (x^i y^j)^{\pm 1} z^k pt \, \cup \, \langle z^2 \rangle (x^i y^{-j})^{\pm 1} z^{k+1} pt;$$

$$(x^i y^j z^k t)^G = \langle x^2, y^2, z \rangle x^i y^j t.$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and the relations in the presentation of G_{49}. □

Proposition C.5. *For G_{50} we have the following commutators:*

$$(p, r) = 1;$$

$$(t, r) = (prt, r) = (pt, r) = x;$$

$$(t, pr) = (pt, pr) = (pt, rt) = y;$$

$$(t, p) = (rt, p) = xy;$$

$$(rt, prt) = xy^{-1}.$$

Thus $G' = \langle x, y, z^2 \rangle$.

The conjugacy classes in G_{50} are: For $i, j, k \in \mathbb{Z}$,

$$(x^i y^j z^k p)^G = \langle xy, xy^{-1}\rangle x^i y^j z^{\pm k} p;$$

$$(x^i y^j z^k r)^G = \langle x, z^2\rangle y^{\pm j} z^k r;$$

$$(x^i y^j z^k pr)^G = \langle y, z^2\rangle x^{\pm i} z^k pr;$$

$$(x^i y^j z^k prt)^G = \langle x^2\rangle x^i y^j z^k prt \,\cup\, \langle x^2\rangle x^{i+1} y^j z^{-k} prt \,\cup\, \langle x^2\rangle x^i y^{-j+1} z^{-k} prt \,\cup\, \langle x^2\rangle x^{i+1} y^{-j+1} z^k prt;$$

$$(x^i y^j z^k rt)^G = \langle y^2\rangle x^i y^j z^k rt \,\cup\, \langle y^2\rangle x^i y^{j+1} z^{-k} rt \,\cup\, \langle y^2\rangle x^{-i+1} y^j z^{-k} rt \,\cup\, \langle y^2\rangle x^{-i+1} y^{j+1} z^k rt;$$

$$(x^i y^j z^k pt)^G = \langle z^2\rangle x^u y^v z^k pt, u \in \{i, -i+1\}, v \in \{j, -j+1\};$$

$$(x^i y^j z^k t)^G = \langle x, y, z^2\rangle z^k t.$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{50}. □

Proposition C.6. *For G_{51} we have the following commutators:*

$$(r,t) = (p,rt) = (pr,pt) = (rt,pt) = (pr,rt) = 1;$$

$$(r,p) = (t,p) = (r,prt) = (pt,r) = (pr,t) = x.$$

Thus $G' = \langle x, y^2, z^2\rangle$.

The conjugacy classes in G_{51} are: For $i, j, k \in \mathbb{Z}$,

$$(x^i y^j z^k p)^G = \langle x^2, y^2\rangle x^i y^j z^k p \,\cup\, \langle x^2, y^2\rangle x^{i+1} y^j z^{-k} p;$$

$$(x^i y^j z^k r)^G = \langle x, z^2\rangle y^{\pm j} z^k r;$$

$$(x^i y^j z^k pr)^G = \langle y^2, z^2\rangle x^i y^j z^k pr \,\cup\, \langle y^2, z^2\rangle x^{1-i} y^j z^k pr;$$

$$(x^i y^j z^k prt)^G = \langle x^2\rangle x^i y^{\pm j} z^k prt \,\cup\, \langle x^2\rangle x^{i+1} y^{\pm j} z^{-k} prt;$$

$$(x^i y^j z^k rt)^G = \langle y^2\rangle x^{\pm i} y^j z^{\pm k} rt;$$

$$(x^i y^j z^k pt)^G = \langle z^2\rangle x^i y^{\pm j} z^k pt \,\cup\, \langle z^2\rangle x^{1-i} y^{\pm j} z^k pt;$$

$$(x^i y^j z^k t)^G = \langle x, y^2, z^2\rangle y^j z^k t.$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{51}. □

Proposition C.7. *For G_{53} we have the following commutators:*

$$\begin{aligned}(t, pr) =& 1;\\ (rt, p) = (prt, r) =& x;\\ (r, p) = (pt, pr) = (rt, pt) =& z;\\ (t, p) = (t, r) =& xz;\\ (pt, r) =& xz^2.\end{aligned}$$

Thus $G' = \langle x, y^2, z\rangle$.

