On Space Groups and Dirichlet–Voronoi Stereohedra

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Preface

This thesis is about space groups and their applications in discrete geometry. It is structured into three different parts. Each part corresponds to one of the three chapters, which we will describe in the following.

In Chapter 1 an introduction to n-dimensional space groups is given. While there are many other texts on space groups, most of them cover only dimension $n \leq 3$, focus very much on crystallographic aspects, or are simply not up-to-date. We therefore tried to remedy the situation by collecting the most important results from this area, especially those that are related to tilings and the algebraic structure of space groups. We made a great effort to include the most important references on space groups. Our hope is that future researchers might find this survey a good starting point for their explorations.

In the second chapter we present a detailed investigation of which Dirichlet–Voronoi stereohedra the tetragonal, trigonal, hexagonal, and cubic groups can generate. A stereohedron is a convex n-dimensional polytope that tiles $\mathbb{R}^n$ by the action of some space group. If this polytope is a Dirichlet–Voronoi domain of some orbit of some space group, the stereohedron is called a Dirichlet–Voronoi stereohedron. Such stereohedra are examples of so-called convex monohedral tiles, whose possible shapes and combinatorial properties are poorly understood in general. In particular it is a long-standing open question whether the number of facets of a convex monohedral tile can be bounded by a function that only depends on the dimension n. With our investigations we want on the one hand to complement the work of Santos et al. [BS01; BS06; SS08; SS11] and on the other hand hope to give a realistic picture of what can be expected from 3-dimensional space groups. To carry out these computations we developed the extensive software suite `plesiohedron`, which is an important part of this thesis and can be found at `github.com/moritzschmitt/plesiohedron`.

Finally, Chapter 3 is devoted to the number $\mathrm{s}(n)$ of isomorphism classes of space groups of $\mathbb{R}^n$. It follows from a theorem by Bieberbach that there are only finitely many nonisomorphic space groups in each dimension. Schwarzenberger showed by counting the orthogonal space groups that

$$\mathrm{s}(n) = 2^{\Omega(n^2)}$$

and Buser later proved

$$\mathrm{s}(n) = 2^{2^{O(n^2)}}.$$

We were able to show that

$$\mathrm{s}(n) = 2^{2^{O(n \log n)}}.$$

For this we develop a new bound on $\mathrm{s}(n)$, which we also use to bound the number of conjugacy classes of finite subgroups in $\mathrm{GL}(n, \mathbb{Z})$. This bound is then evaluated by applying the mass formula of Smith–Minkowski–Siegel.

In Appendix A we concisely provide the necessary background on group cohomology for Chapter 1. This is not new but can also not easily be found in the overwhelming body of literature of homological algebra. Appendix B gives details on how exactly the computations for Chapter 2 were carried out.

Acknowledgements

First and foremost I would like to thank my two advisors Günter M. Ziegler and Ivan Izmestiev. Günter was always available for questions and helpful discussion, and his great mathematical intuition gave me guidance on more than one occasion. I am also grateful for the funding I received from his grants. Ivan listened to my ideas and presentations for hours on end with much patience, and his pointed questions and insightful comments were immensely useful.

Besides my two advisors there are also many other people I wish to thank for discussing questions related to this thesis: Mois Aroyo, Benjamin Assarf, Pavle Blagojević, Nikolai Dolbilin, Alexander Engström, Tobias Finis, Moritz Firsching, Elke Koch, Benjamin Lorenz, Arnau Padrol, Julian Pfeifle, Francisco Santos, Raman Sanyal, Jan-Christoph Schlage-Puchta, Benjamin Schröter, and Christian Stump. Achill Schürmann agreed to be the external referee for this thesis, for which I am much obliged to him.

For this thesis many computations were carried out on the allegro and ZEDAT/HPC clusters of Freie Universität. Both clusters are managed by very competent administrators who patiently answered my many emails and fulfilled all requests I had. Without them a large part of this thesis would not have been possible.

For much needed moral and emotional support I am deeply grateful to my partner Melanie Win Myint. Her contributions to the success of this thesis are immeasurable. Our children Ella and Noah are always enjoyable distractions from less livelier things such as the preparation of this document. Finally, I would like to thank my parents Astrid Bismark-Schmitt and Andreas Schmitt for their constant support and the confidence they equipped me with.

Contents

Chapter 1

A Primer on Euclidean Space Groups

This chapter serves a double purpose. First and foremost it shall serve as a concise introduction to Euclidean space groups. This beautiful part of group theory deserves to be known more widely, and when we started working on it, we quickly found ourselves in agreement with Yale who wrote

> "(...) we struggled to correlate the various notations, incomplete proofs, and partial presentations found in other introductions (...)"
> [Yal68, p. 119]

Yale somewhat remedies the situation for dimensions $n \leq 3$ but does not discuss space groups in higher dimensions. However, higher dimensional space groups are of importance, also for this thesis, and that is why we treat the general case. The other purpose – and this sets our introduction apart from Yale's even in dimension three – is to present a survey of the most important results from the area.

There are many other introductions to space groups. Let us list those known to us together with short comments on what they cover. We refrain from listing the many books on crystallography, even though almost all of them also have space groups as their topic. But on the one hand we found none that covers groups in dimensions higher than three, and often they are not as rigorous as needed by mathematicians. On the other hand they naturally concentrate on topics that are of interest to crystallographers and solid-state scientists but maybe less so to mathematicians.

Marcel Berger. *Geometry I.* Universitext. Springer, 2009: This is the treatment closest in spirit to ours. Space groups are understood as a mean to generate monohedral tilings. Unfortunately, only the planar case is treated and the classification is done only for space groups consisting of positive isometries.

Harold Brown et al. *Crystallographic groups of four-dimensional space.* Wiley, 1978: On the first few pages a readable but incomplete introduction to space group theory is given. The bulk of the book are tables that present the classification of four-dimensional space groups as a tedious list that nowadays would not appear in print.

Johann Jakob Burckhardt. ***Die Bewegungsgruppen der Kristallographie.*** **2nd ed. Birkhäuser, 1966:** Burckhardt gives a very concrete introduction to space groups with strong emphasis on dimensions $n = 2, 3$. He does not discuss any advanced theorems such as the ones by Bieberbach.

John H. Conway, Heidi Burgiel, and Chaim Goodman-Strauss. ***The symmetries of things.*** **A K Peters, 2008:** In this very interesting book an introduction to the powerful orbifold signature is given. This signature is used to classify all three-dimensional space groups. Higher-dimensional space groups are not mentioned in the book.

Harold S. M. Coxeter. ***Introduction to geometry.*** **Wiley, 1989:** This classical work on geometry only provides a superficial introduction to planar space groups in its Chapter 4. Nonetheless it is a nice starting point for further explorations.

Harold S. M. Coxeter and William O. J. Moser. ***Generators and relations for discrete groups.*** **4th ed. Springer, 1980:** Before all 17 two-dimensional space groups are given abstractly as finite presentations in Chap. 4, the authors quickly discuss finite symmetry and rotation groups. It is nicely explained how they arrive at each presentation by using Cayley graphs.

Leonard S. Charlap. ***Bieberbach groups and flat manifolds.*** **Springer, 1986:** A torsion-free space group is called a ***Bieberbach group***. The orbit space of a Bieberbach group Γ is a manifold $M^n = \mathbb{R}^n/\Gamma$ with fundamental group Γ and Riemannian structure inherited from $\mathbb{R}^n$. It is a so-called ***flat manifold***, i.e., a manifold with sectional curvature zero. Moreover, every compact flat manifold can be obtained as an orbit space of a Bieberbach group. Charlap's book starts to discuss Bieberbach's theorems in detail and then proceeds by discussing the algebraic and geometric properties of Bieberbach groups.

Peter Engel. ***Geometric crystallography.*** **Reidel, 1986**
Peter Engel. "Geometric crystallography". In: ***Handbook of convex geometry, Vol. B.*** **North-Holland, 1993:** The first reference is the only one known to us that applies space group actions to construct monohedral tilings and interesting sphere packings. Issues of rigour and clarity make it sometimes difficult to read this book. The second reference is a concise handbook article that contains no proofs. Both works give introductions to general space group theory and cover many more topics from mathematical crystallography.

Daniel R. Farkas. "Crystallographic groups and their mathematics". In: ***Rocky Mountain J. Math.*** **11.4 (1981), pp. 511–552:** This survey article introduces the reader to space groups, mainly from an algebraic point of view.

Birger Iversen. ***Lectures on crystallographic groups.*** **Lecture Notes Series 60. Aarhus Univ., 1990:** In Iversen's book many aspects of space group theory are treated somewhat unsystematically. It is one of the few books that discusses Poincaré's theorem on the relation between fundamental domains and finite presentations of a discrete group.

John G. Ratcliffe. ***Foundations of hyperbolic manifolds.*** **2nd ed. Vol. 149. Grad. Texts in Math. Springer, 2006:** As the title suggests, this books focuses on hyperbolic geometry. Nonetheless it covers a substantial part of the theory of *Euclidean* discrete groups. In particular it contains proofs of Bieberbach's theorems and a superb introduction to Poincaré's theorem.

Rolph L. E. Schwarzenberger. ***N-dimensional crystallography.*** **Res. Notes Math. 41. Pitman, 1980:** Many topics from general crystallography are covered in this book, but its lack of explanations together with Schwarzenberger's fondness for cryptic proofs are no guarantee for a joyful reading.

Andreas Speiser. ***Die Theorie der Gruppen von endlicher Ordnung.*** **Birkhäuser, 1956:** Speiser's book is one of the first systematic accounts of group theory. Despite the title this book also covers a little bit of infinite group theory. In particular a concise introduction to space groups is given.

Andrzej Szczepański. ***Geometry of crystallographic groups.*** **World Scientific, 2012:** The emphasis of this book is again on Bieberbach groups. It contains much material that is already contained in Charlap's book in less readable form, but is valuable as an update on the topic of flat manifolds.

William P. Thurston. ***Three-dimensional geometry and topology.*** **Princeton Univ. Press, 1997:** In Section 4.3 of his book Thurston covers Euclidean discrete groups in general. Within this scope he discussed a few theorems on space groups. He in particular proves generalizations of Bieberbach's theorem that are folklore and were written up here for the first time.

Ernest B. Vinberg and Osip V. Shvartsman. "Discrete groups of motions of spaces of constant curvature". In: ***Geometry II.*** **Springer, 1993:** The authors of this book give an introduction to space groups of spaces of constant curvature. They carefully define all basic terms and list many important theorems (unfortunately without proofs). The list of references of this book is particularly helpful.

Joseph A. Wolf. ***Spaces of constant curvature.*** **5th ed. Publish or Perish, 1984:** As the title suggests, Wolf's book is mainly about spaces of constant curvature per se. It has five parts where parts II and III from a space group point of view are the most interesting. In part II he discusses the Euclidean space form problem and in particular proves Bieberbach's theorems following Auslander [Aus65; Aus60; Aus61]. Part III gives the isometric classification of complete Riemannian manifolds of constant positive curvature.

Hans Wondratschek. "Introduction to space-group symmetry". In: *International tables for crystallography.* Ed. by Theo Hahn. Vol. A. Wiley, 2005. Chap. 8: This article is a contribution to the International Tables for Crystallography. Even though it is written by a crystallographer for crystallographers, the article is very close to current mathematical standard terminology. It includes many references to other parts of the International Tables which makes it a valuable resource for navigating through this literary monstrosity.

Paul B. Yale. *Geometry and symmetry.* Holden-Day, 1968: Yale's book is a general introduction to classical geometry up to dimension 3. In the second chapter it classifies all isometries and continues in Chapter 3 with classification of all finite isometry groups. He then rules out all groups that cannot be crystallographic point groups and constructs from the remaining groups all possible space groups.

1.1 Introduction and Bieberbach's theorems

We will begin with a few remarks on isometries of $\mathbb{R}^n$. The Euclidean group can be written as a semidirect product

$$\mathrm{Isom}(\mathbb{R}^n) \cong \mathrm{O}(n) \ltimes \mathbb{R}^n.$$

The underlying set of this product is $\mathrm{O}(n) \times \mathbb{R}^n$. Hence every isometry $\alpha \in \mathrm{Isom}(\mathbb{R}^n)$ is of the form $\alpha = (A, a)$ with A being the ***linear part*** (or ***rotational*** part) and a being the ***translational part***. Each isometry can be understood as an invertible matrix in $\mathbb{R}^{(n+1)\times(n+1)}$ by embedding $\alpha = (A, a)$ as

$$\alpha \mapsto \begin{bmatrix} A & a \\ 0 & 1 \end{bmatrix} \in \mathrm{GL}(n+1, \mathbb{R}).$$

While this is called the ***linear notation***, we say that $\alpha = (A, a)$ is in ***Frobenius notation***. To save space we will mostly use Frobenius notation, for which we have

$$\alpha\beta = (A, a)(B, b) = (AB, Ab + a)$$

and

$$\alpha^{-1} = (A, a)^{-1} = (A^{-1}, -A^{-1}a).$$

Pure translations are elements of the form (I, t). For further background on classical geometry we suggest Audin [Aud03] and Berger [Ber09a; Ber09b].

The group $\mathrm{Isom}(\mathbb{R}^n)$ is a topological group: it inherits the topology from $\mathrm{GL}(n+1, \mathbb{R})$. We call a subgroup Γ of $\mathrm{Isom}(\mathbb{R}^n)$ a ***discrete group*** if every element of Γ is open with respect to the subspace topology. By using the fact that $\mathrm{O}(n)$ is compact, one can show that this is the same as requiring every orbit

$$\Gamma(x) = \{\gamma(x) : \gamma \in \Gamma\}$$

of a point $x \in \mathbb{R}^n$ to be a discrete set.[1] Among the most famous examples of discrete groups are so-called space groups. These will be defined in terms of fundamental domains for which we need a precise definition first.

[1] Such groups are normally called *discontinuous* or one says that the subgroup action *has discrete orbits*, see [Thu97; Sie43; Rat06].

Definition 1.1.1. Let Γ be a subgroup of $\mathrm{Isom}(\mathbb{R}^n)$. A subset $F \subset \mathbb{R}^n$ is a ***fundamental domain*** if

(i) F is open in $\mathbb{R}^n$,

(ii) F is connected,

(iii) $\{\gamma(F) : \gamma \in \Gamma\}$ are pairwisely disjoint, (***packing property***)

(iv) $\mathbb{R}^n = \bigcup \{\gamma(\mathrm{cl}(F)) : \gamma \in \Gamma\}$. (***covering property***)

We are now ready to introduce our main object of study.

Definition 1.1.2. A ***space group*** of $\mathbb{R}^n$ is a discrete subgroup of $\mathrm{Isom}(\mathbb{R}^n)$ with a bounded fundamental domain.

Remark 1.1.3. Instead of "space group" one encounters also the names *crystallographic group*, *Fedorov group* (especially in literature of Russian origin), and *Raumgruppen*. Sometimes the name *Bieberbach group* is used as well, but nowadays it seems that this name has gone out of fashion and is only used for space groups that are also torsion-free.

Let us illustrate the definition by discussing a few examples that will also be used later on.

Example 1.1.4. (i) Up to isomorphism, there are exactly two space groups in dimension 1. The first one is isomorphic to $\mathbb{Z}$ and the second one is isomorphic to the infinite dihedral group $\mathbb{Z}_2 \ltimes \mathbb{Z}$. The group $\mathbb{Z}$ has as a fundamental domain an open interval of length 1, and the group $\mathbb{Z}_2 \ltimes \mathbb{Z}$ an open interval of length $1/2$.

(ii) Every lattice $L \leq \mathbb{R}^n$ of rank n is a space group. After choosing a basis for L, the open parallelepiped of this basis can be used as a fundamental domain.

(iii) [Cha86, Example 2.3] Consider the isometries

$$\alpha = \begin{bmatrix} 1 & 0 & 1/2 \\ 0 & -1 & 1/2 \\ 0 & 0 & 1 \end{bmatrix} \qquad \beta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1/2 \\ 0 & 0 & 1 \end{bmatrix}$$

and the group $\Gamma = \langle \alpha, \beta \rangle$ generated by them. This group is a space group of $\mathbb{R}^2$ with $\{(x_1, x_2) : 0 < x_i < 1/2\}$ as a fundamental domain. This group is torsion-free as can be easily seen: By using the equalities

$$\alpha\beta = \beta^{-1}\alpha, \quad \alpha^{-1}\beta = \beta^{-1}\alpha^{-1}, \quad \alpha\beta^{-1} = \beta\alpha, \quad \alpha^{-1}\beta^{-1} = \beta\alpha^{-1}$$

it is immediate that every element of Γ is of the form $\beta^k\alpha^l$ for $k, l \in \mathbb{Z}$. Together with

$$(\beta^k\alpha^l)(\beta^r\alpha^s) = \beta^{k+(-1)^l r}\alpha^{l+s}$$

we get that no non-trivial element of Γ can be of finite order.

(iv) The following matrices in $\mathbb{R}^{2\times 2}$

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad A_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad A_3 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \quad A_4 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

form the Klein four-group $V = \{A_1, \ldots, A_4\}$. This group can be used to construct the space group

$$\Gamma = \{(A_i, t) : t \in \mathbb{Z}^2, 1 \leq i \leq 4\},$$

which is isomorphic to $V \ltimes \mathbb{Z}^2$. Since it is a semidirect product, this group has torsion elements. The open square of side length $1/2$ is a fundamental domain.

Space groups played a crucial role in crystallography already in the middle of the 19th century, but they gained real prominence among mathematicians only when Hilbert presented his famous list of problems. In 1900 he published a list of twenty-three problems [Hil00], which were open at that time and which had a strong influence on mathematical research in the 20th century. His eighteenth problem involves space groups. He asked the following question

> Is there in n-dimensional Euclidean space (...) only a finite number of essentially different kinds of groups of motions with a fundamental region? [Hil02].

Hilbert's question was answered in the affirmative by Bieberbach [Bie11] in 1911 by showing that up to isomorphism there are only finitely many space groups in each dimension. Frobenius was quick in pointing out that "isomorphism" is not the right equivalence but "affine conjugation" is, i.e., two groups should be considered as equivalent if they are the same up to a change of the coordinate system. He showed [Fro11] that under this (seemingly finer) sort of equivalence there are still just finitely many. In 1912 finally, Bieberbach proved that for space groups every isomorphism is actually induced by an affine conjugation.

Theorem 1.1.5 (Bieberbach [Bie11; Bie12]). *Let* Γ *be a subgroup of* $\operatorname{Isom}(\mathbb{R}^n)$ *and denote by* T *the set of all translations in* Γ.

(i) Γ *is a space group if and only if* T *is a lattice of rank* n *and* Γ/T *is finite.*

(ii) *Two space groups are isomorphic as abstract groups if and only if they are affinely conjugate.*

(iii) *In each dimension there are only finitely many nonisomorphic space groups.*

Part (iii) will be proven in Chapter 3. A complete proof of this fundamental theorem can be found in the very readable article by Buser [Bus85], see also Buser & Karcher [BK81]. Other proofs include the original one by Bieberbach [Bie11; Bie12], the much simpler one by Frobenius [Fro11] given shortly afterwards, Auslander's [Aus60; Aus61; Aus65], Vinberg's [Vin75], and Oliver's [Oli80]. It is interesting to note what Charlap [Cha86, pp. 41f] writes about Buser's proof: "Peter Buser's new proof resulted from a study of the techniques that Gromov used in his work on almost flat manifolds (...). In fact, Gromov has said that his work on almost flat manifolds resulted from an attempt to understand what's really going on in the proof of Bieberbach's First Theorem."

Low-dimensional classifications

Strictly speaking there are actually infinitely many space groups. But of course the ones that only differ by a change of the affine coordinate system should be identified. Thanks to the Bieberbach theorems we know that this is exactly the same as identifying space groups that are isomorphic as abstract groups. The partition of the set of all space groups into classes of isomorphic groups is therefore the targeted classification. Each class of this partition is called a ***space group type***, where one often uses *space group* and *space group type* synonymous.

For dimension $n \leq 4$ the types of space groups have been completely classified. There is only one type in dimension $n = 0$, and as shown in Example 1.1.4 (i), there are two types in dimension $n = 1$.

Dimension $n = 2$ is the first interesting dimension. In this dimension space groups are also called *wallpaper groups*, *periodic groups*, *plane symmetry groups*, or *plane crystallographic groups*. They were classified for the first time by Fedorov [Fed91a] and later independently by Pólya [Pol24]. There are 17 isomorphism types in total and numerous accounts of their classification can be found. Particularly nice expositions are [CBG08; Joh01].

In dimension $n = 3$ there are 219 isomorphism types. The classification for this dimension is already very involved. It was started by Jordan [Jor67] and then systematically extended by Sohncke [Soh79] to a classification of all orientation-preserving space groups. He later extended his work in [Soh88], but never finished a complete classification. Fedorov [Fed91b] built upon Sohncke's work and derived 218 space group types. Arthur Schoenflies [Sch91], a disciple of Felix Klein, independently obtained 216 different space group types. After comparing results the correct number of 219 types was agreed on. For the interesting history of the discovery see Burckhardt [Bur68]. A modern classification can be found in [Hah05].

The last dimension where a complete classification was given is $n = 4$, a total of 4783 isomorphism types were found. This was done by Brown et al. [Bro+78], with a small mistake that Neubüser et al. [NSW02] corrected.

For higher dimensions a complete classification becomes unlikely, given that for $n = 5$ there are already 222 018 space group types and for $n = 6$ there are 28 927 922. Hence, Plesken & Schulz [PS00] suggest a different approach. They propose to assign to each space group type a unique identifier based on a natural division of the types into $\mathbb{Q}$- and $\mathbb{Z}$-classes and crystal families. Let us define these terms now, as we will need them later as well.

To understand the following definitions, recall that the ***automorphism group*** of a lattice $L \leq \mathbb{R}^n$ of rank n is defined as $\mathrm{Aut}(L) = \{\alpha \in \mathrm{Isom}(\mathbb{R}^n) : \alpha(L) = L\}$. It is easy to show that this group is always finite and is isomorphic to a subgroup of $\mathrm{GL}(n, \mathbb{Z})$. On the other hand, given a finite subgroup G of $\mathrm{GL}(n, \mathbb{Z})$ one can associate a lattice L_G to this subgroup such that its automorphism group has G as a subgroup; see Conway & Sloane [CS99, p. 92] for details. Two such finite subgroups G, H are said to be ***Bravais equivalent*** if $\mathrm{Aut}(L_G)$ and $\mathrm{Aut}(L_H)$ are conjugate in $\mathrm{GL}(n, \mathbb{Z})$. To better understand the following definitions compare with the hierarchy shown in Figure 1.1.

Definition 1.1.6. Two space groups Γ_1 and Γ_2 of $\mathbb{R}^n$ with lattices L_1, L_2 belong to the same ***$\mathbb{Q}$-class*** if their ***point groups*** $\Gamma_1/L_1, \Gamma_2/L_2$ are conjugate in $\mathrm{GL}(n, \mathbb{Q})$. If they are even conjugate in $\mathrm{GL}(n, \mathbb{Z})$, they are in the same ***$\mathbb{Z}$-class***. If the lattices L_1 and L_2 have automorphism groups that are in the same $\mathbb{Q}$-class, we say that Γ_1 and Γ_2 belong to the same ***Bravais system***. And if the lattices have automorphism groups in the same $\mathbb{Z}$-class, the space groups are in the same ***Bravais class***. The $\mathbb{Q}$-classes are combined into ***crystal systems*** by letting two $\mathbb{Q}$-classes be in the same crystal system if they intersect the same Bravais classes. The set of $\mathbb{Z}$-classes is partitioned into ***crystal families*** by

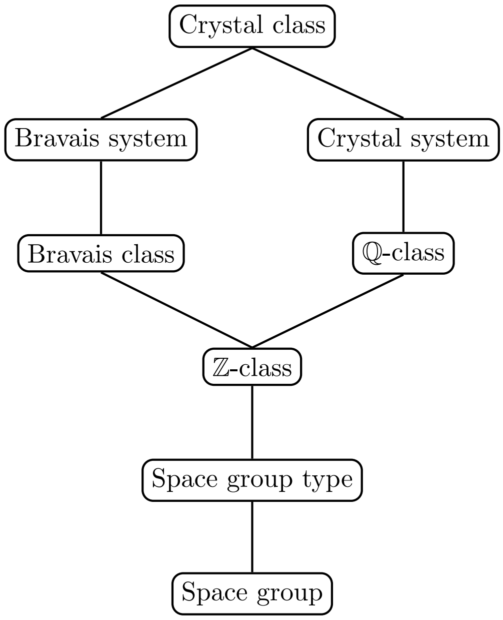


Figure 1.1: Hierarchy of different classifications.

requiring that the finite subgroups $G, H \leq \mathrm{GL}(n, \mathbb{Z})$ are in the same crystal family, if there exist subgroups $F_1, \ldots, F_r$ such that $F_1 = G$ and $F_r = H$ and that F_i, F_{i+1} are $\mathbb{Q}$-equivalent for some i and Bravais equivalent for all others.

Remark 1.1.7. Instead of $\mathbb{Q}$-class and $\mathbb{Z}$-class very often *geometric crystal class* and *arithmetic crystal class* are used, respectively.

Now we will come back to the work of Plesken & Schulz. They begin by taking all finite $\mathbb{Q}$-maximal subgroups of $\mathrm{GL}(n, \mathbb{Z})$ from Plesken & Pohst [PP77a; PP77b], then compute their subgroup structure, and finally compute representatives for each conjugacy class in $\mathrm{GL}(n, \mathbb{Q})$. Then they use the algorithms described in Opgenorth et al. [OPS98] to split the $\mathbb{Q}$-classes into $\mathbb{Z}$-classes. For each $\mathbb{Z}$-class the number of space groups is computed by applying the Zassenhaus algorithm [Zas48].

A fundamentally different way to classify space groups came out of the work by Thurston on orbifolds and was further developed by Conway, Delgado, and Huson. The general definition of *orbifold* is quite involved, see Thurston [Thu97; TM79] and Scott [Sco83]. For us it will be enough to understand an orbifold as the orbit space of the action of a discrete subgroup Γ of $\mathrm{Isom}(\mathbb{R}^n)$. This yields a metric space $M = \mathbb{R}^n/\Gamma$ which for each $p \in M$ has an open neighborhood that is isometric to $\mathrm{B}(p, \varepsilon)/\operatorname{Stab}_\Gamma(p)$.

Conway [Con92; CBG08] developed the *orbifold notation* to describe 2-dimensional orbifolds. He assigns each symbol of the notation a value such that the sum of all symbol values for each orbifold name exactly sums up to the generalized Euler characteristic of the orbifold. Space groups correspond to 2-orbifolds of characteristic 0. By simple arithmetical considerations Conway derives the 17 possible space group types. Later Conway, Delgado, and Huson [Con+01] were able to characterize the three-dimensional space groups by developing the concept of fibered orbifolds, combined with a simple algebraic observation. Similar characterizations for higher dimensions are not available.

Why study space groups?

The answer to this question depends on the point of view. Space groups offer interesting applications to both the algebraist and the geometer. For example, all n-dimensional discrete subgroups of $\mathrm{Isom}(\mathbb{R}^n)$ can be constructed using the classification of k-dimensional space groups for $k \leq n$.

A powerful algebraic application of space groups was given by Felsch et al. [FNP81]. In this article counter-examples to the long-standing class-breadth conjecture were constructed. This conjecture related the breadth and the nilpotency-class of p-groups. The *breadth* $b(G)$ of a p-group G is the size $p^{b(G)}$ of the largest conjugacy class of G, while the *nilpotency class* $c(G)$ is defined as the length of the shortest central series of G. The conjecture stated that

$$c(G) \leq b(G) + 1,$$

but was disproven for 2-groups in the article cited above. For p-groups with $p \geq 3$ it is still open.

On the other hand, for geometers it is probably more relevant that space groups currently provide the only way to easily generate interesting examples of non-planar ***isohedral tilings*** of $\mathbb{R}^n$, i.e., tilings with a transitive symmetry group. All other methods are either very narrow in the possible spectrum of combinatorial types that can be generated or seem to be completely *ad hoc*. This application of space groups will be used extensively in Chapter 2.

Another "geometric" reason to study space groups is their relation to flat manifolds. A Riemannian manifold is *flat* if its sectional curvature is everywhere zero. Equivalently, a flat manifold can be understood as the quotient space $M = \mathbb{R}^n/\Gamma$, where Γ is a torsion-free discrete subgroup of $\mathrm{Isom}(\mathbb{R}^n)$. If M is also compact, the group Γ is a (torsion-free) space group. In this case Γ is isomorphic to the fundamental group of M, and, furthermore, if two such manifolds have isomorphic fundamental groups, then by Bieberbach's theorem they must be affinely equivalent (i.e., there exists a diffeomorphism that preserves the Riemannian connection). Characterizing torsion-free space groups is therefore the same as classifying compact flat manifolds according to their fundamental group or rather up to affine equivalence.

Applications of space groups outside of mathematics can be found everywhere in crystallography [San69; Jan01], solid-state science [Sim13], and chemistry [Dha+10]. Thanks to the Dutch graphic artist M. C. Escher two-dimensional space groups even made their way into art and graphic design; see Schattschneider [GS87; SE05].

1.2 Geometric properties

For a space group Γ of $\mathbb{R}^n$, the ***Dirichlet–Voronoi domain*** of a point $a \in \mathbb{R}^n$ is defined as

$$\mathrm{DV}_\Gamma(a) = \big\{x \in \mathbb{R}^n : \mathrm{d}(x, a) < \mathrm{d}(x, \gamma(a)) \text{ for all } \gamma \in \Gamma - \mathrm{Stab}_\Gamma(a)\big\}.$$

If no confusion arises, we shorten this notation to $\mathrm{DV}(a)$.

Theorem 1.2.1. *Let $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$ be a space group and $a \in \mathbb{R}^n$. Then*

(i) $\mathrm{DV}(a)$ *is the interior of an n-dimensional convex polytope.*

(ii) *If* $\mathrm{Stab}_\Gamma(a) = \{1\}$*, then* $\mathrm{DV}(a)$ *is a fundamental domain for* Γ.

Proof. (i) For $\gamma \in \Gamma - \mathrm{Stab}_\Gamma(a)$ let H_γ be the hyperplane that orthogonally bisects the (nontrivial) segment $\overline{a\gamma(a)}$. Denote the open halfspace induced by H_γ containing a by H_γ^+. We have

$$\mathrm{DV}(a) = \bigcap_{\gamma \in \Gamma} H_\gamma^+.$$

The following argument shows that finitely many halfspaces in the above intersection are enough: Choose a fundamental domain F of Γ. F is bounded and we denote its diameter by $R = \mathrm{diam}(F)$. Consider the set

$$I = \big\{\gamma \in \Gamma : \mathrm{d}(a, \gamma(a)) \leq 2R\big\};$$

since Γ is discrete this set is finite. Now assume that there exists an isometry $\delta \in \Gamma - I$ such that H_δ is a supporting hyperplane of $\mathrm{DV}(a)$. Then there must be a ball B of radius $> 2R$ that contains only a and $\delta(a)$ on the boundary and no other points of $\Gamma(a)$ neither on the boundary nor in the interior. However, at least one tile of the tiling

$$\mathcal{T} = \big\{\gamma(\mathrm{cl}(F)) : \gamma \in \Gamma\big\}$$

is fully contained in B, which means that B cannot be empty – a contradiction. We thus have

$$\mathrm{DV}(a) = \bigcap_{\gamma \in I} H_\gamma^+,$$

so $\mathrm{DV}(a)$ is a polytope. And as the intersection of convex sets, $\mathrm{DV}(a)$ is also convex.

(ii) To show that $\mathrm{DV}(a)$ is a fundamental domain, first note that it is open (as the intersection of finitely many open sets) and connected (due to convexity). Furthermore, for any isometry $\gamma \in \Gamma$ we have

$$\begin{aligned}
&x \in \gamma(\mathrm{DV}(a)) \\
\Longleftrightarrow\ &\gamma^{-1}(x) \in \mathrm{DV}(a) \\
\Longleftrightarrow\ &\forall \delta \in \Gamma - \{1\} : \mathrm{d}(\gamma^{-1}(x), a) < \mathrm{d}(\gamma^{-1}(x), \delta(a)) \\
\Longleftrightarrow\ &\forall \delta \in \Gamma - \{1\} : \mathrm{d}(x, \gamma(a)) < \mathrm{d}(x, \gamma(\delta(a))) \\
\Longleftrightarrow\ &x \in \mathrm{DV}(\gamma(a))
\end{aligned}$$

Using the resulting equality $\gamma(\mathrm{DV}(a)) = \mathrm{DV}(\gamma(a))$, the packing and covering properties of a fundamental domain are imminent for $\mathrm{DV}(a)$. ☐

There is a close connection between fundamental domains, Dirichlet–Voronoi domains, and tilings of $\mathbb{R}^n$.

Definition 1.2.2. A ***tiling*** $\mathcal{T} = \{T_i : i = 1, 2, \ldots\}$ is a collection of closed n-dimensional topological balls which covers $\mathbb{R}^n$, such that

$$\forall\, T_i, T_j \in \mathcal{T} : \operatorname{int}(T_i) \cap \operatorname{int}(T_j) \neq \emptyset \quad \Longrightarrow \quad T_i = T_j.$$

The members $T_i \in \mathcal{T}$ are called ***tiles***. If all tiles are congruent to some fixed ***prototile*** $P \subset \mathbb{R}^n$, the tiling is called ***monohedral***. If the tiles are convex, the tiling is called a ***convex tiling***.

Every fundamental domain (that is topologically an open n-dimensional ball) yields a monohedral tiling of $\mathbb{R}^n$. From Theorem 1.2.1 we know that every Dirichlet–Voronoi fundamental domain gives a convex monohedral tiling where every tile is a polytope. The following implies the partial converse that every convex fundamental domain is automatically polytopal.

Proposition 1.2.3. *If $\mathcal{T}$ is a convex monohedral tiling with a bounded prototile P, then P must be an n-dimensional convex polytope.*

Proof. Fix a tile $T \in \mathcal{T}$, let B be a closed ball containing T, and consider the compact set $N = T + B$. All neighbors of T are contained in N, and since N is of finite volume, there are at most finitely many neighbors $T_1, \ldots, T_m$. By the separation theorems from convex geometry (see [Gru07, Chap. 4]), T can be pairwise separated by hyperplanes from $T_1, \ldots, T_m$. Therefore must T be a convex polytope, and so is P. □

Definition 1.2.4. We define the ***symmetry group*** of a tiling $\mathcal{T}$ as

$$\operatorname{Sym}(\mathcal{T}) = \big\{\alpha \in \operatorname{Isom}(\mathbb{R}^n) : \alpha(\mathcal{T}) = \mathcal{T}\big\}.$$

The tiling $\mathcal{T}$ is ***isohedral*** if $\operatorname{Sym}(\mathcal{T})$ is acting transitively on $\mathcal{T}$. Let S be the prototile of an isohedral tiling.

(i) If S is convex, we call this polytope a ***stereohedron***.

(ii) If S is also a Dirichlet–Voronoi domain of a space group, we call it a ***Dirichlet–Voronoi stereohedron***.

In place of Dirichlet–Voronoi stereohedron also *DV-stereohedron* and *plesiohedron* are used.

Remark 1.2.5. Every isohedral tiling is monohedral. The symmetry group of an isohedral tiling is a space group.

Not all stereohedra are DV-stereohedra. However, it seems to be an open problem if every combinatorial type of a stereohedron can be realized as a DV-stereohedron. Grünbaum & Shephard [GS80, p. 965f.] write about this problem that “there seems to be no grounds to assume that all stereohedra are combinatorially equivalent to plesiohedra.” As Santos noted, such a conjecture would be a vast generalization of Voronoi’s conjecture about Dirichlet–Voronoi domains of *lattices* (see [Gru07, Sect. 32.3] for more information about this conjecture). In Chapter 2 we will investigate three-dimensional Dirichlet–Voronoi stereohedra for orthogonal space groups in detail.

Even though not much is known about possible combinatorial types of stereohedra, we have the following result by Delone [Del61; Što75] that bounds the number of facets.

Theorem 1.2.6. *Let Γ be a space group of $\mathbb{R}^n$ with lattice L and set $h = |\Gamma/L|$. If S is a stereohedron for Γ, then*

$$f_{n-1}(S) \leq 2^n(h+1) - 2. \tag{1.1}$$

More precisely, if $\Gamma_S \leq \Gamma$ is the subgroup of isometries that are symmetries of S, then there is an injection $\Gamma_S \rightarrowtail \Gamma/L$ and for $h' = h/|\Gamma_S|$ we have

$$f_{n-1}(S) \leq 2^n(h'+1) - 2. \tag{1.2}$$

Proof. It is enough to prove (1.2). We will dissect the tiling

$$\mathcal{T} = \big\{\gamma(S) : \gamma \in \Gamma\big\}$$

in the following way: Let $\gamma_1, \ldots, \gamma_h \in \Gamma$ be a transversal of L in Γ. Then by definition

$$\Gamma = \bigcup_{i=1}^{h} L\gamma_i,$$

and we define a ***class*** of the dissection as

$$\mathcal{T}_i = \big\{\tau\gamma_i(S) : \tau \in L\big\}.$$

If $\gamma_i = \gamma_j\delta$ for some $\delta \in \Gamma_S$, we have $\mathcal{T}_i = \mathcal{T}_j$. We thus have h' different classes and without loss of generality we can assume $S \in \mathcal{T}_1$.

Two tiles of $\mathcal{T}$ are called ***neighbors*** if each one has a facet such that the relative interiors of these facets intersect. The bound (1.2) is implied by

(i) #(neighbors of S in $\mathcal{T}_1$) $\leq 2^{n+1} - 2$, and

(ii) #(neighbors of S in $\mathcal{T}_i$) $\leq 2^n$ for $i = 2, \ldots, h'$.

Since $\mathcal{T}_1$ is a lattice packing of S, the first bound follows from a result of Minkowski [Min61] as it is presented by Gruber [Gru07, p. 470; GL87]. The second result we will prove now.

Assume that S has more than 2^n neighbors in $\mathcal{T}_i$ for some $i \in \{2, \ldots, h'\}$. The barycenters of the tiles in $\mathcal{T}_i$ yield a point lattice. Choose one of the points as the origin and fix a lattice basis for the point lattice. With respect to this basis all barycenters are integer linear combinations. Reduce the integer coefficients of the barycenters of all neighbors of S in $\mathcal{T}_i$ modulo 2. Since by assumption there are more than 2^n neighbors, there will be two neighbors S_1 and S_3 whose barycenters are equal after reduction. This means that the lattice vectors t from the barycenter of S_1 to the barycenter of S_3 has even coordinates. Hence, $\frac{1}{2}t$ is also a lattice translation corresponding to a tile S_2 in $\mathcal{T}_i$.

The rest of the argument is best followed by keeping the schematic in Figure 1.2 in mind. Let A_1 be the facet of S_1 and A the facet of S whose relative interiors intersect; and, similarly, let B_3 be the facet of S_3 and B the facet of S whose relative interiors also intersect. We can then choose points

$$a_1 \in \operatorname{relint}(A_1) \cap \operatorname{relint}(A) \quad \text{and} \quad b_3 \in \operatorname{relint}(B_3) \cap \operatorname{relint}(B)$$

and define further points

$$a_2 = a_1 + \frac{1}{2}t \in S_2, \quad a_3 = a_1 + t \in S_3, \quad b_1 = b_3 - t \in S_1, \quad b_2 = b_3 - \frac{1}{2}t \in S_2.$$

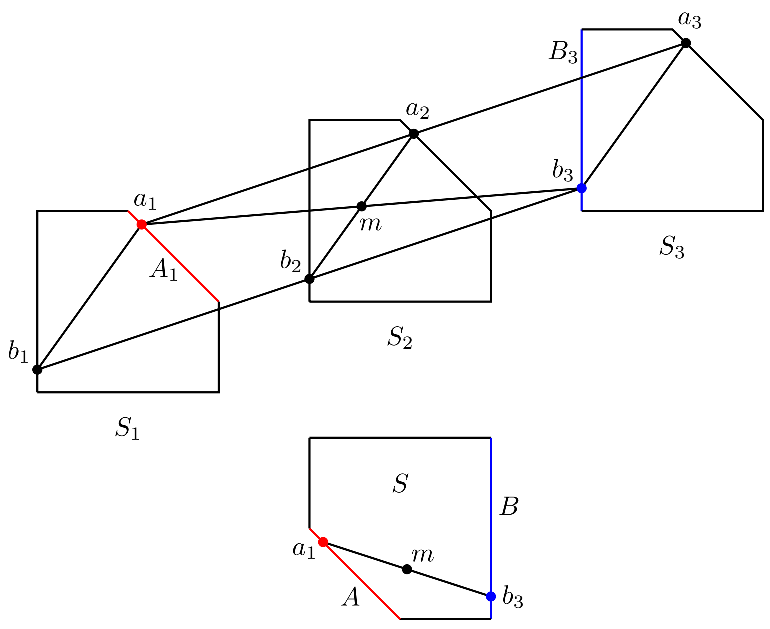


Figure 1.2: The blue dots in the two figures are the same, and similarly for the two red dots.

In the parallelogram $\text{conv}(a_1, a_3, b_3, b_1)$ the segments $\overline{a_1 b_3}$ and $\overline{a_2 b_2}$ intersect in their common midpoint m. Since m lies in the interiors of S_2 and S, we must have $S_2 = S$. This is impossible by the assumption $S \notin \mathcal{T}_i$ for $i = 2, \ldots, h'$. We therefore have at most 2^n neighbors. □

Remark 1.2.7. Tarasov [Tar97] gave a slightly improved bound. He denotes by H the maximal order of $|\Gamma/L|$ for an n-dimensional space group with lattice L and showed that $f_{n-1} \leq 2^n(H - 1/2) - 2$.

For a fixed space group Γ, all fundamental domains are of equal volume.

Proposition 1.2.8. *If Γ is a space group of $\mathbb{R}^n$ and P, Q are fundamental domains of Γ, then* $\text{vol}(P) = \text{vol}(Q)$*.*

Proof. For $\gamma \in \Gamma$, set $P_\gamma = \gamma(\text{cl}(Q)) \cap \text{cl}(P)$. Since both $\text{cl}(P)$ and $\text{cl}(Q)$ are compact, there are only finitely many elements $\gamma_1, \ldots, \gamma_m \in \Gamma$ with $P_{\gamma_i} \neq \emptyset$. Given that P is a fundamental domain, the family $(\gamma_i^{-1}(P_{\gamma_i}))$ must be a dissection of $\text{cl}(Q)$. We therefore get

$$\text{vol}(P) = \sum_{i=1}^{m} \text{vol}(P_{\gamma_i}) = \sum_{i=1}^{m} \text{vol}(\gamma_i^{-1}(P_{\gamma_i})) = \text{vol}(Q).$$

This proves the proposition. □

Remark 1.2.9. The proof even shows that the closures of any two fundamental domains are ***scissors-congruent***; see [Dup12].

The following result is much more general. We denote the volume of a fundamental domain of a space group Γ of $\mathbb{R}^n$ by $\mathrm{vol}(\mathbb{R}^n/\Gamma)$.

Theorem 1.2.10 ([Rat06, Theorem 6.7.3])**.** *If $\Gamma_1 \leq \Gamma_2 \leq \mathrm{Isom}(\mathbb{R}^n)$ are space groups, then*

$$\mathrm{vol}(\mathbb{R}^n/\Gamma_1) = [\Gamma_1 : \Gamma_2]\,\mathrm{vol}(\mathbb{R}^n/\Gamma_2).$$

Fundamental domains of space groups are models of the action's orbit space in the following sense. For a fundamental domain F, let $\mathrm{cl}(F)/\Gamma$ be the set

$$\mathrm{cl}(F)/\Gamma = \big\{\Gamma(x) \cap \mathrm{cl}(F) : x \in \mathrm{cl}(F)\big\}.$$

This is a partition of the subspace $\mathrm{cl}(F)$ and can thus be itself topologized via the quotient topology. The resulting space is homeomorphic to the orbit space $\mathbb{R}^n/\Gamma$.

Proposition 1.2.11. *If F is a fundamental domain for a space group $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$, then*

$$\Phi : \mathrm{cl}(F)/\Gamma \longrightarrow \mathbb{R}^n/\Gamma, \qquad \Gamma(x) \cap \mathrm{cl}(F) \longmapsto \Gamma(x)$$

is a homeomorphism.

Proof. We will show that Φ is a bijective, continuous, open map. The first two properties are almost immediate: If $\Gamma(x) = \Gamma(y)$, then clearly

$$\Gamma(x) \cap \mathrm{cl}(F) = \Gamma(y) \cap \mathrm{cl}(F)$$

from which we get injectivity. For any orbit $\Gamma(x)$, we can find $\gamma \in \Gamma$ with $x \in \gamma(\mathrm{cl}(F))$, i.e., $\gamma^{-1}(x) \in \mathrm{cl}(F)$ and thus

$$\Phi(\Gamma(\gamma^{-1}(x)) \cap \mathrm{cl}(F)) = \Phi(\Gamma(x) \cap \mathrm{cl}(F)) = \Gamma(x).$$

So Φ is also surjective. Continuity is implied by the commutative diagram

$$\begin{array}{ccc} \mathrm{cl}(F) & \overset{i}{\hookrightarrow} & \mathbb{R}^n \\ \downarrow{\scriptstyle p} & & \downarrow{\scriptstyle q} \\ \mathrm{cl}(F)/\Gamma & \overset{\Phi}{\longrightarrow} & \mathbb{R}^n/\Gamma, \end{array}$$

where p and q are quotient maps, and the fact that p is an open map. The last claim follows from $p^{-1}(p(U)) = \bigcup_{\gamma\in\Gamma} \gamma(U)$ for all sets $U \subseteq \mathrm{cl}(F)$.

To show openness of Φ, choose any open subset $U \subseteq \mathrm{cl}(F)/\Gamma$. Then $p^{-1}(U)$ is open in $\mathrm{cl}(F)$, i.e., there exists an open set $V \subseteq \mathbb{R}^n$ such that $p^{-1}(U) = \mathrm{cl}(F) \cap V$. Setting

$$W = \bigcup_{\gamma\in\Gamma} \gamma(\mathrm{cl}(F) \cap V),$$

we get

$$q(W) = q(\mathrm{cl}(F) \cap V) = qi(\mathrm{cl}(F) \cap V) = \Phi p(\mathrm{cl}(F) \cap V) = \Phi(U).$$

Since for any (open) set $O \subseteq \mathbb{R}^n$, we again have $q^{-1}(q(O)) = \bigcup_{\gamma\in\Gamma} \gamma(O)$, the map q is open and thus we only need to prove openness of W.

To this end choose any $w \in W$. We actually may assume that $w \in \operatorname{cl}(F) \cap V$, because $\gamma(W) = W$ for all $\gamma \in \Gamma$. Fix $r > 0$. Since F is a fundamental domain, only finitely many members of $\{\gamma(\operatorname{cl}(F)) : \gamma \in \Gamma\}$ meet $\mathrm{B}(w, r)$, say, $\gamma_1(\operatorname{cl}(F)), \ldots, \gamma_m(\operatorname{cl}(F))$. We have

$$\mathrm{B}(w, r) \subseteq \bigcup_{i=1}^{m} \gamma_i(\operatorname{cl}(F)). \tag{1.3}$$

If $\gamma_i(\operatorname{cl}(F))$ does not contain w, then $\mathrm{B}(w,r) - \gamma_i(\operatorname{cl}(F))$ is an open neighborhood of w. In this case we shrink r to avoid $\gamma_i(\operatorname{cl}(F))$. We therefore may assume that each $\gamma_i(\operatorname{cl}(F))$ contains w, or, put differently, that $\gamma^{-1}(w) \in \operatorname{cl}(F)$ for $i = 1, \ldots, m$. Applying q yields $q(\gamma_i^{-1}(w)) = q(w) \in q(\operatorname{cl}(F) \cap V) = U$, which in turn implies

$$\gamma_i(w) \in q^{-1}(U) = \operatorname{cl}(F) \cap V.$$

This means that $w \in \gamma_i(V)$ for $i = 1, \ldots, m$. Possibly further shrinking of r yields

$$\mathrm{B}(w, r) \subseteq \bigcap_{i=1}^{m} (\gamma_i(V)). \tag{1.4}$$

From (1.3) and (1.4) we can deduce $\mathrm{B}(w, r) \subseteq W$. W is thus open and Φ must be a homeomorphism. □

The orbit space of a space group can not only be considered as a (topological) quotient space but it can also be endowed with a metric in the following way: Given two orbits $\Gamma(x), \Gamma(y)$, we can define the distance function

$$\mathrm{D}(\Gamma(x), \Gamma(y)) = \inf\left\{\mathrm{d}(x', y') : x' \in \Gamma(x), y' \in \Gamma(y)\right\}$$

on $\mathbb{R}^n/\Gamma$. It is laborious but not difficult to show that $(\mathbb{R}^n/\Gamma, \mathrm{D})$ is in fact a metric space. If $\Gamma(x)$ is a point of this metric space it can be shown further that there exists a ball $\mathrm{B}_{\mathrm{D}}(\Gamma(x), r)$ in $\mathbb{R}^n/\Gamma$ which is isometric to the quotient space $\mathrm{B}(x, r)/\operatorname{Stab}_\Gamma(x)$. Details of this construction are given in Bonahon [Bon09].

We will end with topological and geometric characterizations of space groups, which we state without proof.

Theorem 1.2.12. *Let* Γ *be a discrete subgroup of* $\operatorname{Isom}(\mathbb{R}^n)$. *Then the following are equivalent:*

(i) Γ *is a space group.*

(ii) *The orbit space* $\mathbb{R}^n/\Gamma$ *is compact.*

(iii) *The group* $\operatorname{Isom}(\mathbb{R}^n)/\Gamma$ *is compact.*

Remark 1.2.13. A group action of a topological group on a topological space is called ***cocompact*** if the orbit space is compact. Often the group itself is called cocompact. Thus, (ii) could be rephrased as saying that a space group is a discrete, cocompact subgroup of $\operatorname{Isom}(\mathbb{R}^n)$.

1.3 Algebraic properties

From Bieberbach's Theorem 1.1.5 we know that the subgroup of all translations in a space group Γ forms a lattice L of full rank such that the ***(crystallographic) point group*** $P = \Gamma/L$ is finite. (Another name for point group is ***holonomy group***.) Assuming this result, we will now give a concise introduction to algebraic aspects of space groups. We assume familiarity with terminology from homological algebra and a few basic facts from group cohomology that are summarized in Appendix A. Further details can be found in [Rot95; Rot09; Rot10]. If not stated otherwise, we will always assume that Γ is a space group of $\mathbb{R}^n$ with lattice L and point group P.

Proposition 1.3.1. *Let Γ be a space group of $\mathbb{R}^n$. The lattice L is a normal subgroup and the point group P acts on L faithfully by conjugation.*

Proof. Choose an arbitrary element $(A, a) \in \Gamma$. We then have for all $(I, t) \in L$

$$(A, a)(I, t)(A, a)^{-1} = (I, At), \tag{1.5}$$

which is a pure translation and therefore an element of L again. This already shows normality and that P acts on the lattice by conjugation. Since L is of rank n and thus contains a basis of $\mathbb{R}^n$, the above equality also shows that only the identity element of P acts trivially on L. □

As a semidirect product, $\mathrm{Isom}(\mathbb{R}^n) = \mathrm{O}(n) \ltimes \mathbb{R}^n$ comes with the projection

$$\pi : \mathrm{O}(n) \ltimes \mathbb{R}^n \to \mathrm{O}(n), \quad (A, a) \mapsto A \tag{1.6}$$

for which we have $\pi(\Gamma) \cong \Gamma/\ker(\pi) = \Gamma/L$. The point group can hence be identified with the group of all linear parts of Γ. By (1.5), every linear part maps lattice vectors again to lattice vectors. This means that if we represent Γ with respect to a lattice basis of L, the lattice becomes $\mathbb{Z}^n$ and the point group is a finite subgroup of $\mathrm{GL}(n, \mathbb{Z})$. In other words, Γ can be understood as a group extension of $\mathbb{Z}^n$ by a finite unimodular group P that acts faithfully on $\mathbb{Z}^n$. Zassenhaus proved the converse, namely that every such extension is isomorphic to a space group.

Theorem 1.3.2 (Zassenhaus [Zas48])**.** *Let $P \leq \mathrm{GL}(n, \mathbb{Z})$ be a finite group and consider $\mathbb{Z}^n$ as a P-module with the natural action of P on $\mathbb{Z}^n$. Every extension G of $\mathbb{Z}^n$ by P that "realizes the operators" (see Appendix A) is isomorphic to an n-dimensional space group.*

Proof. Let

$$0 \longrightarrow \mathbb{Z}^n \xrightarrow{\ i\ } G \xrightarrow{\ \pi\ } P \longrightarrow 1$$

be an extension that realizes the operators. We will construct a space group $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$ and provide an explicit isomorphism $G \cong \Gamma$. For this purpose choose a basis of $\mathbb{R}^n$ such that $P \leq \mathrm{O}(n)$; this is possible, for details see Berger [Ber09a, Theorem 8.2.5]. Pick a transversal $g_1, \ldots, g_m \in G$ of $\mathbb{Z}^n$ in G such that $\pi(g_i) = A_i \in P$. For arbitrarily chosen $a_1, \ldots, a_m \in \mathbb{R}^n$ define a mapping

$$\Psi : G = \bigcup_{i=1}^{m} g_i\mathbb{Z}^n \to \mathrm{Isom}(\mathbb{R}^n), \qquad g_i t \mapsto (A_i, a_i). \tag{1.7}$$

In general Ψ will not be a homomorphism. For $A_i, A_j \in P$ with $A_iA_j = A_k$ we have

$$(A_i, a_i)(A_j, a_j) = (A_iA_j, A_ia_j + a_i) = (A_k, a_k + t_{ij}) = (I, t_{ij})(A_k, a_k)$$

for some $t_{ij} \in \mathbb{R}^n$. This implies

$$(I, t_{ij}) = (A_i, a_i)(A_j, a_j)(A_k, a_k)^{-1}$$

and induces a mapping

$$f : P \times P \to \mathbb{R}^n, \qquad (A_i, A_j) \mapsto t_{ij}.$$

An arduous calculation shows that f satisfies the cocycle identity and is thus an element of $Z^2(P, \mathbb{R}^n)$. From Lemma A.1 in Appendix A we know that $Z^2(P, \mathbb{R}^n) = B^2(P, \mathbb{R}^n)$, and hence there exists a function $h : P \to \mathbb{R}^n$ satisfying the coboundary identity

$$f(A_i, A_j) = A_ih(A_j) - h(A_iA_j) + h(A_i).$$

Replace each a_i by $a_i - h(A_i)$ in (1.7). This turns Ψ into a homomorphism, which is bijective by construction. □

So every space group corresponds to an element of the second cohomology group $H^2(P, \mathbb{Z}^n)$ and vice versa. However, two different elements of the cohomology group might correspond to isomorphic space groups. The following theorem shows how to partition $H^2(P, \mathbb{Z}^n)$ into classes of nonisomorphic groups.