The conjugacy classes in G_{53} are: For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}(x^i y^j z^k p)^G &= \langle x, y^2\rangle y^j z^u p, u \in \{k, -k-1\};\\ (x^i y^j z^k r)^G &= \langle x, z^2\rangle y^j z^k r \,\cup\, \langle x, z^2\rangle y^{-j} z^{k+1} r;\\ (x^i y^j z^k pr)^G &= \langle y^2, z\rangle x^{\pm i} y^j pr;\\ (x^i y^j z^k prt)^G &= \langle x^2\rangle x^i (y^j z^k)^{\pm 1} prt \,\cup\, \langle x^2\rangle x^{i+1} (y^j z^{-k})^{\pm 1} prt;\\ (x^i y^j z^k rt)^G &= \langle y^2\rangle x^u y^j z^v rt,\ u \in \{i, 1-i\}, v \in \{k, 1-k\};\\ (x^i y^j z^k pt)^G &= \langle z^2\rangle x^u y^j z^k pt \,\cup\, \langle z^2\rangle x^u y^{-j} z^{k+1} pt, u \in \{i, 1-i\};\\ (x^i y^j z^k t)^G &= \langle x^2, y^2, z^2\rangle x^i y^j z^k t \,\cup\, \langle x^2, y^2, z^2\rangle x^{i+1} y^j z^{k+1} t\\ &= \langle xz, x^{-1}z, y^2\rangle x^i y^j z^k t.\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{53}. □

Proposition C.8. *For G_{54} we have the following commutators:*

$$\begin{aligned}(p, rt) =& 1;\\ (r, p) = (t, p) =& x;\\ (t, r) = (rt, pt) = (pt, pr) =& z;\\ (pt, r) =& xz;\\ (pr, t) = (r, prt) =& xz^{-1}.\end{aligned}$$

Thus we have $G' = \langle x, y^2, z\rangle$.

The conjugacy classes in G_{54} *are: For* $i, j, k \in \mathbb{Z}$,

$$
\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2, y^2\rangle x^i y^j z^k p \,\cup\, \langle x^2, y^2\rangle x^{i+1} y^j z^{-k} p;\\
(x^i y^j z^k r)^G &= \langle xz, xz^{-1}\rangle x^i y^j z^k r \,\cup\, \langle xz, xz^{-1}\rangle x^i y^{-j} z^{k+1} r;\\
(x^i y^j z^k pr)^G &= \langle y^2, z\rangle x^u y^j pr,\ u \in \{i, 1-i\};\\
(x^i y^j z^k prt)^G &= \langle x^2\rangle x^i y^{\pm j} z^k prt \,\cup\, \langle x^2\rangle x^{i+1} y^{\pm j} z^{1-k} prt;\\
(x^i y^j z^k rt)^G &= \langle y^2\rangle x^{\pm i} y^j z^u rt,\ u \in \{k, 1-k\};\\
(x^i y^j z^k pt)^G &= \langle z^2\rangle x^i y^j z^k pt, \cup \langle z^2\rangle x^i y^{-j} z^{k+1} pt \,\cup\, \langle z^2\rangle x^{1-i} y^j z^{k+1} pt \,\cup\, \langle z^2\rangle x^{1-i} y^{-j} z^k pt;\\
(x^i y^j z^k t)^G &= \langle x, y^2, z\rangle y^j t.
\end{aligned}
$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{54}. □

Proposition C.9. *For* G_{55} *we have the following commutators:*

$$
\begin{aligned}
(p,t) = (r,pt) = (pr,pt) = (rt,pt) &= 1;\\
(prt, r) &= x^2;\\
(p,r) = (t,r) = (rt,p) = (t,pr) &= xy.
\end{aligned}
$$

It follows that $G' = \langle xy, xy^{-1}, z^2\rangle$.

The conjugacy classes in G_{55} *are: For* $i, j, k \in \mathbb{Z}$,

$$
\begin{aligned}
(x^i y^j z^k p)^G &= \langle xy, xy^{-1}\rangle x^i y^j z^{\pm k} p\\
(x^i y^j z^k r)^G &= \langle x^2, z^2\rangle x^i y^j z^k r \,\cup\, \langle x^2, z^2\rangle x^{i+1} y^{-1-j} z^k r;\\
(x^i y^j z^k pr)^G &= \langle y^2, z^2\rangle x^i y^j z^k pr \,\cup\, \langle y^2, z^2\rangle x^{-1-i} y^{j+1} z^k pr;\\
(x^i y^j z^k prt)^G &= \langle x^2\rangle x^i y^j z^{\pm k} prt \,\cup\, \langle x^2\rangle x^{i+1} y^{1-j} z^{\pm k} prt;\\
(x^i y^j z^k rt)^G &= \langle y^2\rangle x^i y^j z^{\pm k} rt \,\cup\, \langle y^2\rangle x^{1-i} y^{j+1} z^{\pm k} rt;\\
(x^i y^j z^k pt)^G &= \langle z^2\rangle x^{\pm i} y^{\pm j} z^k pt;\\
(x^i y^j z^k t)^G &= \langle xy, xy^{-1}, z^2\rangle x^i y^j z^k t.
\end{aligned}
$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{55}. □

Proposition C.10. *For G_{57} we have the following commutators:*

$$
\begin{aligned}
(prt, r) =& 1;\\
(rt, p) = (t, pr) =& y;\\
(t, p) = (pt, pr) = (rt, pt) =& z;\\
(p, r) =& yz^{-1};\\
(pt, r) =& z^2;\\
(t, r) =& yz.
\end{aligned}
$$

It follows that $G' = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{57} are: For $i, j, k \in \mathbb{Z}$,

$$
\begin{aligned}
(x^iy^jz^kp)^G &= \langle x^2, y\rangle x^iz^kp \,\cup\, \langle x^2, y\rangle x^iz^{-k-1}p;\\
(x^iy^jz^kr)^G &= \langle x^2, z^2\rangle x^iy^jz^kr \,\cup\, \langle x^2, z^2\rangle x^iy^{-j-1}z^{k+1}r;\\
(x^iy^jz^kpr)^G &= \langle y^2, z\rangle x^iy^jpr \,\cup\, \langle y^2, z\rangle x^{-i}y^{j+1}pr;\\
(x^iy^jz^kprt)^G &= \langle x^2\rangle x^iy^uz^{\pm k}prt, u \in \{j, 1-j\};\\
(x^iy^jz^krt)^G &= \langle y^2\rangle x^iy^jz^urt \,\cup\, \langle y^2\rangle x^{-i}y^{j+1}z^urt,\ u \in \{k, 1-k\};\\
(x^iy^jz^kpt)^G &= \langle z^2\rangle x^{\pm i}y^jz^kpt, \cup \langle z^2\rangle x^{\pm i}y^{-j}z^{k+1}pt;\\
(x^iy^jz^kt)^G &= \langle x^2, y, z\rangle x^it.
\end{aligned}
$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{57}. □

Proposition C.11. *For G_{63} we have the following commutators:*

$$
\begin{aligned}
(p, rt) = (pr, t) = (prt, r) =& 1;\\
(r, p) = (t, r) = (t, p) = (pt, pr) = (rt, pt) =& z;\\
(pt, r) =& z^2.
\end{aligned}
$$

It follows that $G' = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{63} *are as follows:*

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2, y^2\rangle x^i y^u z^v p,\ u \in \{j, i+j\}, v \in \{k, -k-1\};\\
(x^i y^j z^k r)^G &= \langle x^2 y^{-1}, z^2\rangle x^i y^j z^k r\\
&\quad \cup \langle x^2 y^{-1}, z^2\rangle x^{-i} y^{-j} z^{k+1} r;\\
(x^i y^j z^k pr)^G &= \langle y, z\rangle x^{\pm i} pr;\\
(x^i y^j z^k prt)^G &= \langle x^2 y^{-1}\rangle (x^i y^j)^{\pm 1} z^{\pm k} prt;\\
(x^i y^j z^k rt)^G &= \langle y\rangle x^{\pm i} z^u rt, u \in \{k, 1-k\};\\
(x^i y^j z^k pt)^G &= \langle z^2\rangle x^i y^{j-\delta(i+2j)} z^{k+\delta} pt, \delta \in \{0,1\},\\
&\quad \cup \langle z^2\rangle (x^i y^{j-\delta(i+2j)})^{-1} z^{k+1-\delta} pt, \delta \in \{0,1\};\\
(x^i y^j z^k t)^G &= \langle x^2, y^2, z\rangle x^i y^u t, u \in \{j, i+j\}.
\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{63}. □