Theorem 1.3.3. *Let $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$ be a space group with lattice $\mathbb{Z}^n$ and point group $P \leq \mathrm{GL}(n, \mathbb{Z})$. The normalizer N of P in $\mathrm{GL}(n, \mathbb{Z})$ acts on $H^2(P, \mathbb{Z}^n)$. There exists a bijective correspondence between the isomorphism classes of extensions and the orbits of the action.*

Proof. Consider $\mathbb{R}^n$ as a P-module with the natural action of P on $\mathbb{R}^n$. Lemma A.1 of Appendix A implies that

$$H^1(P, \mathbb{R}^n) = H^2(P, \mathbb{R}^n) = 0.$$

The long exact cohomology sequence (A.2) of the short exact sequence

$$0 \longrightarrow \mathbb{Z}^n \longrightarrow \mathbb{R}^n \longrightarrow \mathbb{R}^n/\mathbb{Z}^n \longrightarrow 0$$

of P-modules yields

$$H^1(P, \mathbb{R}^n/\mathbb{Z}^n) \cong H^2(P, \mathbb{Z}^n).$$

It is therefore sufficient to define the group action and establish the correspondence for the first cohomology group. To this end choose a derivation $d : P \to \mathbb{R}^n/\mathbb{Z}^n$ from $H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$. We can then define a space group associated to it by setting

$$\Gamma = \big\{(A, d(A) + t) : A \in P \text{ and } t \in \mathbb{Z}^n\big\}.$$

It follows immediately from the defining property of a derivation that Γ is a space group indeed.

By Bieberbach's Theorem 1.1.5 are two space groups Γ, Γ' isomorphic if and only if there exists an affine mapping (B, b) with $\Gamma' = (B, b)\Gamma(B, b)^{-1}$. Since

$$(B, b)(A, d(A) + t)(B, b)^{-1} = (BAB^{-1}, -BAB^{-1}b + Bd(A) + Bt + b),$$

two derivations $d, d' \in H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$ induce isomorphic space groups if and only if for all $A \in P$

$$BAB^{-1} \in P \quad \text{and} \quad d'(A) = -BAB^{-1}b + Bd(A) + b \equiv Bd(A),$$

where "$\equiv$" denotes equality in $H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$. Put differently, we must have $B \in N$ and $d'(A) = Bd(A)$ under the induced action

$$N \times H^1(P, \mathbb{R}^n/\mathbb{Z}^n) \to H^1(P, \mathbb{R}^n/\mathbb{Z}^n), \quad (B, d) \mapsto (A \mapsto Bd(A)).$$

This establishes the bijective correspondence between orbits and isomorphism classes. □

All space groups are finitely presented: This is a corollary of the following more general theorem.

Theorem 1.3.4 ([Joh97, Chap. 10]). *Let $K = \langle X \mid R \rangle$ and $Q = \langle Y \mid S \rangle$ be finitely presented groups. If Γ is a group extension of K by Q*

$$1 \longrightarrow K \xrightarrow{\ i\ } \Gamma \xrightarrow{\ \pi\ } Q \longrightarrow 1,$$

then Γ is also finitely presented.

Corollary 1.3.5. *Every space group is finitely presented.*

Proof. Since every lattice L in $\mathbb{R}^n$ is isomorphic to a free abelian group with basis $X = \{x_1, \ldots, x_n\}$, it is finitely presented as

$$L \cong \langle X \,|\, x_i x_j x_i^{-1} x_j^{-1} = 1 \text{ for all } x_i, x_j \in X \rangle.$$

Furthermore, all point groups are finite and therefore in particular finitely presented. □

The proof of Theorem 1.3.4 is constructive. Yet another method to obtain finite presentations for space groups is by means of Poincaré's Theorem: Given a fundamental domain one calculates so-called cycle and side-pairing relations, which yield a finite presentation. Nice discussions of Poincaré's theorem can be found in Iversen [Ive90] and Ratcliffe [Rat06].

Remark 1.3.6. Finite presentations for space groups can be calculated with the GAP package Cryst [EGN13].

The above Corollary 1.3.5 of course implies in particular that space groups are finitely generated and of countable cardinality. Thus it makes sense to ask for an upper bound on the size of the smallest generating set for n-dimensional space groups. Why would that be interesting? Consider the following situation: Assume we are given an n-dimensional flat manifold like the torus T^n, and we are wondering what finite groups can act freely on it. If F is such a finite group, then $M^n = T^n/F$ is a manifold as well and we have the sequence

$$1 \longrightarrow \pi_1(T^n) \longrightarrow \pi_1(M^n) \longrightarrow F \longrightarrow 1.$$

$\pi_1(M^n)$ is (isomorphic) to an n-dimensional Bieberbach group. Thus a bound on the number of generators of $\pi_1(M^n)$ restricts the possibilities for F.

It is generally believed that the number of generators of a space group in dimension n is bounded by $2n$, while the minimal number of generators of an n-dimensional Bieberbach group is conjectured to be just n.

Example 1.3.7. One can easily see that if the bounds are correct, they are sharp. From Example 1.1.4 we know that in dimension $n = 1$, there are two space groups, namely the Bieberbach group $\mathbb{Z}$ and the infinite dihedral group $\mathbb{Z}_2 \ltimes \mathbb{Z}$ (where $\mathbb{Z}_2$ acts nontrivially on $\mathbb{Z}$). Of course $\mathbb{Z}$ is generated by one element, while the latter group is not torsion-free and thus cannot be generated by just a single element. However, it has the presentation $\langle x, y \mid x^2 = y^2 = 1\rangle$; see Robinson [Rob96, p. 51].

In the following theorem we list all bounds on the number of generators known to us.

Theorem 1.3.8. (i) *The minimal number of generators of an n-dimensional Bieberbach group is bounded by $\leq \sqrt{2n\pi}\, 2^{n-2}$.*

(ii) *Let $\Gamma \leq \mathbb{R}^n$ be a space group such that its point group is a p-group. Furthermore, denote by β_1 the rank of the abelian group $\Gamma/[\Gamma,\Gamma]$ and let $a = 2$ if $p \leq 19$ and $a = 3$ otherwise. Then the minimal number of generators of Γ is bounded by $a(n - \beta_1)/(p - 1) + \beta_1$.*

Pointers to proofs. (i) This bound was proved by Gromov for the minimal number of generators of fundamental groups of general negatively curved n-manifolds; see [Mey89, p. 21] for an exposition.

(ii) This result can be found in Adem et al. [Ade+12, Theorem A]. See Dekimpe & Penninckx [DP09] for slightly weaker results. □

Remark 1.3.9. Closely related to the above discussion is the notion of *growth type* of a finitely generated group. Let S be a finite generating set of a group Γ. The *word length* $\ell_S(\gamma)$ of an element $\gamma \in \Gamma$ is defined to be the smallest n for which there exists $s_1, \ldots, s_n \in S \cup S^{-1}$ such that $\gamma = s_1 \cdots s_n$. One defines for a pair (Γ, S) the *growth function* to be

$$\beta_{(\Gamma,S)} : \mathbb{N} \longrightarrow \mathbb{N}, \qquad k \longmapsto \beta_{(\Gamma,S)}(k) = \#\{\gamma \in \Gamma : \ell_S(\gamma) \leq k\}.$$

One can now define groups of *exponential growth*, *intermediate growth*, or *polynomial growth*, depending on the type of growth function the groups possess.

A famous theorem by Gromov [Gro81] states that a group is of polynomial growth if and only if it is *virtually nilpotent*, that is, if it has a nilpotent[2] subgroup of finite index. In particular every abelian group is nilpotent; thus, every space group is of polynomial growth.

We will continue with a few structural results about space groups, beginning with their subgroups. Of course not every subgroup of a space group is again a space group – some of them are finite – but the large ones are. The following proposition is a direct consequence of Bieberbach's Theorem 1.1.5.

[2]If G is a group, the ***upper central series***

$$1 = Z_0 \leq Z_1 \leq \ldots \leq Z_{n-1} \leq Z_n \leq \ldots$$

is a sequence of subgroups of G, where each Z_n is defined by $Z_n = \{g \in G \mid \forall h \in G : [g,h] \in Z_{n-1}\}$. G is called ***nilpotent*** if $Z_n = G$ for some n. Nilpotent groups are "almost abelian."

Proposition 1.3.10. *Assume* $\Gamma_2 \leq \Gamma_1 \leq \mathrm{Isom}(\mathbb{R}^n)$ *with* $[\Gamma_1 : \Gamma_2] < \infty$*. Then* Γ_1 *is a space group if and only if* Γ_2 *is a space group.*

The lattice of a space group is a maximal abelian subgroup.

Proposition 1.3.11. *Let* Γ *be a space group of* $\mathbb{R}^n$ *and let* L *be its lattice. Then* L *is maximal abelian.*

Proof. Assume that there exists an abelian subgroup M of Γ with $L < M$. Choose $\gamma \in M - L$ and consider the sequence

$$0 \longrightarrow L \xrightarrow{\ i\ } \Gamma \xrightarrow{\ \pi\ } \Gamma/L \longrightarrow 1.$$

From (1.6) we know that Γ/L can be identified with P, and Proposition 1.3.1 shows that P acts faithfully on L. However, if $\Psi : P \to \mathrm{Aut}(L)$ denotes the action, we have the contradiction $\Psi(\pi(\gamma)) = \Psi(1)$. □

The previous theorem has the following nice corollary.

Corollary 1.3.12. *Any abelian space group is a lattice.*

Two subgroups of a group whose intersection is of finite index in both of them are called ***commensurable***. Commensurability is an equivalence relation in the set of all subgroups of a group.

Theorem 1.3.13 ([VGS00, Chap. 1, Prop. 1.10])**.** *Let* Γ_1 *and* Γ_2 *be subgroups of* $\mathrm{Isom}(\mathbb{R}^n)$*, and suppose that their intersection has finite index in both groups. If one of the groups is a space group then so is the other.*

Proposition 1.3.14. *For every space group* Γ*, the center* $\mathrm{Z}(\Gamma)$ *consists of translations.*

Proof. Let $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$ be a space group and

$$\tau_1 = (I, t_1), \ldots, \tau_n = (I, t_n)$$

be a lattice of its basis. For $(A, a) \in \mathrm{Z}(\Gamma)$ we have

$$(I, t_i)(A, a) = (A, t_i + a) \qquad (A, a)(I, t_i) = (A, At_i + a)$$

for every $i = 1, \ldots, n$. Since the lattice is of rank n, however, we must have $A = I$. □

Proposition 1.3.15. *Every space group has only finitely many conjugacy classes of finite subgroups.*

Proof. Let Γ be a space group of $\mathbb{R}^n$ and let $\mathrm{DV}(a) \subset \mathbb{R}^n$ be the Dirichlet–Voronoi domain for some point $a \in \mathbb{R}^n$. If $H \leq \Gamma$ is a finite subgroup, all its isometries fix a common point $x \in \mathbb{R}^n$ (see Yale [Yal68, Theorem 3.5]). Let $\gamma \in \Gamma$ be an isometry, such that $y = \gamma(x) \in \mathrm{DV}(a)$. We then have for all $\delta \in H$, that $\gamma\delta\gamma^{-1}(y) = y$, i.e., H is conjugate to a group of isometries from the set

$$\mathcal{I} = \{\alpha \in \Gamma : \mathrm{cl}(\mathrm{DV}(a)) \cap \alpha(\mathrm{cl}(\mathrm{DV}(a))) \neq \emptyset\}.$$

We will next show that $\mathcal{I}$ is finite, which yields the desired result. Let B be an enclosing ball of $\mathrm{DV}(a)$. Since $\Gamma(a)$ is a discrete set, all but finitely many of the (open) halfspaces defining $\mathrm{DV}(a)$ will contain B. Since $\mathrm{cl}(\mathrm{DV}(a)) \cap \mathrm{cl}(\alpha(\mathrm{DV}(a)))$ will be nonempty if their separating hyperplane induces a halfspace, that does not contain B in its interior, we have $\mathcal{I} < \infty$. □

Every space group can be embedded into another space group of the same dimension, such that the index is finite and such that the supergroup is of particularly simple structure.

Theorem 1.3.16 (Ratcliffe [Rat06])**.** *Let Γ be a space group of $\mathbb{R}^n$ with lattice L and point group P of order m. Then Γ embeds into the semidirect product $\Gamma^* = P \ltimes \frac{1}{m}L$. The supergroup Γ^* is also a space group of $\mathbb{R}^n$ for which we have that $[\Gamma^* : \Gamma] = m^n$.*

Remark 1.3.17. The group Γ^* in the theorem above is called the ***splitting group*** of Γ.

Since the point group P of an n-dimensional space group is conjugate to a subgroup of $\mathrm{O}(n)$ as well as to a subgroup of $\mathrm{GL}(n, \mathbb{Z})$, there exists a restriction on the order of the elements of P. This can be seen as follows: On the one hand, every element $A \in P$ is similar to a matrix of the form

$$A \sim \begin{bmatrix} R_1 & & & & \\ & \ddots & & & \\ & & R_k & & \\ & & & I_\ell & \\ & & & & -I_m \end{bmatrix} \quad \text{with} \quad R_i = \begin{bmatrix} \cos(\phi_i) & -\sin(\phi_i) \\ \sin(\phi_i) & \cos(\phi_i) \end{bmatrix}.$$

This is a result that dates back to Schläfli [Sch66]. On the other hand, the characteristic polynomial $\chi_A(t) \in \mathbb{Z}[t]$ has integer coefficients only. Together this yields, for example, for $n = 2, 3$ that the only possible orders for a lattice symmetry A are

$$\mathrm{ord}(A) = 1, 2, 3, 4, 6.$$

A more general result in this direction was proved by Hiller [Hil85]; see also Baake & Grimm [BG13]. It is best formulated using the ***additive Euler totient function*** $\phi_a : \mathbb{N} \to \mathbb{Z}$ defined as follows:

$$\phi_a(m) = \begin{cases} 0 & m = 1 \\ \phi(p^r) & m = p^r \text{ with } p \text{ prime and } r \geq 1 \\ \phi_a(k) & m = 2k \text{ with } k > 1 \text{ odd} \\ \phi(2^r) + \phi_a(k) & m = 2^r k \text{ with } k > 1 \text{ odd and } r \geq 2 \\ \phi_a(k) + \phi_a(\ell) & m = kl \text{ odd with } k, l > 1 \text{ coprime} \end{cases}$$

Here ϕ denotes the usual Euler totient function.

Theorem 1.3.18. *Let $\Gamma \leq \mathrm{Isom}(\mathbb{R}^n)$ be a space group with point group P. For every element $A \in P$ we have $n \geq \phi_a(\mathrm{ord}(A))$.*

Remark 1.3.19. This theorem is commonly called the ***crystallographic restriction***. The first few values of ϕ_a are

m	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$\phi_a(m)$	0	1	2	2	4	2	6	4	6	4	10	4	12	6	6

We will end by discussing the natural action of a space group and the action of point groups on lattices.

Proposition 1.3.20. *A space group is torsion-free if and only if it acts freely on $\mathbb{R}^n$.*

Proof. ($\Rightarrow$) Assume $\gamma(x) = x$ for some $\gamma \in \Gamma$ and $x \in \mathbb{R}^n$. If we choose the origin to be in x, we get $\gamma \in G = \Gamma \cap \mathrm{O}(n)$. G is a discrete subgroup of a compact group and therefore finite. Hence, G must be trivial and the action has to be free.

($\Leftarrow$) Choose an element $\gamma \in \Gamma$ of finite order and consider $G = \langle \gamma \rangle$. Since this is a finite group of isometries, all elements must have a common fixed point. This implies that G is trivial and Γ therefore torsion-free. $\square$

Given a lattice and a finite group acting on it, how can one construct a space group that realizes this data? Assuming that we write a space group with respect to a basis of its lattice, the question boils down to the construction of a group with lattice $\mathbb{Z}^n$ and point group $P \leq \mathrm{GL}(n, \mathbb{Z})$. There is always an easy solution, namely

$$\Gamma = \big\{(A, a) : A \in P, a \in \mathbb{Z}^n\big\}.$$

This group is isomorphic to the semidirect product $P \ltimes \mathbb{Z}^n$. However, most space groups that realize the data are not semidirect products. Finding all other space groups with the given data involves solving so-called Frobenius congruences. All this is presented in a very accessible form in Souvignier [Sou08].

Theorem 1.3.21 (Auslander & Kuranishi [AK57]). *Given an arbitrary finite group G, there exists a Bieberbach group with point group isomorphic to G.*

Chapter 2

Dirichlet–Voronoi Stereohedra

In a convex monohedral tiling $\mathcal{T}$ of $\mathbb{R}^n$ all tiles are congruent to a convex n-dimensional polytope P, the prototile of $\mathcal{T}$. It is a long-standing open problem if the number of facets of P is bounded by a function depending just on the dimension n; see Brass et al. [BMP06, p. 177f]. For prototiles that are stereohedra we have Delone's bound. However, at least for DV-stereohedra this bound seems to be much too high. To get a more realistic estimate of how many facets a DV-stereohedron can have in $\mathbb{R}^3$, we are going to investigate in this chapter the tetragonal, trigonal, hexagonal, and cubic space groups with respect to what f-vectors their DV-stereohedra possess.

2.1 Setting the stage

Let us recall that a tiling $\mathcal{T} = \{T_i : i = 1, 2, \ldots\}$ is a collection of closed n-dimensional topological balls which covers $\mathbb{R}^n$; the members $T_i \in \mathcal{T}$ are called tiles and they intersect at most in their boundaries. If all tiles are congruent to some fixed prototile $P \subset \mathbb{R}^n$, the tiling is called monohedral.

The fundamental problem to determine all prototiles of monohedral tilings cannot realistically expected to be solved in this generality. It therefore is highly desirable to restrict considerations to convex monohedral tilings. However, even with this restriction prospects of a complete classification are gloomy. Already the case $n = 2$ is open and has an intricate history: Reinhardt's thesis [Rei18] was one of the first systematic investigations of tilings of the plane. Even though he explicitly writes about pentagonal and hexagonal prototiles:

> "Dabei wollen wir die Sechsecke vollständig, die Fünfecke jedoch nur so weit ins Auge fassen, als eine mit ihnen ausgeführte Bedeckung der Ebene ohne das Auftreten singulärer Ecken möglich ist." [Rei18, p. 66],

it was "known" for many years that he had classified *all* planar monohedral tilings. However, the first time a complete classification was actually claimed was only 45 years later by Heesch & Kienzle [HK63]. They applied a classification scheme developed by Heesch in 1932. But shortly afterwards Kershner [Ker68] discovered three more types of pentagonal tiles not included in their classification. Again, a complete classification was claimed, this time by Kershner. He did not include a proof since it "is extremely laborious and will be given elsewhere." Before it could appear Gardner [Gar75b] gave an exposition of Kershner's results prompting the reader Marjorie Rice to submit yet another pentagonal prototile not covered by Kershner's classification [Gar75a]. After that it seems no more claims about full classifications were made and new pentagonal tiles were found very recently by Mann et al. [MMV15].

Given that a full classification of convex monohedral prototiles has not even been achieved for the plane, it seems appropriate to consider more modest problems. A first step in this direction was made by Grünbaum & Shephard [GS77; GS78] by (successfully) classifying all isohedral planar tilings. Furthermore, a list of seven tiling problems (A) – (G) was presented by them in [GS80] of which problem (G) is the following:

(G) *Determine the least upper bound for the number of $(n-1)$-dimensional faces of convex polyhedra which are prototiles of monohedral tilings of $\mathbb{R}^n$.*

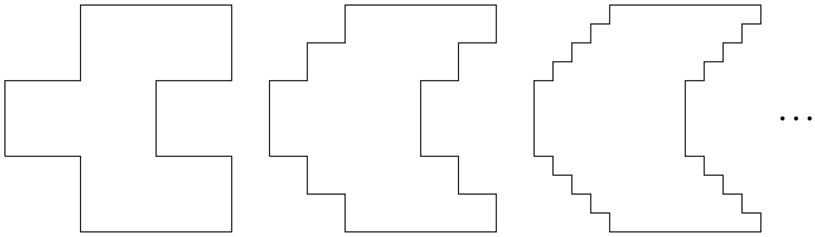
This problem is open for $n \geq 3$ and not much is known. It is not even clear that the number of facets can be bounded at all. We only have Delone's general bound for stereohedra (Theorem 1.2.6) and Tarasov's slight improvement (Remark 1.2.7). Current perception is that these bounds are much too high. We share this assessment and believe it to be supported by results in low dimensions listed in the following table.

dimension	# facets	Delone	Tarasov
$n = 2$	6	50	44
$n = 3$	≥ 38	390	378
$n = 4$	≥ 40	18 446	18 422

Lower bounds for problem (G) are almost always based on the construction of explicit Dirichlet–Voronoi stereohedra. Much research was conducted in this direction; details for the period before 1935 can be found in Nowacki [Now35] and references for later results are given in [Koc73] and [Eng86]. The current record stereohedron has 38 facets and was discovered by Engel [Eng81a]. His discoveries are based on preliminary work by Koch. In her thesis [Koc72], Koch described a fairly efficient way to calculate DV-stereohedra for space groups and did a lot of experiments in subsequent years. Since she lacked the necessary computing power to fully investigate the space group $\mathrm{IT}(214) = I4_132$, she told Engel about it on a conference who went on and used her algorithms, partial results, and the University of Bern's strong computing resources to find his example [Koc15]. In total he discovered four different combinatorial types with 38 facets. None of his presentations are fully rigorous, but we were able to confirm his results.

Starting in 2001, Santos et al. [BS01; BS06; SS08; SS11] studied the upper bound problem for Dirichlet–Voronoi stereohedra in great detail. They gave bounds for the maximal number of facets of DV-stereohedra that are in general much better than Delone's.

Let us conclude this overview by mentioning that if one lessens the restriction in (G), the number of facets is always unbounded. If *convexity* is not required, we have the following prototiles in $\mathbb{R}^2$ with f_1 unbounded.



Giving up monohedrality and only requiring all (convex and bounded) tiles to be of the same combinatorial type, is also not enough to bound the number of facets: For each $k \geq 3$ the plane admits a face-to-face tiling by convex k-gons, see [GS87]. And finally, giving up boundedness but keeping monohedrality and convexity allows for examples with arbitrarily many facets as discovered by Erickson & Kim [EK03].

2.2 Face vectors of DV-stereohedra

To get a realistic estimate of how many facets a DV-stereohedron can have in $\mathbb{R}^3$, we investigated the f-vectors of DV-stereohedra of the tetragonal, trigonal, hexagonal, and cubic space groups. Due to the enormous complexity of this task we decided to not also examine the triclinic, monoclinic, and orthorhombic groups. The triclinic ones are understood anyway (we quickly summarize the results below) and the monoclinic and orthorhombic groups will always yield stereohedra with less than 38 facets [BS01; BS06; SS08; SS11].

The space groups were examined by first fixing a fundamental domain F for a group $\Gamma \leq \mathrm{Isom}(\mathbb{R}^3)$ and then approximating F with an extremely fine point grid. For each point of the grid we then calculated the DV-stereohedron and its f-vector. Here it is important to note that not the whole fundamental domain has to be used but only a fundamental domain of the normalizer $\mathrm{N}(\Gamma)$ of Γ in $\mathrm{Isom}(\mathbb{R}^3)$. The reason for this is simple: For every $\alpha \in \mathrm{N}(\Gamma)$ and every $\beta \in \Gamma$ we have

$$\alpha(\beta(x)) = \beta(\alpha'(x)) \qquad \text{for } x \in \mathbb{R}^3 \text{ and some } \alpha' \in \mathrm{N}(\Gamma).$$

All normalizers of space groups were first calculated by the crystallographer Hirshfeld [Hir68] who did not know about the concept of normalizers. He christened these groups "Cheshire groups", a name that even nowadays can still be encountered. Hirshfeld's article is very short; more details were later given by Gubler [Gub82] and Fischer & Koch [FK83]. All normalizers can be found nicely presented in the International Tables [Hah05, Chap. 15]. The normalizer of a space group does not need to be a space group again. In fact, it does not even need to be a discrete group anymore.

The algorithm for computing the DV-stereohedron of a grid point $x \in F$ with respect to its orbit $\Gamma(x)$ very much depends on using an orthogonal sublattice L' of the space group's lattice $L \leq \Gamma$. Fortunately, the tetragonal, trigonal, hexagonal, and cubic groups are classified in such a way that it is always obvious which orthogonal lattice to use. We denote the basis of such a lattice by b_1', b_2', b_3' (it is worth mentioning that crystallographers normally call exactly the same basis a, b, c). If the normalizer of a space group is not a discrete group anymore, with a fundamental domain that is a lower-dimensional polytope, the directions that are "shrunken" by the normalizer will be denoted by $\varepsilon b_1'$, $\varepsilon b_2'$, or $\varepsilon b_3'$. For details on the algorithm see Appendix B.

Of course one has to wonder how useful such an approximation is with respect to finding a stereohedron with the most number of facets. An assessment can easily be derived from a result of Eggleston et al.: The set of all convex polytopes $\mathcal{P}$ can be turned into a metric space by introducing the Hausdorff metric

$$\delta(P,Q) = \max\big\{ \max_{x\in P}\min_{y\in Q} \mathrm{d}(x,y),\ \max_{y\in Q}\min_{x\in P} \mathrm{d}(x,y)\big\} \qquad \text{for } P,Q\in\mathcal{P}.$$

Eggleston et al. [EGK64] (see also [Grü03, Section 5.3]) proved the lower semicontinuity of the function

$$f_k : \mathcal{P} \longrightarrow \mathbb{Z} \qquad P \longmapsto f_k(P).$$

Furthermore, it is not difficult to show that the function

$$F \longrightarrow \mathcal{P} \qquad x \longmapsto \mathrm{DV}(x)$$

is continuous. Altogether this means that if a point $x \in F$ corresponds to a DV-stereohedron with the most number of facets, there will be a neighborhood $\mathrm{B}(x,r)$ in F, such that $f_k(\mathrm{DV}(y)) = f_k(\mathrm{DV}(x))$ for all $y \in \mathrm{B}(x,r)$. Finding a lower bound for the radius r seems to be difficult, a starting point might be the dissection presented by Koch [Koc72] and Engel [Eng86]. Nonetheless, the above discussion shows that if the grid is fine enough, the approximation is sufficient for finding an extremal stereohedron.

In the following sections we present basic information about the space groups, the fundamental domain of their normalizer that we computed (expressed in the coordinate system of the space group), details on the approximation of the group's fundamental domain, and of course the f-vectors we found together with necessary data to reconstruct the associated DV-stereohedra. All parameter choices were carefully made on basis of experiments conducted before the main computations.

As usual it is impossible to present the massive amount of data generated or to even properly convey the gist of it. We therefore highly encourage the reader to download the data and explore it themselves.

2.2.1 Triclinic groups

The triclinic groups allow for arbitrary 3-dimensional lattices. This generality, however, severely limits the possible space group types. Only two space groups are triclinic, and problem (G) is completely solved for the first one of them; for the second triclinic group IT(2) the problem is solved only for Dirichlet–Voronoi stereohedra.

Space group type $(3,1,1,1,1)$; IT(1) $= P1$

The space group IT(1) corresponds to an arbitrary lattice in $\mathbb{R}^3$. For those lattices Fedorov [Fed85] derived all possible combinatorial types of stereohedra (in this case they are even parallelepipeds), see Conway & Sloane [CS92] for a modern presentation. The possible stereohedra are

stereohedron	f-vector
truncated octahedron	$f = (24, 36, 14)$
hexarhombic dodecahedron	$f = (18, 28, 12)$
rhombic dodecahedron	$f = (14, 24, 12)$
hexagonal prism	$f = (12, 18, 8)$
cube	$f = (8, 12, 6)$

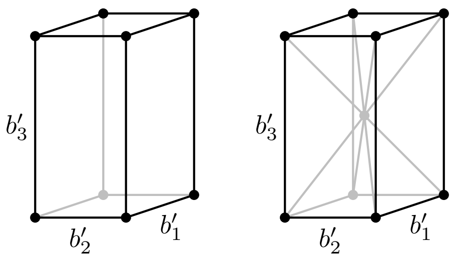
The maximal number of facets for IT(1) is therefore 14.

Space group type $(3, 1, 2, 1, 1)$**;** IT(2) $= P\bar{1}$

This group is already much more complicated then IT(1), even though every orbit decomposes into at most two lattices. In his seminal work Štogrin [Što75] derived all possible combinatorial types of Dirichlet–Voronoi stereohedra. In total there are 165 types; five of them have 20 facets, others have any number from 5 to 19.

2.2.2 Tetragonal groups

Tetragonal groups do not allow for great variation of their metrical parameters. The following types of fundamental parallelepipeds of the sublattice $L' \leq L$ of the space group Γ occur:



primitive (P) body-centered (I)

The lengths of b'_1 and b'_2 have to be equal, the length of b'_3 can be freely chosen. We can therefore encode all lengths by the ***b-ratio*** $\|b'_3\|/\|b'_1\|$. The angles between all pairs of vectors always have to be $\pi/2$.

Space group type $(3, 4, 1, 1, 1)$**;** IT(75) $= P4$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{75} = \operatorname{conv}\left\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$1/2$	$(706/1413, 0, 0)$
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$
$(10, 15, 7)$	$1/2$	$(2825/5652, -1/5652, 0)$

Space group type $(3, 4, 1, 1, 2)$**;** IT(76) $= P4_1$**,** IT(78) $= P4_3$

Normalizer: IT(89) $= P^1422$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{76} = \operatorname{conv}\{(0, 0, 0), (1/2, 0, 0), (1/4, 1/4, 0), (1/4, -1/4, 0)\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Remarks concerning lower bounds: Koch & Fischer [KF72] found a stereohedron with 24 facets for this group.

Metrical parameters: The b-ratio varies from $^1/_2, \ldots, ^7/_2$ in 1001 steps of $^3/_{1000}$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(12, 18, 8)$	$3497/1000$	$(1/4, -1/4, 0)$
$(8, 14, 8)$	2	$(1/4, -1/4, 0)$
$(14, 24, 12)$	2	$(27/148, 23/148, 0)$
$(18, 28, 12)$	$3497/1000$	$(1/2, 0, 0)$
$(24, 36, 14)$	$797/1000$	$(1/2, 0, 0)$
$(24, 38, 16)$	$797/1000$	$(173/3996, 173/3996, 0)$
$(28, 42, 16)$	$797/1000$	$(1079/3996, 919/3996, 0)$
$(32, 48, 18)$	$797/1000$	$(1/4, -1/4, 0)$
$(36, 54, 20)$	$797/1000$	$(1597/3996, 401/3996, 0)$
$(40, 60, 22)$	$797/1000$	$(1807/3996, 191/3996, 0)$
$(44, 66, 24)$	$797/1000$	$(20/333, 44/999, 0)$

Space group type $(3, 4, 1, 1, 3)$**;** IT(77) $= P4_2$

Normalizer: IT(123) $= P^14/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{77} = \operatorname{conv}\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0)\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $^1/_2, \ldots, ^7/_2$ in 1001 steps of $^3/_{1000}$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	$1/2$	$(0,0,0)$
$(12,18,8)$	$1/2$	$(88/1413,0,0)$
$(16,24,10)$	$1/2$	$(706/1413,0,0)$
$(18,28,12)$	$1/2$	$(21/628,-21/628,0)$
$(21,32,13)$	$1/2$	$(2825/5652,-1/5652,0)$
$(24,36,14)$	$1/2$	$(1/4,-1/4,0)$
$(25,38,15)$	$1/2$	$(313/628,-1/5652,0)$
$(28,42,16)$	$1/2$	$(539/5652,-187/5652,0)$

Space group type $(3,4,1,2,1)$**;** $\mathrm{IT}(79) = I4$

Normalizer: $\mathrm{IT}(123) = P^14/mmm$ with basis $\frac{1}{2}(b_1'-b_2'), \frac{1}{2}(b_1'+b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{79} = \mathrm{conv}\left\{(0,0,0),(1/2,0,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2,\ldots,7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	$1/2$	$(1/4,-1/4,0)$
$(8,13,7)$	$1/2$	$(706/1413,0,0)$
$(12,18,8)$	$1/2$	$(103/471,-103/471,0)$
$(14,21,9)$	$1/2$	$(206/471,0,0)$
$(14,23,11)$	$1/2$	$(2825/5652,-1/5652,0)$
$(17,26,11)$	$1/2$	$(2471/5652,-1/5652,0)$
$(18,28,12)$	$7/2$	$(0,0,0)$
$(18,29,13)$	$1/2$	$(2395/5652,-431/5652,0)$
$(21,32,13)$	$1/2$	$(823/1884,-1/1884,0)$
$(24,36,14)$	$1/2$	$(0,0,0)$

Space group type $(3,4,1,2,2)$**;** $\mathrm{IT}(80) = I4_1$

Normalizer: $\mathrm{IT}(125) = P^14/nbm$ with basis $\frac{1}{2}(b_1'-b_2'), \frac{1}{2}(b_1'+b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{80} = \mathrm{conv}\left\{(0,0,0),(1/4,1/4,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(8, 14, 8)$	2	$(0, 0, 0)$
$(19, 29, 12)$	323/250	$(178/1413, 0, 0)$
$(22, 34, 14)$	409/500	$(353/1413, 0, 0)$
$(25, 38, 15)$	797/1000	$(739/5652, 155/5652, 0)$
$(24, 38, 16)$	3497/1000	$(33/157, 18/157, 0)$
$(25, 39, 16)$	1289/1000	$(151/942, 0, 0)$
$(26, 40, 16)$	3497/1000	$(353/1413, 353/1413, 0)$
$(28, 42, 16)$	797/1000	$(1/4, 305/5652, 0)$
$(26, 41, 17)$	797/1000	$(739/5652, 739/5652, 0)$
$(29, 44, 17)$	797/1000	$(739/5652, 497/5652, 0)$
$(30, 45, 17)$	797/1000	$(191/942, 191/942, 0)$
$(28, 44, 18)$	619/500	$(33/157, 18/157, 0)$
$(32, 48, 18)$	3497/1000	$(353/1413, 235/942, 0)$
$(30, 47, 19)$	4/5	$(79/628, 59/628, 0)$
$(33, 50, 19)$	797/1000	$(739/5652, 737/5652, 0)$
$(34, 51, 19)$	797/1000	$(33/157, 33/157, 0)$
$(36, 54, 20)$	3497/1000	$(1/4, 1411/5652, 0)$
$(37, 56, 21)$	797/1000	$(739/5652, 581/5652, 0)$
$(38, 57, 21)$	797/1000	$(1411/5652, 965/5652, 0)$
$(39, 59, 22)$	148/125	$(33/157, 18/157, 0)$
$(40, 60, 22)$	797/1000	$(353/1413, 593/2826, 0)$
$(42, 63, 23)$	797/1000	$(353/1413, 241/1413, 0)$
$(44, 66, 24)$	797/1000	$(1/4, 395/1884, 0)$
$(46, 69, 25)$	317/250	$(377/1884, 559/5652, 0)$
$(48, 72, 26)$	797/1000	$(1/4, 389/1884, 0)$

Space group type $(3, 4, 2, 1, 1)$**;** IT(81) $= P\bar{4}$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{81} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,0)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(249/500,-1/500,0)$
$(10,16,8)$	$4/5$	$(4/25,0,1/4)$
$(12,18,8)$	$3497/1000$	$(62/125,0,1/4)$
$(16,24,10)$	$3497/1000$	$(62/125,0,1/50)$
$(14,24,12)$	$4/5$	$(1/10,-1/10,1/4)$
$(18,28,12)$	$3497/1000$	$(1/4,-1/4,1/4)$
$(18,29,13)$	$4/5$	$(121/250,-1/250,13/100)$
$(19,30,13)$	$4/5$	$(33/100,-17/100,1/4)$
$(21,32,13)$	$3497/1000$	$(249/500,-1/500,1/50)$
$(21,33,14)$	$4/5$	$(31/250,-1/250,13/100)$
$(24,36,14)$	$3497/1000$	$(1/4,-1/4,1/100)$
$(23,36,15)$	$4/5$	$(123/500,-43/500,1/4)$
$(25,38,15)$	$3497/1000$	$(247/500,-1/500,1/50)$
$(28,42,16)$	$3497/1000$	$(31/500,-27/500,1/250)$

Space group type $(3,4,2,2,1)$**;** $\mathrm{IT}(82) = I\bar{4}$

Normalizer: $\mathrm{IT}(139) = I4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{82} = \mathrm{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/8),\\ (1/2,0,1/8),(1/4,-1/4,1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2,\ldots,7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(7,11,6)$	$4/5$	$(17/100,-17/100,0)$
$(8,12,6)$	$3497/1000$	$(1/4,-1/4,0)$
$(6,11,7)$	$4/5$	$(17/50,0,0)$
$(8,13,7)$	$3497/1000$	$(62/125,0,0)$
$(10,16,8)$	$7/2$	$(49/125,0,4/125)$
$(12,18,8)$	$3497/1000$	$(62/125,0,1/8)$
$(13,20,9)$	$3497/1000$	$(0,0,1/8)$
$(14,21,9)$	$797/1000$	$(17/50,0,0)$
$(9,16,9)$	2	$(0,0,1/8)$
$(16,24,10)$	$3497/1000$	$(1/2,0,1/25)$
$(13,22,11)$	$4/5$	$(169/500,-1/500,0)$
$(14,23,11)$	$3497/1000$	$(249/500,-1/500,0)$
$(17,26,11)$	$797/1000$	$(167/500,-1/500,0)$
$(14,24,12)$	$4/5$	$(1/4,-17/100,1/8)$
$(15,25,12)$	$4/5$	$(21/50,0,1/8)$
$(18,28,12)$	$3497/1000$	$(0,0,0)$

f-vector	b-ratio	generating grid point
$(18,29,13)$	$527/1000$	$(41/100,-9/100,0)$
$(19,30,13)$	$7/2$	$(223/500,-27/500,4/125)$
$(21,32,13)$	$797/1000$	$(169/500,-1/500,0)$
$(18,30,14)$	$4/5$	$(3/10,0,1/8)$
$(21,33,14)$	$7/2$	$(2/25,-3/50,1/100)$
$(22,34,14)$	$797/1000$	$(21/50,0,1/8)$
$(23,35,14)$	$3497/1000$	$(62/125,0,1/25)$
$(24,36,14)$	$3497/1000$	$(1/4,-1/4,11/500)$
$(23,36,15)$	$7/2$	$(221/500,-1/20,4/125)$
$(26,39,15)$	$3497/1000$	$(249/500,-1/500,1/25)$
$(25,39,16)$	$797/1000$	$(24/125,-7/125,1/10)$
$(28,42,16)$	$3497/1000$	$(73/250,-1/5,23/1000)$
$(27,42,17)$	$1/2$	$(2/25,-3/50,1/10)$
$(30,45,17)$	$3497/1000$	$(247/500,-1/500,1/25)$
$(29,45,18)$	$527/1000$	$(2/25,-3/50,1/20)$
$(32,48,18)$	$797/1000$	$(201/500,-1/500,101/1000)$
$(31,48,19)$	$32/25$	$(21/125,-3/250,1/20)$
$(34,51,19)$	$3497/1000$	$(241/500,-1/500,3/500)$
$(33,51,20)$	$26/25$	$(27/100,-3/100,1/8)$
$(36,54,20)$	$797/1000$	$(9/100,-19/500,4/125)$
$(35,54,21)$	$32/25$	$(31/250,-1/250,2/25)$
$(38,57,21)$	$3497/1000$	$(219/500,-1/500,9/500)$
$(40,60,22)$	$839/1000$	$(119/500,-21/500,109/1000)$
$(42,63,23)$	$3497/1000$	$(171/500,-1/500,19/1000)$

Space group type $(3,4,3,1,1)$**;** IT(83) $= P4/m$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1'-b_2'), \frac{1}{2}(b_1'+b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{83} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2,\ldots,7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,1/4)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(249/500,-1/500,0)$

Space group type $(3,4,3,1,2)$**;** IT(84) $= P4_2/m$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1'-b_2'), \frac{1}{2}(b_1'+b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{84} = \text{conv}\,\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,1/4)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(107/250,0,107/500)$
$(8,13,7)$	$7/2$	$(49/250,0,117/500)$
$(10,16,8)$	$4/5$	$(4/25,0,0)$
$(12,18,8)$	$3497/1000$	$(62/125,0,31/125)$
$(11,18,9)$	$5/4$	$(3/10,-1/10,61/500)$
$(12,19,9)$	$4/5$	$(101/250,-1/50,47/500)$
$(13,20,9)$	$3497/1000$	$(1/4,-1/4,57/250)$
$(14,21,9)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(9,16,9)$	$4/5$	$(2/25,-2/25,1/25)$
$(14,22,10)$	$4/5$	$(1/5,-2/25,7/250)$
$(16,24,10)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(15,24,11)$	$4/5$	$(16/125,-8/125,4/125)$
$(17,26,11)$	$7/2$	$(207/500,-11/500,109/500)$
$(18,27,11)$	$3497/1000$	$(58/125,-4/125,27/125)$
$(14,24,12)$	$4/5$	$(1/10,-1/10,0)$
$(18,28,12)$	$3497/1000$	$(1/4,-1/4,0)$
$(20,30,12)$	$3497/1000$	$(181/500,-47/500,57/250)$
$(19,30,13)$	$4/5$	$(33/100,-17/100,0)$
$(21,32,13)$	$797/1000$	$(249/500,-1/500,0)$
$(24,36,14)$	$3497/1000$	$(247/500,-1/500,0)$
$(23,36,15)$	$4/5$	$(123/500,-43/500,0)$
$(25,38,15)$	$797/1000$	$(49/100,-1/500,0)$
$(28,42,16)$	$797/1000$	$(121/500,-43/500,0)$

Space group type $(3,4,3,1,3)$**;** IT(85) $= P4/n$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{85} = \text{conv}\,\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(249/500, -1/500, 0)$
$(8, 12, 6)$	3497/1000	$(0, 0, 0)$
$(10, 15, 7)$	3497/1000	$(62/125, 0, 0)$
$(6, 11, 7)$	4/5	$(1/4, -9/100, 1/4)$
$(8, 13, 7)$	3497/1000	$(1/4, -123/500, 1/4)$
$(10, 17, 9)$	1/2	$(13/50, -9/50, 1/5)$
$(14, 21, 9)$	3497/1000	$(1/4, -99/500, 1/500)$
$(11, 20, 11)$	1/2	$(31/100, -17/100, 1/5)$
$(13, 22, 11)$	4/5	$(17/50, 0, 1/4)$
$(14, 23, 11)$	3497/1000	$(62/125, 0, 1/4)$
$(17, 26, 11)$	3497/1000	$(11/25, 0, 1/500)$
$(18, 29, 13)$	3497/1000	$(97/500, -97/500, 1/500)$
$(21, 32, 13)$	3497/1000	$(56/125, 0, 1/500)$

Space group type $(3, 4, 3, 1, 4)$**;** IT(86) $= P4_2/n$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{86} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(0, 0, 1/4)$
$(6, 11, 7)$	4/5	$(1/4, -9/100, 1/4)$
$(8, 13, 7)$	3497/1000	$(1/4, -123/500, 1/4)$
$(10, 16, 8)$	4/5	$(41/100, -9/100, 0)$
$(12, 18, 8)$	3497/1000	$(249/500, -1/500, 0)$
$(13, 20, 9)$	3497/1000	$(1/2, 0, 57/250)$
$(14, 21, 9)$	797/1000	$(1/4, -9/100, 1/4)$
$(9, 16, 9)$	5/4	$(1/2, 0, 9/100)$
$(11, 19, 10)$	7/2	$(1/4, -27/500, 2/125)$
$(16, 24, 10)$	3497/1000	$(1/2, 0, 31/125)$
$(13, 22, 11)$	4/5	$(17/50, 0, 1/4)$
$(14, 23, 11)$	3497/1000	$(62/125, 0, 1/4)$
$(17, 26, 11)$	3497/1000	$(239/500, -11/500, 57/250)$
$(18, 28, 12)$	3497/1000	$(0, 0, 0)$
$(18, 29, 13)$	4/5	$(157/500, -9/100, 3/20)$

f-vector	b-ratio	generating grid point
$(19,30,13)$	$4/5$	$(41/100,-1/500,0)$
$(21,32,13)$	$797/1000$	$(17/50,0,1/4)$
$(20,32,14)$	2	$(3/25,-3/25,1/10)$
$(21,33,14)$	$7/2$	$(19/125,-19/125,121/500)$
$(23,35,14)$	$3497/1000$	$(29/100,-21/100,1/25)$
$(24,36,14)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(22,35,15)$	$7/2$	$(27/500,-27/500,117/500)$
$(23,36,15)$	$4/5$	$(41/100,-43/500,0)$
$(24,37,15)$	$3497/1000$	$(12/25,-1/50,23/100)$
$(25,38,15)$	$797/1000$	$(247/500,-1/500,0)$
$(26,39,15)$	$3497/1000$	$(117/250,0,31/125)$
$(25,39,16)$	$7/2$	$(38/125,0,2/125)$
$(27,41,16)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(28,42,16)$	$3497/1000$	$(58/125,0,29/125)$
$(27,42,17)$	$1/2$	$(56/125,-9/250,53/250)$
$(29,44,17)$	$7/2$	$(223/500,-11/500,117/500)$
$(30,45,17)$	$3497/1000$	$(59/125,0,31/125)$
$(29,45,18)$	$527/1000$	$(9/20,-3/100,23/500)$
$(32,48,18)$	$3497/1000$	$(12/25,0,6/25)$
$(34,51,19)$	$3497/1000$	$(79/250,0,119/500)$
$(36,54,20)$	$3497/1000$	$(62/125,0,31/125)$

Space group type $(3,4,3,2,1)$**;** $\mathrm{IT}(87) = I4/m$

Normalizer: $\mathrm{IT}(123) = P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2')$, $\frac{1}{2}(b_1' + b_2')$, $\frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{87} = \mathrm{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,1/4)$
$(5,9,6)$	$7/2$	$(38/125,0,117/500)$
$(7,11,6)$	$3497/1000$	$(62/125,0,31/125)$
$(8,12,6)$	$3497/1000$	$(0,0,1/4)$
$(10,15,7)$	$3497/1000$	$(247/500,-1/500,1/4)$
$(6,11,7)$	$4/5$	$(17/50,0,0)$
$(8,13,7)$	$3497/1000$	$(62/125,0,0)$
$(10,16,8)$	$4/5$	$(217/500,-17/500,1/5)$
$(12,18,8)$	$3497/1000$	$(47/100,-1/500,31/125)$
$(11,18,9)$	$7/2$	$(151/500,-1/500,117/500)$

f-vector	b-ratio	generating grid point
$(12,19,9)$	3497/1000	$(249/500, -1/500, 31/125)$
$(13,20,9)$	3497/1000	$(0,0,26/125)$
$(14,21,9)$	797/1000	$(17/50,0,0)$
$(9,16,9)$	4/5	$(159/500, -63/500, 11/100)$
$(14,22,10)$	3497/1000	$(237/500, -13/500, 31/125)$
$(16,24,10)$	3497/1000	$(0,0,31/125)$
$(13,22,11)$	4/5	$(169/500, -1/500, 0)$
$(14,23,11)$	3497/1000	$(249/500, -1/500, 0)$
$(17,26,11)$	797/1000	$(167/500, -1/500, 0)$
$(18,28,12)$	3497/1000	$(0,0,0)$
$(18,29,13)$	527/1000	$(41/100, -9/100, 0)$
$(21,32,13)$	797/1000	$(169/500, -1/500, 0)$
$(24,36,14)$	797/1000	$(0,0,0)$

Space group type $(3,4,3,2,2)$**;** IT(88) $= I4_1/a$

Normalizer: IT(134) $= P4_2/nnm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{88} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(0,0,1/8),\\ (1/2,0,1/8),(1/2,1/2,1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 70$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	3497/1000	$(62/125,0,0)$
$(10,15,7)$	3497/1000	$(1/2,0,21/250)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(14,21,9)$	797/1000	$(61/125,0,0)$
$(10,18,10)$	2	$(0,0,1/8)$
$(12,20,10)$	3497/1000	$(0,0,1/8)$
$(13,21,10)$	7/2	$(1/2,38/125,4/125)$
$(15,24,11)$	7/2	$(1/2,57/125,101/1000)$
$(17,26,11)$	3497/1000	$(1/2,0,13/125)$
$(18,27,11)$	797/1000	$(62/125,0,0)$
$(15,25,12)$	4/5	$(3/25,3/25,1/8)$
$(17,27,12)$	899/1000	$(1/2,113/250,1/8)$
$(19,29,12)$	797/1000	$(31/250,31/250,1/8)$
$(20,30,12)$	3497/1000	$(1/2,62/125,0)$
$(17,28,13)$	4/5	$(36/125,1/25,1/8)$
$(18,29,13)$	3497/1000	$(62/125,0,1/8)$
$(19,30,13)$	7/2	$(109/250,13/250,13/1000)$
$(20,31,13)$	797/1000	$(0,0,1/8)$
$(21,32,13)$	3497/1000	$(1/2,0,31/250)$

f-vector	b-ratio	generating grid point
$(21, 33, 14)$	$7/2$	$(38/125, 38/125, 4/125)$
$(22, 34, 14)$	$409/500$	$(0, 0, 0)$
$(23, 35, 14)$	$7/2$	$(101/250, 9/25, 101/1000)$
$(24, 36, 14)$	$3497/1000$	$(1/5, 1/5, 1/20)$
$(21, 34, 15)$	$109/125$	$(19/50, 3/125, 1/8)$
$(22, 35, 15)$	$1/2$	$(29/125, 2/125, 117/1000)$
$(23, 36, 15)$	$7/2$	$(11/25, 49/125, 9/200)$
$(24, 37, 15)$	$797/1000$	$(111/250, 0, 1/8)$
$(25, 38, 15)$	$4/5$	$(1/10, 2/125, 1/40)$
$(26, 39, 15)$	$3497/1000$	$(21/50, 21/50, 21/200)$
$(24, 38, 16)$	$797/1000$	$(1/2, 62/125, 0)$
$(25, 39, 16)$	$3497/1000$	$(58/125, 56/125, 0)$
$(27, 41, 16)$	$7/2$	$(19/250, 19/250, 117/1000)$
$(28, 42, 16)$	$3497/1000$	$(3/250, 3/250, 3/1000)$
$(25, 40, 17)$	$23/25$	$(3/25, 3/25, 1/8)$
$(27, 42, 17)$	$797/1000$	$(19/50, 17/50, 0)$
$(28, 43, 17)$	$797/1000$	$(89/250, 0, 1/8)$
$(29, 44, 17)$	$4/5$	$(21/125, 8/125, 1/10)$
$(30, 45, 17)$	$3497/1000$	$(11/25, 11/25, 11/100)$
$(29, 45, 18)$	$3497/1000$	$(121/250, 103/250, 0)$
$(31, 47, 18)$	$7/2$	$(113/250, 51/125, 101/1000)$
$(32, 48, 18)$	$3497/1000$	$(62/125, 123/250, 0)$
$(31, 48, 19)$	$403/500$	$(21/50, 19/50, 27/250)$
$(32, 49, 19)$	$797/1000$	$(22/125, 12/125, 1/8)$
$(33, 50, 19)$	$4/5$	$(19/125, 4/125, 1/20)$
$(34, 51, 19)$	$3497/1000$	$(62/125, 62/125, 31/250)$
$(33, 51, 20)$	$76/125$	$(11/50, 3/50, 57/500)$
$(35, 53, 20)$	$7/2$	$(62/125, 113/250, 101/1000)$
$(36, 54, 20)$	$3497/1000$	$(62/125, 113/250, 0)$
$(37, 56, 21)$	$7/8$	$(4/25, 1/125, 3/1000)$
$(38, 57, 21)$	$3497/1000$	$(1/250, 1/250, 61/500)$
$(40, 60, 22)$	$3497/1000$	$(62/125, 13/50, 17/1000)$
$(42, 63, 23)$	$3497/1000$	$(62/125, 52/125, 13/125)$

Space group type $(3, 4, 4, 1, 1)$**;** IT(89) $= P422$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{89} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(11, 20, 11)$	$4/5$	$(13/50, -9/50, 1/20)$
$(14, 23, 11)$	$3497/1000$	$(249/500, -1/500, 1/4)$
$(18, 29, 13)$	$3497/1000$	$(111/250, -7/125, 1/500)$

Space group type $(3, 4, 4, 1, 4)$**;** IT(90) $=$ $P42_12$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{90} = \text{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0), (0, 0, 1/4),\\ (1/2, 0, 1/4), (1/4, -1/4, 1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(7, 11, 6)$	$4/5$	$(33/100, -17/100, 1/4)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(31/125, -31/125, 0)$
$(6, 11, 7)$	$4/5$	$(4/25, 0, 1/4)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(249/500, -1/500, 1/50)$
$(14, 21, 9)$	$3497/1000$	$(62/125, 0, 1/50)$
$(18, 28, 12)$	$3497/1000$	$(1/2, 0, 1/4)$
$(17, 28, 13)$	$4/5$	$(41/125, -21/125, 1/4)$
$(18, 29, 13)$	$3497/1000$	$(247/500, -1/500, 1/4)$
$(21, 32, 13)$	$3497/1000$	$(247/500, -1/500, 1/100)$
$(24, 36, 14)$	$3497/1000$	$(1/2, 0, 1/50)$
$(25, 38, 15)$	$3497/1000$	$(247/500, -1/500, 1/50)$

Space group type $(3, 4, 4, 1, 2)$**;** IT(91) $=$ $P4_122$**,** IT(95) $=$ $P4_322$

Normalizer: IT(93) $= P4_222$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{91} = \text{conv}\big\{(0, 0, 0), (1/4, -1/4, 0), (3/4, 1/4, 0), (1/2, 1/2, 0),\\ (0, 0, 1/8), (1/4, -1/4, 1/8), (3/4, 1/4, 1/8), (1/2, 1/2, 1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 50$ [BS06, Corollary 2.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Lemma 4.2 in [BS06] implies that there exists a stereohedron with at least 17 facets for this group.