Proposition C.12. *For G_{64} we have the following commutators:*

$$\begin{aligned}(prt, r) =& 1;\\ (p, r) = (pt, rt) =& yz^{-1};\\ (t, p) = (t, r) = (pt, pr) =& yz;\\ (t, pr) = (rt, p) =& y^2;\\ (pt, r) =& z^2.\end{aligned}$$

It follows that $G' = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{64} are as follows:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}(x^i y^j z^k p)^G &= \langle x^2, y^2\rangle x^i y^u z^k p, u \in \{j, i+j\}\\ &\cup \langle x^2, y^2\rangle x^i y^u z^{-k-1} p, u \in \{j+1, i+j+1\};\\ (x^i y^j z^k r)^G &= \langle x^2 y^{-1}, z^2\rangle x^i y^j z^k r\\ &\cup \langle x^2 y^{-1}, z^2\rangle x^i y^{-i-j-1} z^{k+1} r;\\ (x^i y^j z^k pr)^G &= \langle y, z\rangle x^{\pm i} pr\\ (x^i y^j z^k prt)^G &= \langle x^2 y^{-1}\rangle x^i y^u z^{\pm k} prt, u \in \{j, 2-i-j\};\\ (x^i y^j z^k rt)^G &= \langle y\rangle x^{\pm i} z^u rt, u \in \{k, 1-k\};\\ (x^i y^j z^k pt)^G &= \langle z^2\rangle x^{(1-2\delta_1)i} y^{j+\delta_1 i} z^k pt, \delta_1 \in \{0, 1\}\\ &\cup \langle z^2\rangle x^{(2\delta_2-1)i} y^{1-j-\delta_2 i} z^{k+1} pt, \delta_2 \in \{0, 1\};\\ (x^i y^j z^k t)^G &= \langle x^2, yz, yz^{-1}\rangle y^j z^k t, \ \textit{if } i \textit{ is even},\\ &\langle x^2, y, z\rangle xt \ \textit{if } i \textit{ is odd}.\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{64}. □

Proposition C.13. *Let $G = G_{65}$. Here F is an abelian subgroup of G, thus $G' = K = \langle x^2, y, z^2 \rangle$.*

The conjugacy classes in G_{65} are as follows:

For $i, j, k \in \mathbb{Z}$,

$$(x^i y^j z^k p)^G = \langle x^2, y^2 \rangle x^i y^u z^{\pm k} p,\ u \in \{j, i+j\};$$

$$(x^i y^j z^k r)^G = \langle x^2 y^{-1}, z^2 \rangle (x^i y^j)^{\pm 1} z^k r;$$

$$(x^i y^j z^k pr)^G = \langle y, z^2 \rangle x^{\pm i} z^k pr;$$

$$(x^i y^j z^k prt)^G = \langle x^2 y^{-1} \rangle (x^i y^j)^{\pm 1} z^{\pm k} prt;$$

$$(x^i y^j z^k rt)^G = \langle y \rangle x^{\pm i} z^{\pm k} rt;$$

$$(x^i y^j z^k pt)^G = \langle z^2 \rangle (x^i y^u)^{\pm 1} z^k pt,\ u \in \{j, -i-j\};$$

$$(x^i y^j z^k t)^G = \langle x^2, y^2, z^2 \rangle x^i y^u z^k t,\ u \in \{j, i+j\}.$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{65}. □

Proposition C.14. *For G_{66} we have the following commutators:*

$$(p, r) = (p, t) = (p, rt) = 1;$$

$$(t, r) = (prt, r) = (rt, pt) = (pt, pr) = (t, pr) = (pt, r) = z.$$

It follows that $G' = \langle x^2, y, z \rangle$.

The conjugacy classes in G_{66} are as follows:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2, y^2 \rangle x^i y^u z^{\pm k} p,\ u \in \{j, i+j\};\\
(x^i y^j z^k r)^G &= \langle x^2 y^{-1}, z \rangle (x^i y^j)^{\pm 1} r;\\
(x^i y^j z^k pr)^G &= \langle y, z \rangle x^{\pm i} pr;\\
(x^i y^j z^k prt)^G &= \langle x^2 y^{-1} \rangle (x^i y^j)^{\pm 1} z^u prt,\ u \in \{k, 1-k\};\\
(x^i y^j z^k rt)^G &= \langle y \rangle x^{\pm i} z^u rt, u \in \{k, 1-k\};\\
(x^i y^j z^k pt)^G &= \langle z^2 \rangle (x^i y^j)^{\pm 1} z^k pt\\
&\quad \cup \langle z^2 \rangle (x^{-i} y^{i+j})^{\pm 1} z^{k+1} pt;\\
(x^i y^j z^k t)^G &= \langle x^2, y^2, z^2 \rangle x^i y^j z^k t\\
&\quad \cup \langle x^2, y^2, z^2 \rangle x^i y^{i+j} z^{k+1} t.
\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{66}. □