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 2 000 376 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$4/5$	$(1/50, -1/50, 3/25)$
$(8, 12, 6)$	$4/5$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(3/4, 1/4, 31/250)$
$(10, 16, 8)$	$4/5$	$(1/25, 0, 0)$
$(12, 18, 8)$	$3497/1000$	$(1/4, -1/4, 1/8)$
$(8, 14, 8)$	$14/25$	$(51/100, 49/100, 1/8)$
$(13, 20, 9)$	$4/5$	$(1/2, 995/1998, 1/7992)$
$(9, 16, 9)$	$44/25$	$(1/2, 117/250, 17/200)$
$(11, 19, 10)$	$56/25$	$(127/250, 101/250, 3/200)$
$(15, 23, 10)$	$4/5$	$(13/3996, -1/444, 61/2664)$
$(16, 24, 10)$	$4/5$	$(1/3, 0, 0)$
$(11, 20, 11)$	$88/125$	$(1/2, 121/250, 1/8)$
$(13, 22, 11)$	$4/5$	$(1/2, 997/1998, 1/8)$
$(14, 24, 12)$	$88/125$	$(121/250, 121/250, 1/8)$
$(15, 25, 12)$	$7/2$	$(57/100, 7/20, 2/125)$
$(16, 26, 12)$	$4/5$	$(1/2, 319/666, 1/8)$
$(18, 28, 12)$	$3497/1000$	$(62/125, 62/125, 1/8)$
$(15, 26, 13)$	$4/5$	$(1/2, 23/50, 1/50)$
$(16, 27, 13)$	$4/5$	$(1/50, 1/50, 1/200)$
$(17, 28, 13)$	$4/5$	$(1/3, 0, 1/8)$
$(18, 29, 13)$	$4/5$	$(2/5, 1/5, 0)$
$(19, 30, 13)$	$4/5$	$(1/25, 1/25, 1/50)$
$(20, 31, 13)$	$3497/1000$	$(1/4, -1/4, 0)$
$(21, 32, 13)$	$4/5$	$(985/1998, 319/666, 1/8)$
$(17, 29, 14)$	$4/5$	$(1/2, 23/50, 1/100)$
$(18, 30, 14)$	$44/25$	$(2/125, 2/125, 21/200)$
$(19, 31, 14)$	$4/5$	$(1/2, 29/666, 1/1332)$
$(20, 32, 14)$	$7/2$	$(13/25, 1/5, 61/1000)$
$(21, 33, 14)$	$4/5$	$(12/25, 12/25, 3/25)$
$(22, 34, 14)$	$14/25$	$(7/3996, -1/1332, 61/2664)$
$(23, 35, 14)$	$4/5$	$(19/333, 17/999, 61/2664)$
$(24, 36, 14)$	$797/1000$	$(1/4, -1/4, 0)$
$(20, 33, 15)$	$14/25$	$(271/500, 49/500, 1/8)$
$(21, 34, 15)$	$4/5$	$(1/2, 179/666, 115/3996)$
$(22, 35, 15)$	$4/5$	$(1/2, 29/666, 1/666)$
$(23, 36, 15)$	$7/2$	$(37/100, 7/20, 93/1000)$
$(24, 37, 15)$	$4/5$	$(17/333, 0, 61/2664)$
$(25, 38, 15)$	$4/5$	$(1997/3996, 19/444, 7/2664)$
$(26, 39, 15)$	$14/25$	$(149/3996, -89/3996, 61/2664)$
$(22, 36, 16)$	$4/5$	$(9/50, -3/50, 2/25)$
$(24, 38, 16)$	$4/5$	$(19/37, 1/27, 25/3996)$
$(25, 39, 16)$	$4/5$	$(3/25, 1/25, 1/50)$

f-vector	b-ratio	generating grid point
$(26, 40, 16)$	$14/25$	$(679/1332, 13/1332, 1/8)$
$(27, 41, 16)$	$14/25$	$(151/444, 3/148, 0)$
$(28, 42, 16)$	$4/5$	$(1997/3996, 1075/3996, 5/7992)$
$(24, 39, 17)$	$4/5$	$(3/10, -1/10, 1/20)$
$(26, 41, 17)$	$797/1000$	$(373/500, 123/500, 1/8)$
$(27, 42, 17)$	$4/5$	$(66/125, 11/25, 1/8)$
$(28, 43, 17)$	$4/5$	$(53/1332, -31/3996, 61/2664)$
$(29, 44, 17)$	$14/25$	$(2/37, 8/999, 61/2664)$
$(30, 45, 17)$	$797/1000$	$(309/500, 59/500, 1/8)$
$(28, 44, 18)$	$4/5$	$(131/250, 23/50, 7/100)$
$(29, 45, 18)$	$797/1000$	$(173/250, 69/250, 1/10)$
$(30, 46, 18)$	$14/25$	$(113/222, 5/222, 1/216)$
$(31, 47, 18)$	$14/25$	$(7/333, -2/999, 61/2664)$
$(32, 48, 18)$	$14/25$	$(229/3996, 71/3996, 61/2664)$
$(28, 45, 19)$	$4/5$	$(7/74, -5/74, 17/148)$
$(30, 47, 19)$	$44/25$	$(7/25, -4/25, 1/20)$
$(31, 48, 19)$	$797/1000$	$(29/50, 17/50, 1/20)$
$(32, 49, 19)$	$797/1000$	$(133/250, 113/250, 1/10)$
$(33, 50, 19)$	$3497/1000$	$(84/125, 28/125, 14/125)$
$(34, 51, 19)$	$14/25$	$(677/1332, 347/1332, 263/7992)$
$(32, 50, 20)$	$7/5$	$(139/250, 17/50, 9/200)$
$(33, 51, 20)$	$14/25$	$(1223/1998, 313/1998, 2/27)$
$(35, 53, 20)$	$4/5$	$(131/222, 7/74, 1/36)$
$(36, 54, 20)$	$3497/1000$	$(37/50, 61/250, 31/250)$
$(32, 51, 21)$	$4/5$	$(51/125, -1/25, 33/1000)$
$(35, 54, 21)$	$4/5$	$(13/25, 9/25, 1/40)$
$(36, 55, 21)$	$14/25$	$(506/999, 25/999, 1/296)$
$(37, 56, 21)$	$14/25$	$(101/1998, -5/1998, 61/2664)$
$(38, 57, 21)$	$797/1000$	$(269/500, 19/500, 9/125)$
$(34, 54, 22)$	$4/5$	$(1019/1998, 25/54, 187/3996)$
$(34, 54, 22)$	$4/5$	$(133/250, 23/50, 51/500)$
$(37, 57, 22)$	$4/5$	$(47/111, -17/333, 23/999)$
$(39, 59, 22)$	$14/25$	$(527/999, 32/999, 1/72)$
$(40, 60, 22)$	$14/25$	$(223/444, 355/1332, 239/7992)$
$(39, 60, 23)$	$4/5$	$(131/250, 1/10, 1/50)$
$(41, 62, 23)$	$797/1000$	$(269/500, 19/500, 9/500)$
$(42, 63, 23)$	$797/1000$	$(207/500, -43/500, 41/1000)$
$(41, 63, 24)$	$4/5$	$(139/250, 3/50, 1/40)$
$(43, 65, 24)$	$14/25$	$(1063/1998, 71/1998, 1/54)$
$(44, 66, 24)$	$14/25$	$(409/666, 103/666, 62/999)$
$(46, 69, 25)$	$14/25$	$(355/666, 67/1998, 11/666)$
$(48, 72, 26)$	$14/25$	$(538/999, 13/333, 71/2664)$

Space group type $(3, 4, 4, 1, 5)$**;** $\mathrm{IT}(92) = P4_12_12$**,** $\mathrm{IT}(96) = P4_32_12$

Normalizer: $\mathrm{IT}(93) = P4_222$ with basis $\frac{1}{2}(b'_1 - b'_2)$, $\frac{1}{2}(b'_1 + b'_2)$, $\frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{92} = \text{conv}\big\{(0,0,0),(1/4,-1/4,0),(3/4,1/4,0),(1/2,1/2,0),\\ (0,0,1/8),(1/4,-1/4,1/8),(3/4,1/4,1/8),(1/2,1/2,1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 64$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 2 000 376 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	$7/5$	$(0,0,1/8)$
$(12,18,8)$	$7/5$	$(1/2,997/1998,1/8)$
$(13,20,9)$	$3497/1000$	$(1/2,1/2,43/1000)$
$(15,23,10)$	$3497/1000$	$(1/4,123/500,31/500)$
$(16,24,10)$	$7/5$	$(1/2,1/2,499/3996)$
$(14,24,12)$	$14/25$	$(51/100,1/100,0)$
$(15,25,12)$	$7/5$	$(1/2,9/74,0)$
$(16,26,12)$	$7/5$	$(377/999,0,1/7992)$
$(18,28,12)$	$7/5$	$(761/1332,95/1332,0)$
$(16,27,13)$	2	$(1/4,-1/4,1/8)$
$(17,28,13)$	$4/5$	$(7/20,1/20,0)$
$(18,29,13)$	$7/5$	$(1/2,49/1998,799/7992)$
$(19,30,13)$	$7/5$	$(769/1332,1/12,101/7992)$
$(20,31,13)$	$7/5$	$(2243/3996,245/3996,125/1998)$
$(21,32,13)$	$797/1000$	$(73/100,27/100,23/200)$
$(16,28,14)$	$4/5$	$(2/25,0,1/8)$
$(18,30,14)$	$4/5$	$(23/50,23/50,0)$
$(21,33,14)$	$7/5$	$(475/999,0,799/7992)$
$(22,34,14)$	$7/5$	$(499/999,1/3,83/666)$
$(24,36,14)$	$7/5$	$(2455/3996,617/3996,3/74)$
$(22,35,15)$	$7/5$	$(1/2,49/666,133/2664)$
$(23,36,15)$	$7/5$	$(623/1332,35/444,125/1998)$
$(24,37,15)$	$797/1000$	$(9/20,7/20,0)$
$(25,38,15)$	$7/5$	$(1927/3996,3/148,13/108)$
$(26,39,15)$	$7/5$	$(46/999,-16/999,61/2664)$
$(16,30,16)$	$4/5$	$(1/2,1/10,1/8)$
$(22,36,16)$	$4/5$	$(1/2,3/10,1/8)$
$(24,38,16)$	$797/1000$	$(1/2,113/250,1/8)$
$(25,39,16)$	$7/5$	$(560/999,160/999,445/7992)$
$(26,40,16)$	$7/5$	$(23/222,23/222,23/888)$
$(27,41,16)$	$797/1000$	$(12/25,0,3/25)$
$(28,42,16)$	$7/5$	$(133/1998,91/1998,61/2664)$
$(26,41,17)$	$797/1000$	$(48/125,19/125,0)$
$(27,42,17)$	$7/5$	$(293/666,71/666,25/999)$
$(28,43,17)$	$3497/1000$	$(1/4,7/500,123/1000)$
$(29,44,17)$	$797/1000$	$(273/500,227/500,1/8)$
$(30,45,17)$	$7/5$	$(49/999,-7/999,61/2664)$

f-vector	b-ratio	generating grid point
$(26, 42, 18)$	$26/25$	$(37/100, -13/500, 1/8)$
$(27, 43, 18)$	$797/1000$	$(197/500, 91/500, 0)$
$(29, 45, 18)$	$7/5$	$(289/666, 391/1998, 11/3996)$
$(30, 46, 18)$	$7/5$	$(1997/3996, 1/4, 499/3996)$
$(31, 47, 18)$	$797/1000$	$(91/250, 23/250, 0)$
$(32, 48, 18)$	$7/5$	$(22/333, 44/999, 61/2664)$
$(30, 47, 19)$	$1/2$	$(59/125, 0, 99/1000)$
$(31, 48, 19)$	$7/5$	$(1/3, 80/999, 799/7992)$
$(32, 49, 19)$	$4/5$	$(2/25, 2/125, 1/10)$
$(33, 50, 19)$	$797/1000$	$(49/100, 43/500, 0)$
$(34, 51, 19)$	$7/5$	$(85/1998, -29/1998, 61/2664)$
$(33, 51, 20)$	$7/5$	$(10/27, 0, 869/7992)$
$(34, 52, 20)$	$7/5$	$(497/999, 2/9, 55/444)$
$(35, 53, 20)$	$797/1000$	$(117/250, 33/250, 0)$
$(36, 54, 20)$	$7/5$	$(73/999, 22/333, 61/2664)$
$(35, 54, 21)$	$7/5$	$(421/1332, 199/1332, 125/1998)$
$(37, 56, 21)$	$797/1000$	$(59/125, 16/125, 0)$
$(38, 57, 21)$	$797/1000$	$(129/250, 21/50, 1/8)$
$(34, 54, 22)$	$67/50$	$(17/100, -1/500, 1/8)$
$(37, 57, 22)$	$4/5$	$(107/250, -3/250, 3/25)$
$(39, 59, 22)$	$797/1000$	$(56/125, 0, 14/125)$
$(40, 60, 22)$	$7/5$	$(1951/3996, 1/3996, 1/7992)$
$(41, 62, 23)$	$7/5$	$(223/666, 5/54, 11/148)$
$(42, 63, 23)$	$797/1000$	$(263/500, 197/500, 1/8)$
$(43, 65, 24)$	$1061/1000$	$(51/125, 1/25, 1/10)$
$(44, 66, 24)$	$797/1000$	$(57/125, 2/125, 1/8)$
$(43, 66, 25)$	$23/25$	$(43/100, 1/20, 1/8)$
$(46, 69, 25)$	$797/1000$	$(223/500, 17/500, 1/8)$
$(48, 72, 26)$	$797/1000$	$(113/250, 9/250, 1/8)$
$(50, 75, 27)$	$797/1000$	$(9/20, 19/500, 1/8)$
$(52, 78, 28)$	$7/5$	$(1163/3996, 59/1332, 827/7992)$
$(54, 81, 29)$	$7/5$	$(583/1998, 103/1998, 29/296)$

Space group type $(3, 4, 4, 1, 3)$**;** $\mathrm{IT}(93) = P4_222$

Normalizer: $\mathrm{IT}(123) = P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{93} = \mathrm{conv}\,\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,1/4)$
$(7,11,6)$	$4/5$	$(33/100,-17/100,0)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(107/250,0,107/500)$
$(8,13,7)$	$7/2$	$(49/250,0,117/500)$
$(10,16,8)$	$4/5$	$(17/50,-4/25,1/4)$
$(12,18,8)$	$3497/1000$	$(62/125,0,31/125)$
$(13,20,9)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(9,16,9)$	$4/5$	$(2/25,-2/25,21/100)$
$(16,24,10)$	$3497/1000$	$(1/4,-1/4,1/50)$
$(13,22,11)$	$41/25$	$(38/125,-49/250,4/25)$
$(17,26,11)$	$3497/1000$	$(58/125,-9/250,107/500)$
$(14,24,12)$	$4/5$	$(1/10,-1/10,1/4)$
$(18,28,12)$	$3497/1000$	$(1/4,-1/4,1/4)$
$(20,32,14)$	$7/2$	$(87/250,-19/125,117/500)$
$(24,36,14)$	$797/1000$	$(1/4,-1/4,1/4)$
$(22,35,15)$	$7/2$	$(201/500,-49/500,1/125)$
$(23,36,15)$	$4/5$	$(133/500,-117/500,1/5)$
$(24,37,15)$	$3497/1000$	$(27/100,-23/100,1/50)$
$(25,39,16)$	$7/2$	$(173/500,-3/20,117/500)$
$(26,40,16)$	$4/5$	$(21/250,-13/250,1/5)$
$(27,41,16)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(27,42,17)$	$7/2$	$(31/125,-49/250,9/500)$
$(30,45,17)$	$3497/1000$	$(231/500,-17/500,107/500)$
$(29,45,18)$	$7/2$	$(83/250,-17/125,117/500)$
$(32,48,18)$	$3497/1000$	$(247/500,-1/500,123/500)$
$(31,48,19)$	$4/5$	$(19/250,-9/125,1/5)$
$(34,51,19)$	$3497/1000$	$(67/250,-57/250,1/50)$
$(33,51,20)$	$4/5$	$(6/125,-2/125,121/500)$
$(36,54,20)$	$3497/1000$	$(58/125,-4/125,27/125)$
$(38,57,21)$	$3497/1000$	$(3/10,-9/50,6/25)$
$(40,60,22)$	$3497/1000$	$(113/250,-1/50,27/125)$

Space group type $(3,4,4,1,6)$**;** $\mathrm{IT}(94) = P4_22_12$

Normalizer: $\mathrm{IT}(123) = P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{94} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/4)$
$(10, 15, 7)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(6, 11, 7)$	$4/5$	$(17/50, 0, 0)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 0)$
$(10, 16, 8)$	$7/2$	$(27/250, 0, 109/500)$
$(12, 18, 8)$	$3497/1000$	$(249/500, -1/500, 0)$
$(12, 19, 9)$	$4/5$	$(169/500, -1/500, 0)$
$(13, 20, 9)$	$3497/1000$	$(1/4, -1/4, 57/250)$
$(14, 21, 9)$	$3497/1000$	$(59/250, -59/250, 31/125)$
$(9, 16, 9)$	$5/4$	$(1/4, -1/4, 9/100)$
$(11, 19, 10)$	$7/2$	$(38/125, 0, 117/500)$
$(16, 24, 10)$	$3497/1000$	$(1/4, -1/4, 31/125)$
$(14, 23, 11)$	$3497/1000$	$(249/500, -1/500, 1/4)$
$(17, 26, 11)$	$3497/1000$	$(229/500, -21/500, 26/125)$
$(15, 25, 12)$	2	$(4/25, 0, 1/5)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(16, 27, 13)$	2	$(23/100, -7/100, 1/5)$
$(18, 29, 13)$	$527/1000$	$(41/100, -9/100, 1/4)$
$(19, 30, 13)$	$7/2$	$(151/500, -1/500, 117/500)$
$(21, 32, 13)$	$797/1000$	$(17/100, -17/100, 0)$
$(20, 32, 14)$	2	$(33/100, -17/100, 1/5)$
$(21, 33, 14)$	$7/2$	$(201/500, -49/500, 121/500)$
$(22, 34, 14)$	$3497/1000$	$(3/125, 0, 31/125)$
$(23, 35, 14)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(24, 36, 14)$	$3497/1000$	$(1/2, 0, 31/125)$
$(22, 35, 15)$	$7/2$	$(38/125, -49/250, 117/500)$
$(23, 36, 15)$	$1/2$	$(41/100, -7/100, 17/100)$
$(24, 37, 15)$	$3497/1000$	$(33/100, -17/100, 59/250)$
$(26, 39, 15)$	$3497/1000$	$(237/500, -13/500, 31/125)$
$(25, 39, 16)$	$7/2$	$(121/500, -31/500, 117/500)$
$(27, 41, 16)$	$3497/1000$	$(131/500, -119/500, 31/125)$
$(28, 42, 16)$	$3497/1000$	$(247/500, -1/500, 123/500)$
$(27, 42, 17)$	$7/2$	$(103/500, -49/500, 23/100)$
$(30, 45, 17)$	$3497/1000$	$(57/125, -1/25, 26/125)$
$(29, 45, 18)$	$7/2$	$(3/50, -6/125, 109/500)$
$(32, 48, 18)$	$3497/1000$	$(23/50, -9/250, 53/250)$
$(31, 48, 19)$	$7/2$	$(61/500, -23/500, 28/125)$
$(34, 51, 19)$	$3497/1000$	$(79/250, -39/250, 59/250)$
$(33, 51, 20)$	$7/2$	$(53/500, -1/500, 109/500)$
$(36, 54, 20)$	$3497/1000$	$(9/20, -3/100, 21/100)$
$(38, 57, 21)$	$3497/1000$	$(31/100, -73/500, 57/250)$
$(40, 60, 22)$	$3497/1000$	$(49/250, -6/125, 57/250)$

Space group type $(3, 4, 4, 2, 1)$**;** $\mathrm{IT}(97) = I422$

Normalizer: $\mathrm{IT}(123) = P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{97} = \text{conv}\,\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f**-vector**	**b-ratio**	**generating grid point**
$(5,8,5)$	$4/5$	$(169/500,-1/500,0)$
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,0)$
$(5,9,6)$	$7/2$	$(38/125,0,117/500)$
$(7,11,6)$	$3497/1000$	$(62/125,0,31/125)$
$(8,12,6)$	$3497/1000$	$(0,0,1/4)$
$(10,15,7)$	$3497/1000$	$(59/125,0,31/125)$
$(6,11,7)$	$4/5$	$(17/50,0,0)$
$(8,13,7)$	$3497/1000$	$(62/125,0,0)$
$(10,16,8)$	$3497/1000$	$(247/500,-1/500,1/4)$
$(12,18,8)$	$797/1000$	$(17/100,-17/100,0)$
$(12,19,9)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(13,20,9)$	$3497/1000$	$(0,0,26/125)$
$(14,21,9)$	$797/1000$	$(17/50,0,0)$
$(9,16,9)$	$5/4$	$(2/5,-1/10,6/125)$
$(12,20,10)$	$4/5$	$(149/500,-17/100,1/5)$
$(14,22,10)$	$3497/1000$	$(237/500,-13/500,1/500)$
$(16,24,10)$	$3497/1000$	$(0,0,31/125)$
$(14,23,11)$	$3497/1000$	$(249/500,-1/500,1/4)$
$(13,23,12)$	$23/25$	$(99/250,-7/250,1/10)$
$(15,25,12)$	$7/2$	$(151/500,-1/500,117/500)$
$(16,26,12)$	$3497/1000$	$(247/500,-1/500,123/500)$
$(18,28,12)$	$3497/1000$	$(0,0,0)$
$(17,28,13)$	$4/5$	$(151/500,-51/500,1/10)$
$(18,29,13)$	$527/1000$	$(41/100,-9/100,1/4)$
$(17,29,14)$	$7/2$	$(28/125,-49/250,1/500)$
$(19,31,14)$	$4/5$	$(3/10,-12/125,51/500)$
$(20,32,14)$	$3497/1000$	$(59/125,-3/125,1/500)$
$(24,36,14)$	$797/1000$	$(0,0,0)$
$(21,34,15)$	$1/2$	$(29/125,-8/125,2/25)$
$(24,37,15)$	$797/1000$	$(153/500,-49/500,13/125)$
$(23,37,16)$	$7/5$	$(13/125,-13/250,9/50)$
$(26,40,16)$	$3497/1000$	$(47/100,-1/500,31/125)$
$(26,41,17)$	$3497/1000$	$(47/100,-13/500,1/500)$
$(28,43,17)$	$797/1000$	$(34/125,-3/50,1/500)$
$(30,46,18)$	$3497/1000$	$(21/50,-13/250,31/125)$

Space group type $(3,4,4,2,2)$**;** IT(98) $= I4_122$

Normalizer: IT(134) $= P4_2/nnm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{98} = \operatorname{conv}\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(0,0,1/8),\\ (1/2,0,1/8),(1/2,1/2,1/8)\}$$

Upper bound on number of facets: $f_2 \leq 70$ (Theorem 1.2.6)

Remarks concerning lower bounds: In [BS06, Example 4.5] a stereohedron with 29 facets was constructed for this group.

Metrical parameters: Initially we let the b-ratio vary from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. For each step we used 1 008 126 grid points in the approximating grid. An analysis of the results suggested that it would be interesting to use a finer grid for the b-ratios 377/250 and 38/25. In these cases, the approximating grids had 1 000 981 800 points.

f-vector	b-ratio	generating grid point
(10, 15, 7)	38/25	(1/2, 315/1259, 1257/10072)
(8, 13, 7)	7/2	(1/2, 87/250, 109/1000)
(12, 18, 8)	38/25	(993/2518, 133/1259, 0)
(8, 14, 8)	2	(0, 0, 0)
(14, 21, 9)	38/25	(1/2, 629/1259, 1/5036)
(10, 18, 10)	2	(1/2, 62/125, 0)
(12, 20, 10)	3497/1000	(1/2, 62/125, 0)
(13, 21, 10)	7/2	(1/2, 19/125, 109/1000)
(16, 24, 10)	797/1000	(62/125, 1/250, 0)
(13, 22, 11)	7/5	(13/50, 13/50, 21/200)
(14, 23, 11)	38/25	(885/2518, 885/2518, 1/8)
(15, 24, 11)	7/2	(1/2, 38/125, 2/125)
(17, 26, 11)	38/25	(713/2518, 713/2518, 713/10072)
(14, 24, 12)	2	(1/2, 0, 0)
(15, 25, 12)	797/1000	(62/125, 62/125, 1/8)
(16, 26, 12)	7/2	(49/125, 0, 4/125)
(17, 27, 12)	797/1000	(41/125, 41/125, 1/8)
(18, 28, 12)	38/25	(727/2518, 0, 1/8)
(20, 30, 12)	38/25	(1/2, 921/2518, 921/10072)
(16, 27, 13)	2	(0, 0, 1/8)
(17, 28, 13)	38/25	(993/2518, 629/2518, 0)
(18, 29, 13)	5/4	(1/2, 2/5, 3/500)
(19, 30, 13)	4/5	(8/25, 33/250, 3/25)
(20, 31, 13)	38/25	(1/2, 1/2, 169/5036)
(21, 32, 13)	38/25	(323/1259, 613/2518, 565/5036)
(22, 33, 13)	38/25	(1/2, 889/2518, 889/10072)
(16, 28, 14)	7/2	(87/250, 87/250, 109/1000)
(18, 30, 14)	4/5	(1/2, 13/50, 1/8)
(20, 32, 14)	797/1000	(62/125, 62/125, 31/250)

f-vector	b-ratio	generating grid point
$(21, 33, 14)$	$4/5$	$(21/50, 0, 1/8)$
$(22, 34, 14)$	$38/25$	$(629/1259, 629/1259, 629/5036)$
$(23, 35, 14)$	$797/1000$	$(62/125, 0, 1/8)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 1/8)$
$(20, 33, 15)$	2	$(3/10, 6/25, 27/1000)$
$(21, 34, 15)$	$797/1000$	$(62/125, 1/250, 31/250)$
$(22, 35, 15)$	$7/2$	$(87/250, 19/125, 109/1000)$
$(23, 36, 15)$	$7/2$	$(31/125, 19/125, 109/1000)$
$(24, 37, 15)$	$38/25$	$(487/1259, 487/1259, 487/5036)$
$(25, 38, 15)$	$38/25$	$(767/2518, 246/1259, 781/10072)$
$(26, 39, 15)$	$797/1000$	$(21/50, 0, 1/8)$
$(22, 36, 16)$	$14/25$	$(13/50, 13/50, 0)$
$(23, 37, 16)$	$38/25$	$(385/1259, 385/1259, 385/5036)$
$(24, 38, 16)$	$797/1000$	$(1/2, 13/50, 1/8)$
$(25, 39, 16)$	$38/25$	$(849/2518, 205/1259, 565/5036)$
$(26, 40, 16)$	$38/25$	$(849/2518, 849/2518, 0)$
$(27, 41, 16)$	$38/25$	$(333/1259, 593/2518, 565/5036)$
$(28, 42, 16)$	$38/25$	$(229/2518, 227/2518, 57/2518)$
$(26, 41, 17)$	$797/1000$	$(62/125, 62/125, 0)$
$(27, 42, 17)$	$7/2$	$(19/50, 19/125, 109/1000)$
$(28, 43, 17)$	$38/25$	$(659/2518, 300/1259, 565/5036)$
$(29, 44, 17)$	$797/1000$	$(61/125, 2/125, 0)$
$(30, 45, 17)$	$38/25$	$(1129/2518, 564/1259, 565/5036)$
$(25, 41, 18)$	$1/2$	$(69/250, 32/125, 2/25)$
$(26, 42, 18)$	2	$(3/10, 6/25, 3/25)$
$(27, 43, 18)$	2	$(8/25, 6/25, 3/25)$
$(28, 44, 18)$	$7/2$	$(107/250, 19/125, 109/1000)$
$(29, 45, 18)$	$38/25$	$(1215/2518, 1171/2518, 317/5036)$
$(30, 46, 18)$	$3497/1000$	$(121/250, 103/250, 121/1000)$
$(31, 47, 18)$	$38/25$	$(471/1259, 319/1259, 565/5036)$
$(32, 48, 18)$	$38/25$	$(1129/2518, 129/2518, 565/5036)$
$(28, 45, 19)$	$527/1000$	$(9/25, 7/25, 1/10)$
$(29, 46, 19)$	2	$(23/50, 2/5, 1/20)$
$(30, 47, 19)$	$7/2$	$(109/250, 87/250, 109/1000)$
$(31, 48, 19)$	$38/25$	$(1171/2518, 449/2518, 625/5036)$
$(32, 49, 19)$	$38/25$	$(476/1259, 398/1259, 1/8)$
$(33, 50, 19)$	$38/25$	$(496/1259, 374/1259, 565/5036)$
$(34, 51, 19)$	$38/25$	$(1129/2518, 559/1259, 565/5036)$
$(29, 47, 20)$	$4/5$	$(91/250, 3/10, 1/10)$
$(30, 48, 20)$	2	$(2/5, 17/50, 39/1000)$
$(32, 50, 20)$	$7/2$	$(109/250, 19/125, 109/1000)$
$(33, 51, 20)$	$38/25$	$(611/1259, 1171/2518, 247/5036)$
$(34, 52, 20)$	$703/500$	$(107/250, 97/250, 1/20)$
$(35, 53, 20)$	$38/25$	$(1129/2518, 397/1259, 565/5036)$
$(36, 54, 20)$	$38/25$	$(1129/2518, 517/2518, 565/5036)$
$(31, 50, 21)$	$5/4$	$(59/125, 93/250, 8/125)$
$(34, 53, 21)$	$7/2$	$(54/125, 47/125, 119/1000)$
$(35, 54, 21)$	$38/25$	$(1235/2518, 1059/2518, 217/2518)$
$(36, 55, 21)$	$797/1000$	$(1/2, 62/125, 1/500)$

f-vector	b-ratio	generating grid point
$(37,56,21)$	$38/25$	$(1093/2518,321/1259,565/5036)$
$(38,57,21)$	$38/25$	$(1129/2518,446/1259,565/5036)$
$(34,54,22)$	$797/1000$	$(9/25,7/25,1/10)$
$(36,56,22)$	$4/5$	$(9/25,37/125,1/10)$
$(37,57,22)$	$38/25$	$(508/1259,405/1259,317/5036)$
$(38,58,22)$	$3497/1000$	$(8/25,6/25,31/250)$
$(39,59,22)$	$38/25$	$(1129/2518,739/2518,565/5036)$
$(40,60,22)$	$38/25$	$(1129/2518,553/1259,565/5036)$
$(38,59,23)$	$5/4$	$(123/250,49/125,8/125)$
$(39,60,23)$	$38/25$	$(1237/2518,1171/2518,67/5036)$
$(40,61,23)$	$821/1000$	$(1/2,63/250,123/1000)$
$(41,62,23)$	$38/25$	$(1129/2518,357/1259,565/5036)$
$(42,63,23)$	$38/25$	$(1129/2518,859/2518,565/5036)$
$(40,62,24)$	$5/4$	$(12/25,19/50,8/125)$
$(41,63,24)$	$38/25$	$(1215/2518,427/1259,317/5036)$
$(42,64,24)$	$119/100$	$(17/50,67/250,1/10)$
$(43,65,24)$	$38/25$	$(1129/2518,721/2518,565/5036)$
$(44,66,24)$	$38/25$	$(781/2518,333/1259,565/5036)$
$(43,66,25)$	$4/5$	$(113/250,13/50,3/25)$
$(44,67,25)$	$106/125$	$(1/2,33/125,14/125)$
$(45,68,25)$	$38/25$	$(1121/2518,645/2518,565/5036)$
$(46,69,25)$	$38/25$	$(491/1259,827/2518,565/5036)$
$(44,68,26)$	$38/25$	$(595/1259,753/2518,467/5036)$
$(45,69,26)$	$4/5$	$(73/250,13/50,9/100)$
$(46,70,26)$	$89/100$	$(3/10,63/250,3/25)$
$(47,71,26)$	$797/1000$	$(2/5,7/25,1/10)$
$(48,72,26)$	$38/25$	$(645/2518,315/1259,1257/10072)$
$(46,71,27)$	$38/25$	$(1247/2518,443/1259,625/10072)$
$(47,72,27)$	$4/5$	$(69/250,32/125,1/20)$
$(48,73,27)$	$7/5$	$(57/125,32/125,3/25)$
$(49,74,27)$	$797/1000$	$(36/125,63/250,59/500)$
$(50,75,27)$	$797/1000$	$(1/2,83/250,83/1000)$
$(49,75,28)$	$4/5$	$(39/125,32/125,1/10)$
$(50,76,28)$	$439/500$	$(3/10,63/250,3/25)$
$(51,77,28)$	$38/25$	$(596/1259,807/2518,803/10072)$
$(52,78,28)$	$797/1000$	$(101/250,69/250,101/1000)$
$(50,77,29)$	$38/25$	$(629/1259,897/2518,625/10072)$
$(52,79,29)$	$419/250$	$(121/250,91/250,1/20)$
$(53,80,29)$	$403/500$	$(73/250,63/250,59/500)$
$(54,81,29)$	$797/1000$	$(51/125,69/250,51/500)$
$(53,81,30)$	$41/25$	$(62/125,17/50,3/50)$
$(54,82,30)$	$433/500$	$(3/10,63/250,3/25)$
$(55,83,30)$	$403/500$	$(73/250,63/250,119/1000)$
$(56,84,30)$	$797/1000$	$(71/250,32/125,71/1000)$
$(55,84,31)$	$44/25$	$(123/250,19/50,1/25)$
$(57,86,31)$	$493/500$	$(87/250,63/250,3/25)$
$(58,87,31)$	$797/1000$	$(39/125,33/125,39/500)$
$(59,89,32)$	$803/1000$	$(73/250,63/250,119/1000)$
$(60,90,32)$	$409/500$	$(37/125,63/250,119/1000)$

f-vector	b-ratio	generating grid point
$(62, 93, 33)$	$403/500$	$(39/125, 63/250, 117/1000)$
$(63, 95, 34)$	$38/25$	$(625/1259, 727/2518, 231/2518)$
$(66, 99, 35)$	$727/500$	$(62/125, 41/125, 79/1000)$

Space group type $(3, 4, 5, 1, 1)$**;** IT(99) $= P4mm$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{99} = \text{conv}\left\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$1/2$	$(2825/5652, -1/5652, 0)$
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$

Space group type $(3, 4, 5, 1, 5)$**;** IT(100) $= P4bm$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{100} = \text{conv}\left\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$1/2$	$(353/1413, -353/1413, 0)$
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$
$(10, 15, 7)$	$1/2$	$(2825/5652, -1/5652, 0)$

Space group type $(3,4,5,1,4)$**;** IT(101) $= P4_2cm$

Normalizer: IT(123) $= P^14/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{101} = \mathrm{conv}\left\{(0,0,0),(1/2,0,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$1/2$	$(706/1413,0,0)$
$(8,12,6)$	$1/2$	$(0,0,0)$
$(12,18,8)$	$1/2$	$(2825/5652,-1/5652,0)$
$(16,24,10)$	$1/2$	$(206/471,-59/942,0)$
$(18,28,12)$	$1/2$	$(21/628,-21/628,0)$
$(24,36,14)$	$1/2$	$(1/4,-1/4,0)$

Space group type $(3,4,5,1,8)$**;** IT(102) $= P4_2nm$

Normalizer: IT(123) $= P^14/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{102} = \mathrm{conv}\left\{(0,0,0),(1/2,0,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	$1/2$	$(1/2,0,0)$
$(8,13,7)$	$1/2$	$(706/1413,0,0)$
$(12,18,8)$	$1/2$	$(2825/5652,-1/5652,0)$
$(14,21,9)$	$1/2$	$(206/471,0,0)$
$(16,24,10)$	$1/2$	$(206/471,-59/942,0)$
$(18,28,12)$	$7/2$	$(0,0,0)$
$(21,32,13)$	$1/2$	$(103/471,-103/471,0)$

f-vector	b-ratio	generating grid point
$(24, 36, 14)$	$1/2$	$(0, 0, 0)$

Space group type $(3, 4, 5, 1, 3)$**;** IT(103) $= P4cc$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{103} = \operatorname{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$1/2$	$(706/1413, 0, 0)$
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$
$(14, 23, 11)$	$1/2$	$(2825/5652, -1/5652, 0)$
$(18, 29, 13)$	$1/2$	$(2395/5652, -431/5652, 0)$

Space group type $(3, 4, 5, 1, 7)$**;** IT(104) $= P4nc$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{104} = \operatorname{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$1/2$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$1/2$	$(2825/5652, -1/5652, 0)$
$(8, 13, 7)$	$1/2$	$(706/1413, 0, 0)$
$(12, 18, 8)$	$1/2$	$(103/471, -103/471, 0)$
$(14, 21, 9)$	$1/2$	$(206/471, 0, 0)$
$(18, 28, 12)$	$7/2$	$(0, 0, 0)$

f-vector	b-ratio	generating grid point
$(18, 29, 13)$	$1/2$	$(941/1884, -1/5652, 0)$
$(21, 32, 13)$	$1/2$	$(2471/5652, -1/5652, 0)$
$(24, 36, 14)$	$1/2$	$(0, 0, 0)$
$(25, 38, 15)$	$1/2$	$(823/1884, -1/1884, 0)$

Space group type $(3, 4, 5, 1, 2)$**;** $\mathrm{IT}(105) = P4_2mc$

Normalizer: $\mathrm{IT}(123) = P^14/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{105} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$
$(12, 18, 8)$	$1/2$	$(2825/5652, -1/5652, 0)$
$(16, 24, 10)$	$1/2$	$(706/1413, 0, 0)$
$(18, 28, 12)$	$7/2$	$(1/2, 0, 0)$
$(24, 36, 14)$	$1/2$	$(1/2, 0, 0)$

Space group type $(3, 4, 5, 1, 6)$**;** $\mathrm{IT}(106) = P4_2bc$

Normalizer: $\mathrm{IT}(123) = P^14/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{106} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\}$$

Upper bound on number of facets: $f_2 \leq 22$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$1/2$	$(0, 0, 0)$
$(10, 15, 7)$	$1/2$	$(2825/5652, -1/5652, 0)$

f-vector	b-ratio	generating grid point
$(14, 23, 11)$	$1/2$	$(353/1413, -353/1413, 0)$
$(18, 28, 12)$	$1/2$	$(706/1413, 0, 0)$
$(18, 29, 13)$	$1/2$	$(193/942, -193/942, 0)$
$(24, 36, 14)$	$1/2$	$(67/157, 0, 0)$
$(28, 42, 16)$	$1/2$	$(596/1413, -13/2826, 0)$

Space group type $(3, 4, 5, 2, 1)$**;** IT(107) $=$ $I4mm$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{107} = \operatorname{conv}\left\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$1/2$	$(2825/5652, -1/5652, 0)$
$(8, 12, 6)$	$1/2$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$1/2$	$(2471/5652, -1/5652, 0)$
$(8, 13, 7)$	$1/2$	$(706/1413, 0, 0)$
$(12, 18, 8)$	$1/2$	$(103/471, -103/471, 0)$
$(14, 21, 9)$	$1/2$	$(206/471, 0, 0)$
$(18, 28, 12)$	$7/2$	$(0, 0, 0)$
$(24, 36, 14)$	$1/2$	$(0, 0, 0)$

Space group type $(3, 4, 5, 2, 2)$**;** IT(108) $=$ $I4cm$

Normalizer: IT(123) $= P^1 4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \varepsilon b'_3$

Reduced fundamental domain:

$$R_{108} = \operatorname{conv}\left\{(0,0,0), (1/2,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$1/2$	$(353/1413,-353/1413,0)$
$(8,12,6)$	$1/2$	$(0,0,0)$
$(10,16,8)$	$1/2$	$(941/1884,-1/5652,0)$
$(14,22,10)$	$1/2$	$(2393/5652,-431/5652,0)$
$(14,23,11)$	$1/2$	$(2825/5652,-1/5652,0)$
$(18,29,13)$	$1/2$	$(2395/5652,-431/5652,0)$

Space group type $(3,4,5,2,3)$**;** $\mathrm{IT}(109) = I4_1md$

Normalizer: $\mathrm{IT}(125) = P^14/nbm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{109} = \mathrm{conv}\left\{(0,0,0),(1/4,1/4,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2,\ldots,7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	$3497/1000$	$(1/4,-1/4,0)$
$(12,18,8)$	$3497/1000$	$(0,0,0)$
$(8,14,8)$	2	$(0,0,0)$
$(14,21,9)$	$797/1000$	$(1/4,107/628,0)$
$(16,24,10)$	$797/1000$	$(241/1413,241/1413,0)$
$(18,27,11)$	$797/1000$	$(1/4,65/5652,0)$
$(19,29,12)$	$323/250$	$(178/1413,0,0)$
$(22,34,14)$	$409/500$	$(353/1413,0,0)$
$(25,38,15)$	$797/1000$	$(41/314,0,0)$
$(24,38,16)$	$283/200$	$(0,0,0)$
$(25,39,16)$	$1289/1000$	$(151/942,0,0)$
$(26,40,16)$	$1157/1000$	$(5/2826,0,0)$
$(28,42,16)$	$797/1000$	$(353/1413,0,0)$
$(32,48,18)$	$797/1000$	$(0,0,0)$
$(36,54,20)$	$1157/1000$	$(0,0,0)$

Space group type $(3,4,5,2,4)$**;** $\mathrm{IT}(110) = I4_1cd$

Normalizer: $\mathrm{IT}(125) = P^14/nbm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \varepsilon b_3'$

Reduced fundamental domain:

$$R_{110} = \mathrm{conv}\left\{(0,0,0),(1/4,1/4,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 44$ [BS06, Proposition 3.4] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(14, 24, 12)$	2	$(0, 0, 0)$
$(18, 28, 12)$	3497/1000	$(0, 0, 0)$
$(18, 29, 13)$	3497/1000	$(353/1413, 353/1413, 0)$
$(21, 32, 13)$	797/1000	$(33/157, 0, 0)$
$(24, 36, 14)$	3497/1000	$(1/4, 1411/5652, 0)$
$(26, 39, 15)$	797/1000	$(33/157, 65/471, 0)$
$(28, 42, 16)$	3497/1000	$(353/1413, 235/942, 0)$
$(30, 45, 17)$	797/1000	$(33/157, 33/157, 0)$
$(32, 48, 18)$	797/1000	$(671/2826, 515/2826, 0)$
$(34, 51, 19)$	797/1000	$(28/157, 28/157, 0)$
$(36, 54, 20)$	797/1000	$(1217/5652, 353/1884, 0)$
$(38, 57, 21)$	797/1000	$(1111/5652, 265/1884, 0)$
$(40, 60, 22)$	527/1000	$(344/1413, 583/2826, 0)$

Space group type $(3, 4, 6, 1, 1)$**;** IT(111) $= P\bar{4}2m$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{111} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(249/500, -1/500, 0)$
$(8, 12, 6)$	3497/1000	$(0, 0, 0)$
$(10, 16, 8)$	4/5	$(17/50, -4/25, 1/4)$
$(12, 18, 8)$	3497/1000	$(249/500, -1/500, 1/4)$
$(16, 24, 10)$	3497/1000	$(13/50, -6/25, 1/100)$
$(14, 24, 12)$	4/5	$(1/10, -1/10, 1/4)$
$(18, 28, 12)$	3497/1000	$(1/4, -1/4, 1/4)$
$(24, 36, 14)$	3497/1000	$(1/4, -1/4, 1/100)$

Space group type $(3,4,6,1,2)$; IT(112) $= P\bar{4}2c$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{112} = \operatorname{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,0)$
$(7,11,6)$	$4/5$	$(33/100,-17/100,1/4)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(62/125,0,31/125)$
$(8,13,7)$	$7/2$	$(49/125,0,4/125)$
$(10,16,8)$	$4/5$	$(4/25,0,1/4)$
$(12,18,8)$	$3497/1000$	$(62/125,0,1/4)$
$(13,20,9)$	$3497/1000$	$(1/2,0,31/125)$
$(16,24,10)$	$3497/1000$	$(1/2,0,1/25)$
$(14,23,11)$	$3497/1000$	$(249/500,-1/500,0)$
$(14,24,12)$	$4/5$	$(1/50,-1/50,3/20)$
$(18,28,12)$	$3497/1000$	$(1/2,0,1/4)$
$(18,29,13)$	$527/1000$	$(41/100,-9/100,0)$
$(19,30,13)$	$7/2$	$(223/500,-27/500,4/125)$
$(21,33,14)$	$29/25$	$(12/125,-9/250,3/20)$
$(24,36,14)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(23,36,15)$	$7/2$	$(221/500,-1/20,4/125)$
$(26,39,15)$	$3497/1000$	$(249/500,-1/500,1/25)$
$(28,42,16)$	$3497/1000$	$(1/4,-103/500,11/500)$
$(30,45,17)$	$3497/1000$	$(247/500,-1/500,1/25)$

Space group type $(3,4,6,1,3)$; IT(113) $= P\bar{4}2_1m$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{113} = \operatorname{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(31/125, -31/125, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(249/500, -1/500, 0)$
$(6, 11, 7)$	$4/5$	$(4/25, 0, 1/4)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 1/4)$
$(10, 16, 8)$	$4/5$	$(4/25, -4/25, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(12, 19, 9)$	$4/5$	$(41/125, -21/125, 1/4)$
$(14, 21, 9)$	$3497/1000$	$(62/125, 0, 1/50)$
$(16, 24, 10)$	$3497/1000$	$(31/125, -31/125, 1/100)$
$(14, 24, 12)$	$5/4$	$(1/4, -1/4, 1/10)$
$(18, 28, 12)$	$3497/1000$	$(1/4, -1/4, 1/4)$
$(19, 30, 13)$	$4/5$	$(33/100, -17/100, 1/4)$
$(21, 32, 13)$	$3497/1000$	$(249/500, -1/500, 1/50)$
$(24, 36, 14)$	$3497/1000$	$(1/4, -1/4, 1/100)$

Space group type $(3, 4, 6, 1, 4)$**;** $\mathrm{IT}(114) = P\bar{4}2_1c$

Normalizer: $\mathrm{IT}(123) = P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{114} = \mathrm{conv}\,\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0), (0, 0, 1/4), (1/2, 0, 1/4), (1/4, -1/4, 1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(7, 11, 6)$	$4/5$	$(17/100, -17/100, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/4)$
$(10, 15, 7)$	$3497/1000$	$(249/500, -1/500, 0)$
$(6, 11, 7)$	$4/5$	$(17/50, 0, 0)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 0)$
$(10, 16, 8)$	$7/2$	$(27/250, 0, 109/500)$
$(12, 18, 8)$	$3497/1000$	$(52/125, 0, 26/125)$
$(13, 20, 9)$	$3497/1000$	$(0, 0, 26/125)$
$(14, 21, 9)$	$797/1000$	$(17/50, 0, 0)$
$(11, 19, 10)$	$7/2$	$(38/125, 0, 117/500)$
$(16, 24, 10)$	$3497/1000$	$(0, 0, 31/125)$
$(14, 23, 11)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(14, 24, 12)$	2	$(1/5, -1/5, 3/25)$
$(15, 25, 12)$	2	$(4/25, 0, 1/5)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(17, 28, 13)$	$4/5$	$(169/500, -1/500, 0)$

f-vector	b-ratio	generating grid point
$(18, 29, 13)$	$3497/1000$	$(247/500, -1/500, 0)$
$(19, 30, 13)$	$7/2$	$(19/125, -19/125, 117/500)$
$(21, 32, 13)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(21, 33, 14)$	$7/2$	$(151/500, -1/500, 117/500)$
$(22, 34, 14)$	$3497/1000$	$(3/125, 0, 31/125)$
$(24, 36, 14)$	$3497/1000$	$(1/4, -1/4, 31/125)$
$(23, 36, 15)$	$7/2$	$(53/500, -1/500, 109/500)$
$(25, 38, 15)$	$797/1000$	$(169/500, -1/500, 0)$
$(26, 39, 15)$	$3497/1000$	$(59/250, -59/250, 31/125)$
$(25, 39, 16)$	$1/2$	$(107/250, -1/50, 21/500)$
$(28, 42, 16)$	$3497/1000$	$(31/125, -51/250, 11/500)$
$(30, 45, 17)$	$3497/1000$	$(23/50, -9/250, 53/250)$
$(29, 45, 18)$	$1/2$	$(81/500, -69/500, 1/50)$
$(32, 48, 18)$	$797/1000$	$(43/250, -41/250, 1/250)$
$(34, 51, 19)$	$3497/1000$	$(29/500, -1/500, 61/250)$
$(36, 54, 20)$	$797/1000$	$(17/100, -83/500, 1/500)$

Space group type $(3, 4, 6, 2, 1)$**;** IT(115) $= P\bar{4}m2$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{115} = \text{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(7, 11, 6)$	$4/5$	$(33/100, -17/100, 1/4)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 16, 8)$	$4/5$	$(4/25, 0, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(62/125, 0, 1/4)$
$(16, 24, 10)$	$3497/1000$	$(62/125, 0, 1/50)$
$(18, 28, 12)$	$3497/1000$	$(1/2, 0, 1/4)$
$(24, 36, 14)$	$3497/1000$	$(1/2, 0, 1/50)$

Space group type $(3, 4, 6, 2, 2)$**;** IT(116) $= P\bar{4}c2$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{116} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	3497/1000	$(62/125,0,1/4)$
$(8,12,6)$	3497/1000	$(0,0,0)$
$(10,16,8)$	4/5	$(17/50,-4/25,1/4)$
$(12,18,8)$	3497/1000	$(52/125,0,26/125)$
$(13,20,9)$	3497/1000	$(1/4,-1/4,31/125)$
$(9,16,9)$	4/5	$(2/25,-2/25,21/100)$
$(16,24,10)$	3497/1000	$(62/125,0,31/125)$
$(14,23,11)$	3497/1000	$(249/500,-1/500,0)$
$(17,26,11)$	3497/1000	$(229/500,-21/500,26/125)$
$(14,24,12)$	4/5	$(1/10,-1/10,1/4)$
$(18,28,12)$	3497/1000	$(1/4,-1/4,1/4)$
$(18,29,13)$	527/1000	$(41/100,-9/100,0)$
$(20,32,14)$	2	$(33/100,-17/100,1/5)$
$(21,33,14)$	7/2	$(201/500,-49/500,1/125)$
$(23,35,14)$	3497/1000	$(249/500,-1/500,31/125)$
$(24,36,14)$	3497/1000	$(1/2,0,31/125)$
$(22,35,15)$	7/2	$(38/125,-49/250,2/125)$
$(23,36,15)$	1/2	$(1/5,-3/50,1/10)$
$(24,37,15)$	3497/1000	$(27/100,-23/100,1/50)$
$(26,39,15)$	3497/1000	$(237/500,-13/500,1/500)$
$(25,39,16)$	11/10	$(3/50,-2/125,13/500)$
$(27,41,16)$	3497/1000	$(67/250,-29/125,9/500)$
$(28,42,16)$	3497/1000	$(247/500,-1/500,123/500)$
$(27,42,17)$	7/2	$(31/125,-49/250,9/500)$
$(30,45,17)$	3497/1000	$(57/125,-1/25,26/125)$
$(29,45,18)$	4/5	$(1/10,-1/50,1/5)$
$(32,48,18)$	3497/1000	$(23/50,-9/250,53/250)$
$(31,48,19)$	4/5	$(3/50,-13/250,3/20)$
$(34,51,19)$	3497/1000	$(67/250,-57/250,1/50)$
$(36,54,20)$	3497/1000	$(113/250,-4/125,21/100)$
$(38,57,21)$	3497/1000	$(119/500,-99/500,1/50)$

Space group type $(3,4,6,2,3)$**;** IT(117) $= P\bar{4}b2$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{117} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 22$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	3497/1000	$(31/125,-31/125,0)$
$(8,12,6)$	3497/1000	$(0,0,0)$
$(10,15,7)$	3497/1000	$(249/500,-1/500,0)$
$(14,23,11)$	3497/1000	$(31/125,-31/125,1/4)$
$(18,28,12)$	3497/1000	$(62/125,0,1/4)$
$(18,29,13)$	3497/1000	$(109/500,-109/500,1/500)$
$(24,36,14)$	3497/1000	$(247/500,-1/500,1/4)$
$(28,42,16)$	3497/1000	$(11/50,-27/125,1/500)$