Proposition C.15. *For G_{67} we have the following commutators:*

$$\begin{aligned}
&(r, pt) = (r, prt) = 1;\\
&(p, r) = (pt, pr) = (pt, rt) = (t, p) = (t, r) = y;\\
&(rt, p) = (t, pr) = y^2.
\end{aligned}$$

It follows that $G' = K = \langle x^2, y, z^2 \rangle$.

The conjugacy classes in G_{67} are:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^iy^jz^kp)^G &= \langle x^2, y^2\rangle x^iy^uz^kp, u \in \{i, i+j\} \\
&\cup \langle x^2, y^2\rangle x^iy^uz^{-k}p, u \in \{j+1, i+j+1\}; \\
(x^iy^jz^kr)^G &= \langle x^2y^{-1}, z^2\rangle x^iy^uz^kr, u \in \{j, -i-j-1\}; \\
(x^iy^jz^kpr)^G &= \langle y, z^2\rangle x^{\pm i}z^kpr; \\
(x^iy^jz^kprt)^G &= \langle x^2y^{-1}\rangle x^iy^uz^{\pm k}prt, u \in \{j, 2-i-j\}; \\
(x^iy^jz^krt)^G &= \langle y\rangle x^{\pm i}z^{\pm k}rt; \\
(x^iy^jz^kpt)^G &= \langle z^2\rangle x^iy^uz^kpt, u \in \{j, 1-i-j\} \\
&\cup \langle z^2\rangle x^{-i}y^uz^kpt, u \in \{i+j, 1-j\} \\
(x^iy^jz^kt)^G &= \langle x^2, y, z^2\rangle x^iz^kt.
\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{67}. □

Proposition C.16. *For G_{68} we have the following commutators:*

$$\begin{aligned}
(p, rt) =& 1; \\
(t, r) = (rt, pt) = (pt, pr) =& z; \\
(p, r) = (p, t) =& x^{-2}y; \\
(r, pt) =& x^{-2}yz^{-1}; \\
(pr, t) = (r, prt) =& x^2y^{-1}z^{-1}.
\end{aligned}$$

It follows that $G' = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{68} are:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2, y^2 \rangle x^i y^u z^k p, u \in \{j, i+j\}, \\
&\cup \langle x^2, y^2 \rangle x^i y^u z^{-k} p, u \in \{j+1, i+j+1\}; \\
(x^i y^j z^k r)^G &= \langle x^2 y^{-1}, z^2 \rangle x^i y^u z^v r, u \in \{j, -i-j\}, v \in \{k, k-1\}; \\
(x^i y^j z^k pr)^G &= \langle y, z^2 \rangle x^u z^v pr, u \in \{i, 2-i\}, v \in \{k, k-1\}; \\
(x^i y^j z^k prt)^G &= \langle x^2 y^{-1} \rangle (x^i y^j)^{\pm 1} z^u prt, u \in \{k, 1-k\}; \\
(x^i y^j z^k rt)^G &= \langle y \rangle x^{\pm i} z^u rt, u \in \{k, 1-k\}; \\
(x^i y^j z^k pt)^G &= \langle z^2 \rangle x^i y^j z^k (y^{-i-2j} z)^\delta pt, \delta \in \{0, 1\}, \\
&\cup \langle z^2 \rangle x^{2-i} y^{-j-1} z^k (y^{i+2j} z)^\delta pt, \delta \in \{0, 1\}; \\
(x^i y^j z^k t)^G &= \langle x^2, y, z \rangle x^i t.
\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{68}. □

Proposition C.17. *The following pertains to G_{69}.*

Here F is an abelian subgroup of G, thus $G' = K = \langle x^2, y^2, z \rangle$.