Space group type $(3,4,6,2,4)$**;** IT(118) $= P\bar{4}n2$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{118} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 38$ [BS06, Proposition 2.5] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(7,11,6)$	4/5	$(17/100,-17/100,0)$
$(8,12,6)$	3497/1000	$(0,0,1/4)$
$(10,15,7)$	3497/1000	$(249/500,-1/500,0)$
$(6,11,7)$	4/5	$(4/25,0,1/4)$
$(8,13,7)$	3497/1000	$(62/125,0,1/4)$
$(10,16,8)$	7/2	$(38/125,0,117/500)$
$(12,18,8)$	3497/1000	$(62/125,0,31/125)$
$(12,19,9)$	4/5	$(41/125,-21/125,1/4)$
$(13,20,9)$	3497/1000	$(1/4,-1/4,31/125)$
$(14,21,9)$	3497/1000	$(249/500,-1/500,1/25)$
$(9,16,9)$	5/4	$(1/4,-1/4,4/25)$

f-vector	b-ratio	generating grid point
$(16,24,10)$	$3497/1000$	$(1/4,-1/4,1/50)$
$(13,22,11)$	$41/25$	$(49/250,-49/250,4/25)$
$(17,26,11)$	$3497/1000$	$(31/125,-31/125,31/125)$
$(15,25,12)$	$4/5$	$(16/125,0,1/5)$
$(18,28,12)$	$3497/1000$	$(0,0,0)$
$(16,27,13)$	$4/5$	$(149/500,-17/100,1/5)$
$(17,28,13)$	$4/5$	$(169/500,-1/500,0)$
$(18,29,13)$	$3497/1000$	$(247/500,-1/500,0)$
$(19,30,13)$	$4/5$	$(33/100,-17/100,1/4)$
$(21,32,13)$	$797/1000$	$(249/500,-1/500,1/4)$
$(18,30,14)$	$4/5$	$(4/25,0,9/100)$
$(20,32,14)$	$7/2$	$(19/125,-19/125,117/500)$
$(22,34,14)$	$797/1000$	$(4/25,0,123/500)$
$(23,35,14)$	$3497/1000$	$(59/125,0,31/125)$
$(24,36,14)$	$797/1000$	$(0,0,0)$
$(22,35,15)$	$7/2$	$(49/250,-49/250,2/125)$
$(23,36,15)$	$4/5$	$(117/500,-117/500,1/5)$
$(24,37,15)$	$3497/1000$	$(61/250,-61/250,1/50)$
$(25,38,15)$	$797/1000$	$(169/500,-1/500,0)$
$(25,39,16)$	$7/2$	$(173/500,-3/20,2/125)$
$(27,41,16)$	$3497/1000$	$(31/125,-31/125,1/50)$
$(28,42,16)$	$797/1000$	$(62/125,0,31/125)$
$(27,42,17)$	$7/8$	$(59/250,-12/125,101/500)$
$(28,43,17)$	$44/25$	$(27/250,-7/250,1/25)$
$(29,44,17)$	$797/1000$	$(2/5,-12/125,6/25)$
$(30,45,17)$	$3497/1000$	$(247/500,-1/500,123/500)$
$(26,42,18)$	2	$(1/4,-1/20,1/20)$
$(29,45,18)$	$7/2$	$(111/250,-13/250,4/125)$
$(31,47,18)$	$797/1000$	$(4/25,-17/250,1/20)$
$(32,48,18)$	$3497/1000$	$(67/250,-57/250,1/50)$
$(31,48,19)$	$7/2$	$(147/500,-49/500,1/50)$
$(33,50,19)$	$3497/1000$	$(9/20,-3/500,3/100)$
$(34,51,19)$	$3497/1000$	$(131/500,-111/500,1/50)$
$(33,51,20)$	$7/2$	$(219/500,-23/500,4/125)$
$(36,54,20)$	$3497/1000$	$(227/500,-21/500,17/500)$
$(35,54,21)$	$41/25$	$(79/250,-1/25,1/10)$
$(37,56,21)$	$3497/1000$	$(2/5,-3/250,3/100)$
$(38,57,21)$	$3497/1000$	$(43/250,-18/125,9/500)$
$(37,57,22)$	$7/2$	$(38/125,-1/250,119/500)$
$(40,60,22)$	$3497/1000$	$(12/25,-2/125,19/500)$
$(42,63,23)$	$3497/1000$	$(247/500,-1/500,1/25)$
$(44,66,24)$	$3497/1000$	$(229/500,-1/500,31/125)$

Space group type $(3,4,6,3,1)$**;** IT(119) $= I\bar{4}m2$

Normalizer: IT(139) $= I4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{119} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/8),(1/2,0,1/8),(1/4,-1/4,1/8)\}$$

Upper bound on number of facets: $f_2 \le 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \le 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5,8,5)$	4/5	$(169/500,-1/500,0)$
$(6,9,5)$	3497/1000	$(249/500,-1/500,0)$
$(7,11,6)$	7/2	$(223/500,-27/500,4/125)$
$(8,12,6)$	3497/1000	$(1/4,-1/4,0)$
$(10,15,7)$	3497/1000	$(249/500,-1/500,1/25)$
$(6,11,7)$	4/5	$(17/50,0,0)$
$(8,13,7)$	3497/1000	$(62/125,0,0)$
$(10,16,8)$	7/2	$(49/125,0,4/125)$
$(12,18,8)$	3497/1000	$(62/125,0,1/8)$
$(12,19,9)$	4/5	$(34/125,-1/125,1/8)$
$(13,20,9)$	3497/1000	$(0,0,1/8)$
$(14,21,9)$	3497/1000	$(247/500,-1/500,1/25)$
$(9,16,9)$	2	$(0,0,1/8)$
$(16,24,10)$	3497/1000	$(1/2,0,1/25)$
$(18,27,11)$	797/1000	$(149/500,-1/500,3/40)$
$(15,25,12)$	4/5	$(21/50,0,1/8)$
$(18,28,12)$	3497/1000	$(0,0,0)$
$(18,30,14)$	4/5	$(3/10,0,1/8)$
$(22,34,14)$	797/1000	$(21/50,0,1/8)$
$(23,35,14)$	3497/1000	$(62/125,0,1/25)$
$(24,36,14)$	797/1000	$(0,0,0)$
$(28,42,16)$	797/1000	$(38/125,0,1/8)$

Space group type $(3,4,6,3,2)$**;** IT(120) $= I\bar{4}c2$

Normalizer: IT(139) $= I4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{120} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/8),(1/2,0,1/8),(1/4,-1/4,1/8)\}$$

Upper bound on number of facets: $f_2 \le 40$ [BS06, Corollary 3.5] for points with trivial stabilizer and $f_2 \le 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(31/125, -31/125, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 16, 8)$	$3497/1000$	$(247/500, -1/500, 0)$
$(12, 19, 9)$	$3497/1000$	$(31/125, -31/125, 1/8)$
$(9, 16, 9)$	$5/4$	$(1/10, -1/10, 6/125)$
$(14, 22, 10)$	$3497/1000$	$(121/500, -121/500, 1/1000)$
$(14, 23, 11)$	$3497/1000$	$(249/500, -1/500, 0)$
$(18, 28, 12)$	$3497/1000$	$(62/125, 0, 1/8)$
$(18, 29, 13)$	$527/1000$	$(41/100, -9/100, 0)$
$(21, 33, 14)$	$7/2$	$(69/250, -7/250, 1/500)$
$(24, 36, 14)$	$3497/1000$	$(247/500, -1/500, 31/250)$
$(23, 36, 15)$	$1/2$	$(16/125, -9/125, 31/250)$
$(25, 39, 16)$	$7/2$	$(69/250, -49/250, 1/500)$
$(28, 42, 16)$	$3497/1000$	$(27/125, -49/250, 1/200)$
$(30, 45, 17)$	$3497/1000$	$(54/125, -13/250, 1/1000)$
$(32, 48, 18)$	$527/1000$	$(189/500, -59/500, 1/1000)$
$(34, 51, 19)$	$3497/1000$	$(61/250, -6/25, 1/1000)$

Space group type $(3, 4, 6, 4, 1)$**;** IT(121) $= I\bar{4}2m$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{121} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 70$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(169/500, -1/500, 0)$
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(5, 9, 6)$	$7/2$	$(38/125, 0, 117/500)$
$(7, 11, 6)$	$3497/1000$	$(62/125, 0, 31/125)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/4)$
$(10, 15, 7)$	$3497/1000$	$(59/125, 0, 31/125)$
$(6, 11, 7)$	$4/5$	$(17/50, 0, 0)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 0)$
$(10, 16, 8)$	$3497/1000$	$(247/500, -1/500, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(12, 19, 9)$	$7/2$	$(151/500, -1/500, 117/500)$
$(13, 20, 9)$	$3497/1000$	$(0, 0, 26/125)$
$(14, 21, 9)$	$797/1000$	$(17/50, 0, 0)$
$(14, 22, 10)$	$527/1000$	$(51/250, -23/125, 1/4)$

f-vector	b-ratio	generating grid point
$(16, 24, 10)$	$3497/1000$	$(27/100, -23/100, 1/50)$
$(14, 23, 11)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(14, 24, 12)$	2	$(1/5, -1/5, 3/25)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(20, 30, 12)$	$797/1000$	$(43/250, -41/250, 1/250)$
$(18, 29, 13)$	$527/1000$	$(49/250, -49/250, 1/4)$
$(19, 30, 13)$	$7/2$	$(19/125, -19/125, 117/500)$
$(24, 36, 14)$	$3497/1000$	$(1/4, -1/4, 31/125)$
$(26, 39, 15)$	$3497/1000$	$(59/250, -59/250, 31/125)$
$(30, 45, 17)$	$797/1000$	$(21/125, -21/125, 1/250)$

Space group type $(3, 4, 6, 4, 2)$**;** IT(122) $= I\bar{4}2d$

Normalizer: IT(134) $= P4_2/nnm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{122} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (0,0,1/8), (1/2,0,1/8), (1/2,1/2,1/8)\}$$

Upper bound on number of facets: $f_2 \leq 70$ (Theorem 1.2.6)

Metrical parameters: Initially we let the b-ratio vary from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. For each step we used 1 008 126 grid points in the approximating grid. An analysis of the results suggested that it would be interesting to use a finer grid for the b-ratio 5/4. In this case, the approximating grid had 1 000 981 800 points.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	$5/4$	$(875/2518, 875/2518, 0)$
$(10, 15, 7)$	$3497/1000$	$(1/2, 1/2, 21/250)$
$(8, 13, 7)$	$7/2$	$(1/2, 87/250, 109/1000)$
$(12, 18, 8)$	$5/4$	$(1121/2518, 1121/2518, 0)$
$(8, 14, 8)$	2	$(0, 0, 0)$
$(12, 19, 9)$	2	$(63/250, 63/250, 31/250)$
$(14, 21, 9)$	$283/200$	$(1/2, 62/125, 1/500)$
$(10, 18, 10)$	2	$(1/2, 62/125, 0)$
$(12, 20, 10)$	$3497/1000$	$(1/2, 62/125, 0)$
$(13, 21, 10)$	$7/2$	$(1/2, 19/125, 109/1000)$
$(16, 24, 10)$	$797/1000$	$(62/125, 62/125, 0)$
$(15, 24, 11)$	$7/2$	$(1/2, 38/125, 2/125)$
$(17, 26, 11)$	$3497/1000$	$(1/2, 26/125, 13/250)$
$(14, 24, 12)$	2	$(1/2, 0, 0)$
$(15, 25, 12)$	$3497/1000$	$(62/125, 62/125, 1/8)$
$(16, 26, 12)$	$7/2$	$(49/125, 0, 4/125)$
$(17, 27, 12)$	$5/4$	$(1/2, 983/2518, 0)$
$(18, 28, 12)$	$3497/1000$	$(1/2, 0, 0)$
$(20, 30, 12)$	$3497/1000$	$(1/2, 62/125, 31/250)$

f-vector	b-ratio	generating grid point
$(16, 27, 13)$	$4/5$	$(23/50, 23/50, 1/8)$
$(18, 29, 13)$	$5/4$	$(1121/2518, 1121/2518, 1/8)$
$(19, 30, 13)$	$5/4$	$(96/1259, 75/2518, 75/5036)$
$(20, 31, 13)$	$5/4$	$(1/2, 629/1259, 0)$
$(21, 32, 13)$	$5/4$	$(1121/2518, 0, 1/8)$
$(22, 33, 13)$	$3497/1000$	$(1/2, 51/125, 51/500)$
$(18, 30, 14)$	$7/2$	$(87/250, 87/250, 109/1000)$
$(19, 31, 14)$	$4/5$	$(21/50, 9/25, 0)$
$(20, 32, 14)$	$5/4$	$(629/1259, 629/1259, 1/8)$
$(21, 33, 14)$	$5/4$	$(546/1259, 74/1259, 1109/10072)$
$(22, 34, 14)$	$5/4$	$(629/1259, 1257/2518, 0)$
$(23, 35, 14)$	$797/1000$	$(62/125, 0, 1/8)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 1/8)$
$(20, 33, 15)$	2	$(3/10, 6/25, 123/1000)$
$(21, 34, 15)$	$4/5$	$(87/250, 6/25, 0)$
$(22, 35, 15)$	$7/2$	$(38/125, 38/125, 4/125)$
$(23, 36, 15)$	$5/4$	$(546/1259, 300/1259, 1109/10072)$
$(24, 37, 15)$	$797/1000$	$(87/250, 59/250, 0)$
$(25, 38, 15)$	$3497/1000$	$(62/125, 63/250, 31/250)$
$(26, 39, 15)$	$797/1000$	$(21/50, 0, 1/8)$
$(21, 35, 16)$	$4/5$	$(23/50, 33/125, 1/8)$
$(22, 36, 16)$	2	$(2/5, 17/50, 89/1000)$
$(23, 37, 16)$	$4/5$	$(17/50, 83/250, 0)$
$(24, 38, 16)$	$7/2$	$(109/250, 87/250, 109/1000)$
$(25, 39, 16)$	$7/2$	$(48/125, 19/125, 109/1000)$
$(26, 40, 16)$	$5/4$	$(1245/2518, 619/1259, 0)$
$(27, 41, 16)$	$797/1000$	$(62/125, 61/125, 0)$
$(28, 42, 16)$	$5/4$	$(56/1259, 111/2518, 1131/10072)$
$(25, 40, 17)$	$797/1000$	$(23/50, 67/250, 1/8)$
$(26, 41, 17)$	$7/2$	$(109/250, 19/125, 109/1000)$
$(27, 42, 17)$	$5/4$	$(592/1259, 875/2518, 627/5036)$
$(28, 43, 17)$	$797/1000$	$(54/125, 46/125, 0)$
$(29, 44, 17)$	$5/4$	$(1/2, 389/1259, 389/5036)$
$(30, 45, 17)$	$5/4$	$(115/1259, 113/2518, 57/5036)$
$(28, 44, 18)$	$7/2$	$(23/50, 26/125, 9/200)$
$(29, 45, 18)$	$5/4$	$(546/1259, 329/1259, 1109/10072)$
$(30, 46, 18)$	$797/1000$	$(89/250, 63/250, 0)$
$(31, 47, 18)$	$5/4$	$(1/2, 442/1259, 221/2518)$
$(32, 48, 18)$	$5/4$	$(229/2518, 227/2518, 57/2518)$
$(30, 47, 19)$	$1157/1000$	$(1/2, 62/125, 1/500)$
$(31, 48, 19)$	$5/4$	$(617/1259, 1225/2518, 619/5036)$
$(32, 49, 19)$	$797/1000$	$(91/250, 9/25, 0)$
$(33, 50, 19)$	$5/4$	$(1/2, 427/1259, 427/5036)$
$(34, 51, 19)$	$5/4$	$(1129/2518, 1115/2518, 565/5036)$
$(32, 50, 20)$	2	$(121/250, 19/50, 2/25)$
$(33, 51, 20)$	$5/4$	$(544/1259, 663/2518, 136/1259)$
$(35, 53, 20)$	$5/4$	$(628/1259, 1255/2518, 1/8)$
$(36, 54, 20)$	$3497/1000$	$(34/125, 34/125, 31/250)$
$(35, 54, 21)$	$5/4$	$(626/1259, 1227/2518, 8/1259)$

f-vector	b-ratio	generating grid point
$(36, 55, 21)$	$797/1000$	$(1/2, 62/125, 1/500)$
$(37, 56, 21)$	$5/4$	$(1/2, 839/2518, 839/10072)$
$(38, 57, 21)$	$5/4$	$(1129/2518, 687/2518, 565/5036)$
$(36, 56, 22)$	$5/4$	$(1/2, 521/1259, 555/10072)$
$(37, 57, 22)$	$5/4$	$(1247/2518, 1067/2518, 209/10072)$
$(38, 58, 22)$	$571/500$	$(59/125, 41/125, 3/50)$
$(39, 59, 22)$	$3497/1000$	$(123/250, 33/125, 123/1000)$
$(40, 60, 22)$	$5/4$	$(1129/2518, 679/2518, 565/5036)$
$(38, 59, 23)$	$5/4$	$(1/2, 592/1259, 8/1259)$
$(39, 60, 23)$	$5/4$	$(629/1259, 1233/2518, 8/1259)$
$(40, 61, 23)$	$821/1000$	$(1/2, 63/250, 123/1000)$
$(41, 62, 23)$	$797/1000$	$(61/125, 44/125, 1/20)$
$(42, 63, 23)$	$797/1000$	$(61/125, 63/250, 61/500)$
$(41, 63, 24)$	$4/5$	$(1/2, 113/250, 1/40)$
$(43, 65, 24)$	$5/4$	$(1/2, 877/2518, 877/10072)$
$(44, 66, 24)$	$797/1000$	$(62/125, 63/250, 31/250)$
$(43, 66, 25)$	$5/4$	$(629/1259, 604/1259, 16/1259)$
$(44, 67, 25)$	$5/4$	$(1/2, 1257/2518, 3/10072)$
$(45, 68, 25)$	$797/1000$	$(123/250, 73/250, 9/100)$
$(46, 69, 25)$	$797/1000$	$(1/2, 42/125, 21/250)$
$(45, 69, 26)$	$5/4$	$(1195/2518, 667/2518, 1195/10072)$
$(47, 71, 26)$	$821/1000$	$(1/2, 32/125, 121/1000)$
$(48, 72, 26)$	$797/1000$	$(59/125, 32/125, 59/500)$
$(47, 72, 27)$	$5/4$	$(615/1259, 667/2518, 1195/10072)$
$(49, 74, 27)$	$527/1000$	$(123/250, 73/250, 9/100)$
$(50, 75, 27)$	$797/1000$	$(1/2, 83/250, 83/1000)$
$(49, 75, 28)$	$5/4$	$(1251/2518, 967/2518, 683/10072)$
$(51, 77, 28)$	$227/250$	$(58/125, 69/250, 1/10)$
$(52, 78, 28)$	$821/1000$	$(62/125, 32/125, 121/1000)$
$(53, 80, 29)$	$121/125$	$(12/25, 7/25, 1/10)$
$(54, 81, 29)$	$5/4$	$(622/1259, 633/2518, 1253/10072)$
$(56, 84, 30)$	$881/1000$	$(58/125, 63/250, 123/1000)$
$(58, 87, 31)$	$5/4$	$(629/1259, 1249/2518, 3/2518)$

Space group type $(3, 4, 7, 1, 1)$**;** IT(123) $= P4/mmm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$; so the normalizer is identical with the group itself but the basis is different.

Reduced fundamental domain:

$$R_{123} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), \\ (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \dots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,0)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$

Space group type $(3,4,7,1,2)$**;** IT(124) $= P4/mcc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{124} = \text{conv}\,\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,1/4)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(12,19,9)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(9,16,9)$	$4/5$	$(57/250,-51/250,27/125)$
$(14,22,10)$	$3497/1000$	$(237/500,-13/500,31/125)$
$(14,23,11)$	$3497/1000$	$(249/500,-1/500,0)$
$(18,29,13)$	$527/1000$	$(41/100,-9/100,0)$

Space group type $(3,4,7,1,5)$**;** IT(125) $= P4/nbm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{125} = \text{conv}\,\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,0)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,16,8)$	$3497/1000$	$(62/125,0,1/4)$
$(8,14,8)$	$4/5$	$(17/50,0,1/20)$
$(14,22,10)$	$3497/1000$	$(54/125,0,1/500)$

f-vector	b-ratio	generating grid point
$(14, 23, 11)$	$3497/1000$	$(249/500, -1/500, 1/4)$
$(18, 29, 13)$	$3497/1000$	$(97/500, -97/500, 1/500)$

Space group type $(3, 4, 7, 1, 6)$**;** IT(126) $= P4/nnc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{126} = \text{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(17/50, 0, 1/4)$
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(5, 9, 6)$	$7/2$	$(1/4, -27/500, 2/125)$
$(7, 11, 6)$	$3497/1000$	$(1/4, -123/500, 1/500)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(1/4, -111/500, 1/500)$
$(6, 11, 7)$	$4/5$	$(1/4, -9/100, 1/4)$
$(8, 13, 7)$	$3497/1000$	$(1/4, -123/500, 1/4)$
$(14, 21, 9)$	$797/1000$	$(1/4, -9/100, 1/4)$
$(11, 20, 11)$	$5/4$	$(43/100, -7/100, 9/50)$
$(13, 22, 11)$	$7/2$	$(38/125, 0, 2/125)$
$(14, 23, 11)$	$3497/1000$	$(62/125, 0, 31/125)$
$(17, 28, 13)$	$1/2$	$(2/5, 0, 1/5)$
$(18, 29, 13)$	$3497/1000$	$(28/125, -28/125, 1/500)$
$(20, 31, 13)$	$3497/1000$	$(59/125, 0, 1/500)$
$(24, 37, 15)$	$3497/1000$	$(56/125, 0, 1/250)$

Space group type $(3, 4, 7, 1, 13)$**;** IT(127) $= P4/mbm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{127} = \text{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from 1/2, …, 7/2 in 1001 steps of 3/1000. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(31/125, -31/125, 0)$
$(8, 12, 6)$	3497/1000	$(0, 0, 0)$
$(10, 15, 7)$	3497/1000	$(249/500, -1/500, 0)$

Space group type $(3, 4, 7, 1, 14)$**;** IT(128) $= P4/mnc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2)$, $\frac{1}{2}(b'_1 + b'_2)$, $\frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{128} = \text{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0), (0, 0, 1/4), (1/2, 0, 1/4), (1/4, -1/4, 1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from 1/2, …, 7/2 in 1001 steps of 3/1000. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(31/125, -31/125, 1/4)$
$(5, 9, 6)$	7/2	$(38/125, 0, 117/500)$
$(7, 11, 6)$	3497/1000	$(62/125, 0, 31/125)$
$(8, 12, 6)$	3497/1000	$(0, 0, 1/4)$
$(10, 15, 7)$	3497/1000	$(249/500, -1/500, 0)$
$(6, 11, 7)$	4/5	$(17/50, 0, 0)$
$(8, 13, 7)$	3497/1000	$(62/125, 0, 0)$
$(12, 18, 8)$	797/1000	$(17/100, -17/100, 0)$
$(12, 19, 9)$	4/5	$(81/250, -17/250, 16/125)$
$(13, 20, 9)$	3497/1000	$(0, 0, 26/125)$
$(14, 21, 9)$	3497/1000	$(47/100, -1/500, 31/125)$
$(13, 21, 10)$	7/2	$(151/500, -1/500, 117/500)$
$(14, 22, 10)$	3497/1000	$(247/500, -1/500, 123/500)$
$(16, 24, 10)$	3497/1000	$(0, 0, 31/125)$
$(18, 27, 11)$	3497/1000	$(213/500, -23/500, 31/125)$
$(18, 28, 12)$	3497/1000	$(0, 0, 0)$
$(17, 28, 13)$	4/5	$(169/500, -1/500, 0)$
$(18, 29, 13)$	3497/1000	$(247/500, -1/500, 0)$
$(21, 32, 13)$	797/1000	$(167/500, -1/500, 0)$
$(24, 36, 14)$	797/1000	$(0, 0, 0)$
$(25, 38, 15)$	797/1000	$(169/500, -1/500, 0)$

Space group type $(3, 4, 7, 1, 9)$; IT(129) $= P4/nmm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{129} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(17/50, 0, 1/4)$
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(56/125, 0, 1/500)$
$(6, 11, 7)$	$4/5$	$(1/4, -9/100, 1/4)$
$(8, 13, 7)$	$3497/1000$	$(1/4, -123/500, 1/4)$
$(14, 21, 9)$	$3497/1000$	$(1/4, -99/500, 1/500)$

Space group type $(3, 4, 7, 1, 10)$; IT(130) $= P4/ncc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{130} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(6, 11, 7)$	2	$(1/4, -9/100, 1/20)$
$(8, 13, 7)$	$3497/1000$	$(1/4, -123/500, 1/500)$
$(10, 16, 8)$	$3497/1000$	$(62/125, 0, 1/4)$
$(12, 19, 9)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(14, 21, 9)$	$3497/1000$	$(1/4, -111/500, 1/500)$
$(9, 16, 9)$	$5/4$	$(3/20, -3/20, 6/125)$
$(14, 22, 10)$	$3497/1000$	$(28/125, -28/125, 1/500)$

f-vector	b-ratio	generating grid point
$(14, 23, 11)$	3497/1000	$(249/500, -1/500, 1/4)$
$(15, 25, 12)$	4/5	$(4/25, 0, 9/100)$
$(16, 26, 12)$	3497/1000	$(62/125, 0, 31/125)$
$(18, 29, 13)$	527/1000	$(223/500, -27/500, 1/4)$
$(20, 31, 13)$	3497/1000	$(59/125, 0, 1/500)$
$(17, 29, 14)$	4/5	$(173/500, -3/20, 57/500)$
$(19, 31, 14)$	4/5	$(217/500, -9/500, 21/100)$
$(20, 32, 14)$	3497/1000	$(113/500, -111/500, 1/500)$
$(22, 34, 14)$	3497/1000	$(52/125, 0, 31/125)$
$(24, 37, 15)$	527/1000	$(209/500, -37/500, 31/125)$
$(26, 40, 16)$	3497/1000	$(59/125, 0, 31/125)$
$(26, 41, 17)$	3497/1000	$(28/125, -11/50, 1/500)$

Space group type $(3, 4, 7, 1, 3)$**;** IT(131) $= P4_2/mmc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{131} = \operatorname{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/4, -1/4, 0), (0, 0, 1/4), (1/2, 0, 1/4), (1/4, -1/4, 1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(62/125, 0, 1/4)$
$(7, 11, 6)$	7/2	$(87/250, -19/125, 117/500)$
$(8, 12, 6)$	3497/1000	$(0, 0, 0)$
$(10, 15, 7)$	3497/1000	$(107/250, 0, 107/500)$
$(8, 13, 7)$	7/2	$(49/250, 0, 117/500)$
$(10, 16, 8)$	4/5	$(4/25, 0, 0)$
$(12, 18, 8)$	3497/1000	$(62/125, 0, 31/125)$
$(13, 20, 9)$	3497/1000	$(1/2, 0, 26/125)$
$(16, 24, 10)$	3497/1000	$(1/2, 0, 31/125)$
$(18, 28, 12)$	3497/1000	$(1/2, 0, 0)$
$(24, 36, 14)$	797/1000	$(1/2, 0, 0)$