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2 z^{-1}, y^2 z^{-1} \rangle x^i y^j z^u p,\ u \in \{k, -i-j-k\} \\
&\cup \langle x^2 z^{-1}, y^2 z^{-1} \rangle x^i y^{-j} z^u p,\ u \in \{j+k, -i-k\}; \\
(x^i y^j z^k r)^G &= \langle x^2, z \rangle x^i y^j z^u r,\ u \in \{k, -i-j-k\} \\
&\cup \langle x^2, z \rangle x^i y^{-j} z^u r,\ u \in \{j+k, -i-k\}; \\
(x^i y^j z^k pr)^G &= \langle y^2, z \rangle x^{\pm i} y^j pr; \\
(x^i y^j z^k prt)^G &= \langle x^2 z^{-1} \rangle (x^i y^j)^{\pm 1} z^u prt, u \in \{k, 1-k\}; \\
(x^i y^j z^k rt)^G &= \langle y^2 z^{-1} \rangle x^{\pm i} z^u rt, u \in \{k, 1-k\}; \\
(x^i y^j z^k pt)^G &= \langle z \rangle x^{\pm i} y^{\pm j} pt; \\
(x^i y^j z^k t)^G &= \langle x^2, y^2, z^2 \rangle x^i y^j z^u t, u \in \{k, j+k, i+k\}.
\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{69}. □

Proposition C.18. *For G_{72} we have the following commutators:*

$$\begin{aligned}(p,t) = (pt,rt) = (pt,pr) = (pt,r) = (pt,prt) &= 1;\\ (p,r) = (t,r) = (t,pr) = (rt,p) &= x^2z^{-1};\\ (r,pr) = (rt,prt) &= x^2y^{-2}z^{-1};\\ (rt,pr) &= y^2.\end{aligned}$$

It follows that $G' = K = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{72} are:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}(x^iy^jz^kp)^G &= \langle x^2z^{-1}, y^2\rangle(x^iy^jz^k)^{\pm 1}p\\ &\quad\cup \langle x^2z^{-1}, y^2\rangle(x^iy^{i+j}z^k)^{\pm 1}p;\\ (x^iy^jz^kr)^G &= \langle x^2y^{-1}, z^2\rangle x^iy^jz^ur, u \in \{k, i+k\}\\ &\quad\cup \langle x^2y^{-1}, z^2\rangle x^{-i}y^{-j-1}z^ur, u \in \{k+1, i+k+1\};\\ (x^iy^jz^kpr)^G &= \langle yz, yz^{-1}\rangle x^iy^jz^upr, u \in \{k, i+k\}\\ &\quad\cup \langle yz, yz^{-1}\rangle x^{-i-2}y^jz^upr, u \in \{k+1, i+k+1\};\\ (x^iy^jz^kprt)^G &= \langle x^2y^{-1}z^{-1}\rangle x^iy^jz^uprt, u \in \{k, -i-k\}\\ &\quad\cup \langle x^2y^{-1}z^{-1}\rangle x^{-i}y^{1-j}z^uprt, u \in \{-k, i+k\};\\ (x^iy^jz^krt)^G &= \langle y\rangle x^iz^urt, u \in \{k, -i-k\}\\ &\quad\cup \langle y\rangle x^{2-i}z^urt, u \in \{i+k-1, -k-1\};\\ (x^iy^jz^kpt)^G &= \langle z\rangle(x^iy^u)^{\pm 1}pt, u \in \{j, -i-j\};\\ (x^iy^jz^kt)^G &= \langle x^2, y^2, z\rangle y^jt \quad \textit{if } i \textit{ is even},\\ &\quad \textit{or } \langle x^2, y, z\rangle xt \quad \textit{if } i \textit{ is odd}.\end{aligned}$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{72}. □

Proposition C.19. *For G_{73} we have the following commutators:*

$$(p,r) = x^{-2}y^2; \qquad (p,t) = x^{-2}y;$$

$$(t,r) = yz; \qquad (pr,r) = x^2;$$

$$(rt,p) = (prt,rt) = y; \qquad (rt,pr) = y^2z;$$

$$(pt,r) = x^2y^{-1}z; \qquad (pr,t) = x^2y^{-2}z^{-1};$$

$$(pt,pr) = (rt,pt) = z; \qquad (r,prt) = (pt,prt) = x^2y^{-1}z^{-1}.$$

Therefore $G' = K = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{73} are:

For $i,j,k \in \mathbb{Z}$,

$$(x^iy^jz^kp)^G = \langle x^2z^{-1}, y\rangle x^iz^kp \ \cup\ \langle x^2z^{-1}, y\rangle x^iz^{-i-k-1}p \ \text{ if } i \text{ is even,}$$

$$\langle x^2z^{-1}, y^2\rangle x^iy^jz^kp \ \cup\ \langle x^2z^{-1}, y^2\rangle x^iy^{j+1}z^{-i-k-1}p; \ \text{ if } i \text{ is odd;}$$

$$(x^iy^jz^kr)^G = \langle x^2y^{-1}, z^2\rangle x^iy^jz^ur,\ u \in \{k, i+k+1\}$$

$$\cup \langle x^2y^{-1}, z^2\rangle x^iy^{-1-i-j}z^ur,\ u \in \{i+k, 1+k\};$$

$$(x^iy^jz^kpr)^G = \langle y,z\rangle x^upr, u \in \{i, 2-i\}, \ \text{ if } i \text{ is even,}$$

$$\langle yz, yz^{-1}\rangle x^iy^jz^k(x^{2-2i}z)^\delta pr, \delta \in \{0,1\} \ \text{ if } i \text{ is odd;}$$

$$(x^iy^jz^kprt)^G = \langle x^2y^{-1}z^{-1}\rangle x^iy^uz^vprt, u \in \{j, 1-i-j\}, v \in \{k, -i-k\};$$

$$(x^iy^jz^krt)^G = \langle y\rangle x^iz^urt,\ u \in \{k, 1-i-k\}$$

$$\cup \langle y\rangle x^{-i}z^urt,\ u \in \{i+k, 1-k\};$$

$$(x^iy^jz^kpt)^G = \langle z\rangle x^iy^upt,\ u \in \{j, -i-j\}$$

$$\cup \langle z\rangle x^{2-i}y^upt,\ u \in \{i+j-1, -1-j\};$$

$$(x^iy^jz^kt)^G = \langle x^2, y, z\rangle x^it.$$

Proof. This follows from Lemma C.1, Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{73}. □

Proposition C.20. *For G_{74} we have the following commutators:*

$$(r, prt) = (r, pt) = (prt, pt) = 1;$$

$$(p, r) = (t, p) = (pr, r) = (t, r) = (pt, pr) = (pt, rt) = y;$$

$$(rt, p) = (t, pr) = (prt, rt) = y^2;$$

$$(rt, pr) = y^3.$$

Therefore $G' = K = \langle x^2, y, z\rangle$.

The conjugacy classes in G_{74} are:

For $i, j, k \in \mathbb{Z}$,

$$\begin{aligned}
(x^i y^j z^k p)^G &= \langle x^2 z^{-1}, y^2\rangle x^i y^u z^k p,\ u \in \{j, i+j\}\\
&\cup \langle x^2 z^{-1}, y^2\rangle x^i y^u z^{-i-k} p,\ u \in \{i+j+1, j+1\};\\
(x^i y^j z^k r)^G &= \langle x^2 y^{-1}, z^2\rangle x^i y^u z^v r,\ u \in \{j, -i-j-1\},\ v \in \{k, i+k\};\\
(x^i y^j z^k pr)^G &= \langle yz, yz^{-1}\rangle x^{\pm 1} y^j z^k pr\\
&\cup \langle yz, yz^{-1}\rangle x^{\pm i} y^{j+1} z^{i+k} pr;\\
(x^i y^j z^k prt)^G &= \langle x^2 y^{-1} z^{-1}\rangle x^i y^u z^v prt,\ u \in \{j, 2-j-i\}\ v \in \{k, -i-k\};\\
(x^i y^j z^k rt)^G &= \langle y\rangle (x^i z^u)^{\pm 1} rt,\ u \in \{k, -i-k\};\\
(x^i y^j z^k pt)^G &= \langle z\rangle x^i y^u pt,\ u \in \{j, 1-i-j\}\\
&\cup \langle z\rangle x^{-i} y^u pt,\ u \in \{i+j, 1-j\};\\
(x^i y^j z^k t)^G &= \langle x^2, y, z^2\rangle z^k t \ \text{ if } i \text{ is even},\\
&\quad \langle x^2, yz, yz^{-1}\rangle x y^j z^k t \text{ if } i \text{ is odd}.
\end{aligned}$$

Proof. This follows from Proposition A.1, Proposition C.2, and from the relations in the presentation of G_{74}. □