Space group type $(3, 4, 7, 1, 4)$**;** IT(132) $= P4_2/mcm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{132} = \text{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(62/125,0,1/4)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(249/500,-1/500,31/125)$
$(8,13,7)$	$7/2$	$(201/500,-49/500,121/500)$
$(10,16,8)$	$4/5$	$(17/50,-4/25,0)$
$(12,18,8)$	$3497/1000$	$(249/500,-1/500,0)$
$(13,20,9)$	$3497/1000$	$(1/4,-1/4,57/250)$
$(9,16,9)$	$4/5$	$(2/25,-2/25,1/25)$
$(16,24,10)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(14,24,12)$	$4/5$	$(1/10,-1/10,0)$
$(18,28,12)$	$3497/1000$	$(1/4,-1/4,0)$
$(24,36,14)$	$797/1000$	$(1/4,-1/4,0)$

Space group type $(3,4,7,1,7)$**;** IT(133) $= P4_2/nbc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2)$, $\frac{1}{2}(b'_1 + b'_2)$, $\frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{133} = \text{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 40$ [BS06, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,0)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,16,8)$	$3497/1000$	$(62/125,0,1/4)$
$(12,18,8)$	$3497/1000$	$(62/125,0,0)$
$(13,20,9)$	$3497/1000$	$(1/4,-123/500,1/500)$
$(9,16,9)$	$4/5$	$(1/4,-9/100,2/25)$
$(16,24,10)$	$3497/1000$	$(1/4,-111/500,31/125)$

f-vector	b-ratio	generating grid point
$(11, 20, 11)$	$5/4$	$(43/100, -7/100, 9/50)$
$(14, 23, 11)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(18, 28, 12)$	$3497/1000$	$(1/4, -123/500, 0)$
$(18, 29, 13)$	$3497/1000$	$(28/125, -28/125, 1/500)$
$(21, 33, 14)$	$7/5$	$(3/20, -13/100, 1/20)$
$(24, 36, 14)$	$3497/1000$	$(62/125, 0, 31/125)$
$(23, 36, 15)$	$1/2$	$(1/10, 0, 1/20)$
$(25, 39, 16)$	$7/2$	$(38/125, 0, 121/500)$
$(28, 42, 16)$	$3497/1000$	$(59/125, 0, 31/125)$
$(27, 42, 17)$	$4/5$	$(77/500, -51/500, 1/20)$
$(30, 45, 17)$	$3497/1000$	$(103/250, 0, 31/125)$
$(32, 48, 18)$	$3497/1000$	$(79/250, 0, 1/250)$
$(34, 51, 19)$	$3497/1000$	$(56/125, 0, 31/125)$

Space group type $(3, 4, 7, 1, 8)$**;** IT(134) $= P4_2/nnm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2)$, $\frac{1}{2}(b'_1 + b'_2)$, $\frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{134} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(17/50, 0, 1/4)$
$(6, 9, 5)$	$3497/1000$	$(62/125, 0, 1/4)$
$(5, 9, 6)$	$7/2$	$(1/4, -71/500, 4/125)$
$(7, 11, 6)$	$3497/1000$	$(1/4, -89/500, 9/250)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/4)$
$(10, 15, 7)$	$3497/1000$	$(1/4, -123/500, 1/500)$
$(8, 13, 7)$	$3497/1000$	$(1/4, -123/500, 1/4)$
$(10, 16, 8)$	$4/5$	$(41/100, -9/100, 0)$
$(12, 18, 8)$	$3497/1000$	$(249/500, -1/500, 0)$
$(12, 19, 9)$	$7/2$	$(38/125, 0, 2/125)$
$(13, 20, 9)$	$3497/1000$	$(1/4, -1/4, 31/125)$
$(14, 21, 9)$	$797/1000$	$(1/4, -123/500, 1/4)$
$(9, 16, 9)$	$5/4$	$(1/2, 0, 9/100)$
$(14, 22, 10)$	$4/5$	$(93/250, 0, 1/5)$
$(15, 23, 10)$	$7/2$	$(87/250, 0, 121/500)$
$(16, 24, 10)$	$3497/1000$	$(58/125, 0, 29/125)$
$(13, 22, 11)$	$41/25$	$(27/500, -27/500, 9/100)$
$(16, 25, 11)$	$4/5$	$(43/125, -1/10, 11/50)$

f-vector	b-ratio	generating grid point
$(17, 26, 11)$	$3497/1000$	$(239/500, -11/500, 57/250)$
$(18, 27, 11)$	$3497/1000$	$(62/125, 0, 31/125)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(22, 33, 13)$	$797/1000$	$(42/125, 0, 31/125)$
$(20, 32, 14)$	$7/2$	$(49/250, -49/250, 4/125)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 0)$
$(22, 35, 15)$	$7/2$	$(19/125, -19/125, 121/500)$
$(23, 36, 15)$	$4/5$	$(8/125, -8/125, 1/5)$
$(24, 37, 15)$	$3497/1000$	$(12/25, -1/50, 23/100)$
$(25, 39, 16)$	$4/5$	$(109/500, -109/500, 1/5)$
$(27, 41, 16)$	$3497/1000$	$(249/500, -1/500, 31/125)$
$(30, 45, 17)$	$797/1000$	$(219/500, -31/500, 47/250)$
$(34, 51, 19)$	$797/1000$	$(11/125, -11/125, 1/500)$

Space group type $(3, 4, 7, 1, 15)$**;** IT(135) $= P4_2/mbc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2)$, $\frac{1}{2}(b'_1 + b'_2)$, $\frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{135} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 0)$
$(10, 15, 7)$	$3497/1000$	$(249/500, -1/500, 0)$
$(12, 19, 9)$	$3497/1000$	$(31/125, -31/125, 31/125)$
$(13, 20, 9)$	$3497/1000$	$(62/125, 0, 31/125)$
$(9, 16, 9)$	$4/5$	$(4/25, 0, 2/25)$
$(14, 22, 10)$	$3497/1000$	$(59/250, -59/250, 31/125)$
$(16, 24, 10)$	$3497/1000$	$(59/125, 0, 31/125)$
$(14, 23, 11)$	$3497/1000$	$(31/125, -31/125, 0)$
$(15, 24, 11)$	$1/2$	$(7/25, -1/5, 22/125)$
$(18, 27, 11)$	$3497/1000$	$(247/500, -1/500, 123/500)$
$(18, 28, 12)$	$3497/1000$	$(62/125, 0, 0)$
$(20, 30, 12)$	$3497/1000$	$(54/125, -1/25, 31/125)$
$(18, 29, 13)$	$527/1000$	$(49/250, -49/250, 0)$
$(24, 36, 14)$	$3497/1000$	$(247/500, -1/500, 0)$
$(28, 42, 16)$	$527/1000$	$(193/500, -13/500, 0)$

Space group type $(3,4,7,1,16)$**;** IT(136) $= P4_2/mnm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{136} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	3497/1000	$(249/500,-1/500,1/4)$
$(5,9,6)$	7/2	$(38/125,0,117/500)$
$(7,11,6)$	3497/1000	$(62/125,0,31/125)$
$(8,12,6)$	3497/1000	$(0,0,1/4)$
$(10,15,7)$	3497/1000	$(249/500,-1/500,31/125)$
$(6,11,7)$	4/5	$(17/50,0,0)$
$(8,13,7)$	3497/1000	$(62/125,0,0)$
$(9,14,7)$	7/2	$(151/500,-1/500,117/500)$
$(10,16,8)$	4/5	$(17/50,-4/25,0)$
$(12,18,8)$	3497/1000	$(249/500,-1/500,0)$
$(12,19,9)$	4/5	$(169/500,-1/500,0)$
$(13,20,9)$	3497/1000	$(1/4,-1/4,57/250)$
$(14,21,9)$	3497/1000	$(59/250,-59/250,31/125)$
$(9,16,9)$	5/4	$(1/4,-1/4,9/100)$
$(16,24,10)$	3497/1000	$(1/4,-1/4,31/125)$
$(18,28,12)$	3497/1000	$(0,0,0)$
$(19,30,13)$	4/5	$(17/100,-17/100,0)$
$(21,32,13)$	797/1000	$(17/100,-17/100,0)$
$(24,36,14)$	797/1000	$(0,0,0)$

Space group type $(3,4,7,1,11)$**;** IT(137) $= P4_2/nmc$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{137} = \text{conv}\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5,8,5)$	$4/5$	$(17/50,0,1/4)$
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,0)$
$(7,11,6)$	$7/2$	$(49/250,-49/250,4/125)$
$(8,12,6)$	$3497/1000$	$(0,0,0)$
$(10,15,7)$	$3497/1000$	$(71/250,-27/125,17/500)$
$(8,13,7)$	$3497/1000$	$(1/4,-123/500,1/4)$
$(10,16,8)$	$7/2$	$(1/4,-71/500,4/125)$
$(12,18,8)$	$3497/1000$	$(62/125,0,0)$
$(13,20,9)$	$3497/1000$	$(1/4,-1/4,31/125)$
$(14,21,9)$	$3497/1000$	$(141/500,-107/500,17/500)$
$(11,19,10)$	$5/4$	$(1/4,-1/20,24/125)$
$(16,24,10)$	$3497/1000$	$(1/4,-1/4,1/25)$
$(15,25,12)$	2	$(1/4,-9/100,1/20)$
$(18,28,12)$	$3497/1000$	$(1/4,-1/4,1/4)$
$(22,34,14)$	$3497/1000$	$(1/4,-123/500,1/500)$
$(24,36,14)$	$797/1000$	$(1/4,-1/4,1/4)$

Space group type $(3,4,7,1,12)$**;** IT(138) $= P4_2/ncm$

Normalizer: IT(123) $= P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{138} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/2,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(249/500,-1/500,1/4)$
$(7,11,6)$	$4/5$	$(41/100,-43/500,0)$
$(8,12,6)$	$3497/1000$	$(0,0,1/4)$
$(10,15,7)$	$3497/1000$	$(12/25,-1/50,23/100)$
$(6,11,7)$	2	$(1/4,-9/100,1/20)$
$(8,13,7)$	$3497/1000$	$(1/4,-123/500,1/500)$
$(10,16,8)$	$3497/1000$	$(62/125,0,1/4)$
$(12,18,8)$	$3497/1000$	$(249/500,-1/500,0)$
$(12,19,9)$	2	$(17/50,0,1/5)$
$(13,20,9)$	$3497/1000$	$(1/2,0,57/250)$
$(14,21,9)$	$3497/1000$	$(34/125,0,31/125)$
$(9,16,9)$	$5/4$	$(1/2,0,9/100)$
$(14,22,10)$	$1/2$	$(3/20,-9/100,1/20)$
$(15,23,10)$	$7/2$	$(87/250,-17/125,121/500)$
$(16,24,10)$	$3497/1000$	$(58/125,0,29/125)$

f-vector	b-ratio	generating grid point
$(18, 27, 11)$	$3497/1000$	$(62/125, 0, 31/125)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(20, 30, 12)$	$797/1000$	$(123/250, 0, 1/500)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 0)$

Space group type $(3, 4, 7, 2, 1)$**;** IT(139) $=$ $I4/mmm$

Normalizer: IT(123) $=$ $P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{139} = \text{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$7/2$	$(151/500, -1/500, 117/500)$
$(6, 9, 5)$	$3497/1000$	$(249/500, -1/500, 0)$
$(5, 9, 6)$	$7/2$	$(38/125, 0, 117/500)$
$(7, 11, 6)$	$3497/1000$	$(62/125, 0, 31/125)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/4)$
$(10, 15, 7)$	$3497/1000$	$(59/125, 0, 31/125)$
$(6, 11, 7)$	$4/5$	$(17/50, 0, 0)$
$(8, 13, 7)$	$3497/1000$	$(62/125, 0, 0)$
$(12, 18, 8)$	$797/1000$	$(17/100, -17/100, 0)$
$(13, 20, 9)$	$3497/1000$	$(0, 0, 26/125)$
$(14, 21, 9)$	$797/1000$	$(17/50, 0, 0)$
$(16, 24, 10)$	$3497/1000$	$(0, 0, 31/125)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 0)$

Space group type $(3, 4, 7, 2, 2)$**;** IT(140) $=$ $I4/mcm$

Normalizer: IT(123) $=$ $P4/mmm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{140} = \text{conv}\{(0,0,0), (1/2,0,0), (1/4,-1/4,0), (0,0,1/4), (1/2,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Examples of stereohedra with 8 facets are known for this group, see [BS01, Example 2.5].

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(249/500, -1/500, 1/4)$
$(8, 12, 6)$	3497/1000	$(0, 0, 0)$
$(7, 12, 7)$	7/2	$(28/125, -49/250, 31/125)$
$(9, 14, 7)$	3497/1000	$(247/500, -1/500, 123/500)$
$(10, 16, 8)$	3497/1000	$(247/500, -1/500, 0)$
$(11, 17, 8)$	3497/1000	$(47/100, -13/500, 31/125)$
$(12, 19, 9)$	3497/1000	$(249/500, -1/500, 31/125)$
$(9, 16, 9)$	5/4	$(2/5, -1/10, 101/500)$
$(14, 22, 10)$	3497/1000	$(237/500, -13/500, 31/125)$
$(14, 23, 11)$	3497/1000	$(249/500, -1/500, 0)$
$(18, 29, 13)$	527/1000	$(41/100, -9/100, 0)$

Space group type $(3, 4, 7, 2, 3)$**;** $\mathrm{IT}(141) = I4_1/amd$

Normalizer: $\mathrm{IT}(134) = P4_2/nnm$ with basis $\frac{1}{2}(b_1' - b_2'), \frac{1}{2}(b_1' + b_2'), \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{141} = \mathrm{conv}\big\{(0, 0, 0), (1/2, 0, 0), (1/2, 1/2, 0), (0, 0, 1/8), (1/2, 0, 1/8), (1/2, 1/2, 1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Examples of stereohedra with 18 facets are known for this group, see [BS01, Example 2.9].

Metrical parameters: Initially we let the b-ratio vary from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. For each step we used 1 008 126 grid points in the approximating grid. An analysis of the results suggested that it would be interesting to use a finer grid for the b-ratio 1/2. In this case, the approximating grid had 1 000 981 800 points.

f-vector	b-ratio	generating grid point
$(7, 11, 6)$	7/2	$(13/50, 9/50, 9/200)$
$(8, 12, 6)$	3497/1000	$(54/125, 54/125, 27/250)$
$(10, 15, 7)$	3497/1000	$(1/2, 0, 21/250)$
$(7, 12, 7)$	4/5	$(36/125, 1/25, 1/8)$
$(8, 13, 7)$	3497/1000	$(62/125, 0, 1/8)$
$(10, 16, 8)$	4/5	$(1/5, 2/125, 1/20)$
$(11, 17, 8)$	7/2	$(53/125, 53/125, 117/1000)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

f-vector	b-ratio	generating grid point
$(9, 15, 8)$	$4/5$	$(19/50, 19/50, 1/8)$
$(12, 19, 9)$	$4/5$	$(1/25, 1/25, 1/8)$
$(13, 20, 9)$	$797/1000$	$(62/125, 0, 1/8)$
$(14, 21, 9)$	$3497/1000$	$(62/125, 62/125, 31/250)$
$(10, 18, 10)$	2	$(0, 0, 1/8)$
$(12, 20, 10)$	$3497/1000$	$(0, 0, 1/8)$
$(14, 22, 10)$	$797/1000$	$(19/50, 19/50, 1/8)$
$(15, 23, 10)$	$797/1000$	$(44/125, 17/250, 1/10)$
$(16, 24, 10)$	$797/1000$	$(26/125, 26/125, 1/8)$
$(15, 24, 11)$	$7/2$	$(1/2, 87/250, 117/1000)$
$(16, 25, 11)$	$797/1000$	$(62/125, 62/125, 0)$
$(17, 26, 11)$	$3497/1000$	$(1/2, 0, 13/125)$
$(18, 27, 11)$	$797/1000$	$(62/125, 0, 0)$
$(15, 25, 12)$	$4/5$	$(1/2, 19/50, 1/8)$
$(16, 26, 12)$	$5/4$	$(1/2, 7/25, 7/100)$
$(17, 27, 12)$	$797/1000$	$(56/125, 81/250, 3/25)$
$(18, 28, 12)$	$4/5$	$(47/125, 7/125, 2/25)$
$(19, 29, 12)$	$797/1000$	$(2/5, 19/50, 1/10)$
$(20, 30, 12)$	$3497/1000$	$(1/2, 62/125, 0)$
$(20, 31, 13)$	$797/1000$	$(0, 0, 1/8)$
$(21, 32, 13)$	$3497/1000$	$(1/2, 0, 31/250)$
$(22, 33, 13)$	$3497/1000$	$(1/2, 123/250, 1/1000)$
$(20, 32, 14)$	$797/1000$	$(1/2, 19/50, 1/8)$
$(21, 33, 14)$	$527/1000$	$(56/125, 81/250, 3/25)$
$(22, 34, 14)$	$4/5$	$(2/5, 12/125, 1/10)$
$(23, 35, 14)$	$797/1000$	$(1/2, 0, 31/250)$
$(24, 36, 14)$	$797/1000$	$(97/250, 97/250, 97/1000)$
$(23, 36, 15)$	$299/250$	$(1/2, 62/125, 1/500)$
$(24, 37, 15)$	$1/2$	$(53/125, 101/250, 3/50)$
$(25, 38, 15)$	$527/1000$	$(2/5, 2/5, 1/10)$
$(26, 39, 15)$	$797/1000$	$(101/250, 101/250, 101/1000)$
$(24, 38, 16)$	$797/1000$	$(1/2, 62/125, 0)$
$(26, 40, 16)$	$1/2$	$(103/250, 3/50, 1/20)$
$(28, 42, 16)$	$797/1000$	$(0, 0, 0)$
$(26, 41, 17)$	$5/4$	$(1/2, 3/10, 93/1000)$
$(27, 42, 17)$	$4/5$	$(1/2, 107/250, 3/40)$
$(29, 44, 17)$	$427/500$	$(1/2, 123/250, 11/1000)$
$(30, 45, 17)$	$797/1000$	$(62/125, 69/250, 121/1000)$
$(29, 45, 18)$	$1/2$	$(1/2, 865/2518, 3/10072)$
$(31, 47, 18)$	$797/1000$	$(1/2, 52/125, 13/125)$
$(32, 48, 18)$	$527/1000$	$(49/125, 49/125, 107/1000)$
$(30, 47, 19)$	$1157/1000$	$(1/2, 62/125, 1/500)$
$(31, 48, 19)$	$5/4$	$(1/2, 2/5, 8/125)$
$(33, 50, 19)$	$106/125$	$(1/2, 123/250, 11/1000)$
$(34, 51, 19)$	$797/1000$	$(1/2, 2/5, 1/10)$
$(33, 51, 20)$	$409/500$	$(1/2, 62/125, 1/500)$
$(36, 55, 21)$	$797/1000$	$(1/2, 62/125, 1/500)$
$(37, 56, 21)$	$959/1000$	$(1/2, 121/250, 3/200)$
$(38, 57, 21)$	$797/1000$	$(1/2, 47/125, 31/250)$

f-vector	b-ratio	generating grid point
$(39, 60, 23)$	$4/5$	$(1/2, 119/250, 1/40)$
$(40, 61, 23)$	$1/2$	$(1/2, 629/1259, 1/5036)$
$(43, 65, 24)$	$797/1000$	$(1/2, 41/125, 41/500)$
$(44, 67, 25)$	$169/200$	$(1/2, 121/250, 3/200)$
$(46, 69, 25)$	$797/1000$	$(1/2, 93/250, 93/1000)$
$(47, 71, 26)$	$821/1000$	$(1/2, 62/125, 3/1000)$
$(50, 75, 27)$	$797/1000$	$(1/2, 89/250, 89/1000)$
$(54, 81, 29)$	$527/1000$	$(1/2, 89/250, 89/1000)$

Space group type $(3, 4, 7, 2, 4)$**;** IT(142) $= I4_1/acd$

Normalizer: IT(134) $= P4_2/nnm$ with basis $\frac{1}{2}(b'_1 - b'_2), \frac{1}{2}(b'_1 + b'_2), \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{142} = \text{conv}\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (0,0,1/8), (1/2,0,1/8), (1/2,1/2,1/8)\}$$

Upper bound on number of facets: $f_2 \leq 80$ [BS06, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 134$ in general (Theorem 1.2.6).

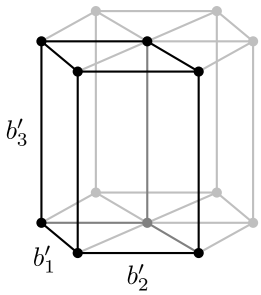
Metrical parameters: Initially we let the b-ratio vary from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. For each step we used 1 008 126 grid points in the approximating grid. An analysis of the results suggested that it would be interesting to use a finer grid for the b-ratio 253/500. In this case, the approximating grid had 1 000 981 800 points.

f-vector	b-ratio	generating grid point
$(7, 11, 6)$	$4/5$	$(1/2, 23/50, 1/8)$
$(8, 12, 6)$	$3497/1000$	$(0, 0, 1/8)$
$(12, 18, 8)$	$3497/1000$	$(1/2, 62/125, 0)$
$(13, 20, 9)$	$3497/1000$	$(1/2, 0, 13/125)$
$(10, 18, 10)$	$4/5$	$(23/50, 23/50, 1/8)$
$(16, 24, 10)$	$3497/1000$	$(1/2, 0, 31/250)$
$(11, 20, 11)$	$4/5$	$(3/10, 0, 1/8)$
$(12, 21, 11)$	$4/5$	$(1/25, 1/25, 1/8)$
$(13, 22, 11)$	$3497/1000$	$(62/125, 0, 1/8)$
$(17, 26, 11)$	$3497/1000$	$(1/2, 52/125, 13/125)$
$(15, 25, 12)$	$4/5$	$(47/250, 1/25, 1/8)$
$(16, 26, 12)$	$797/1000$	$(56/125, 0, 1/8)$
$(18, 28, 12)$	$3497/1000$	$(0, 0, 0)$
$(17, 28, 13)$	$527/1000$	$(111/250, 0, 1/8)$
$(18, 29, 13)$	$4/5$	$(123/250, 123/250, 1/40)$
$(20, 31, 13)$	$797/1000$	$(26/125, 26/125, 1/8)$
$(21, 32, 13)$	$527/1000$	$(1/5, 1/5, 1/8)$
$(19, 31, 14)$	$4/5$	$(11/25, 13/50, 1/8)$
$(20, 32, 14)$	$7/2$	$(1/2, 38/125, 4/125)$
$(21, 33, 14)$	$3497/1000$	$(23/50, 3/10, 0)$

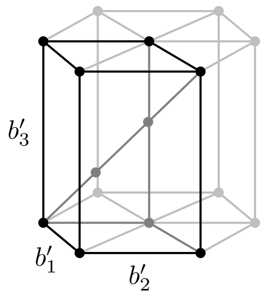
f-vector	b-ratio	generating grid point
$(22, 34, 14)$	$3497/1000$	$(62/125, 62/125, 0)$
$(23, 35, 14)$	$3497/1000$	$(93/250, 93/250, 0)$
$(24, 36, 14)$	$3497/1000$	$(109/250, 109/250, 109/1000)$
$(20, 33, 15)$	2	$(13/250, 9/250, 9/500)$
$(22, 35, 15)$	$7/2$	$(1/2, 87/250, 117/1000)$
$(23, 36, 15)$	$7/2$	$(57/125, 38/125, 4/125)$
$(24, 37, 15)$	$3497/1000$	$(1/2, 109/250, 109/1000)$
$(25, 38, 15)$	$797/1000$	$(103/250, 103/250, 0)$
$(26, 39, 15)$	$797/1000$	$(23/50, 23/50, 23/200)$
$(25, 39, 16)$	$3497/1000$	$(23/50, 3/10, 33/1000)$
$(27, 41, 16)$	$3497/1000$	$(1/2, 62/125, 31/250)$
$(28, 42, 16)$	$3497/1000$	$(93/250, 93/250, 93/1000)$
$(27, 42, 17)$	$7/2$	$(56/125, 101/250, 14/125)$
$(29, 44, 17)$	$7/2$	$(2/5, 63/250, 117/1000)$
$(30, 45, 17)$	$3497/1000$	$(58/125, 58/125, 29/250)$
$(26, 42, 18)$	2	$(11/25, 2/5, 19/500)$
$(29, 45, 18)$	$7/2$	$(87/250, 87/250, 117/1000)$
$(31, 47, 18)$	$3497/1000$	$(12/25, 2/125, 1/500)$
$(32, 48, 18)$	$3497/1000$	$(33/250, 33/250, 31/250)$
$(31, 48, 19)$	$3497/1000$	$(23/50, 3/10, 4/125)$
$(33, 50, 19)$	$3497/1000$	$(93/250, 93/250, 61/500)$
$(34, 51, 19)$	$3497/1000$	$(62/125, 62/125, 31/250)$
$(33, 51, 20)$	$3497/1000$	$(23/50, 3/10, 27/1000)$
$(35, 53, 20)$	$797/1000$	$(17/125, 17/125, 57/500)$
$(36, 54, 20)$	$3497/1000$	$(13/50, 13/50, 31/250)$
$(35, 54, 21)$	$1/2$	$(9/50, 9/50, 31/500)$
$(37, 56, 21)$	$7/2$	$(69/250, 31/250, 117/1000)$
$(38, 57, 21)$	$3497/1000$	$(93/250, 93/250, 31/250)$
$(40, 60, 22)$	$3497/1000$	$(27/250, 27/250, 7/1000)$
$(42, 63, 23)$	$3497/1000$	$(123/250, 13/50, 31/250)$
$(44, 66, 24)$	$797/1000$	$(4/25, 27/250, 113/1000)$
$(46, 69, 25)$	$503/1000$	$(31/125, 49/250, 1/500)$

2.2.3 Trigonal groups

In the case of the trigonal and hexagonal crystal systems we need to apply a change of basis to get cuboidal fundamental parallelepipeds for the sublattice L'. The space groups of these systems are given in the IT with respect to sublattice parallelepipeds of the following types:



primitive
(P)



rhombohedral
(R)

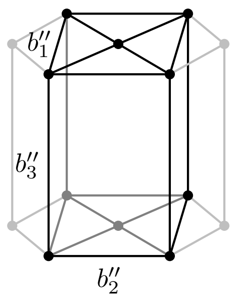
The lengths of b'_1 and b'_2 have to be equal, the length of b'_3 can be freely chosen. The angle between b'_1 and b'_2 must be $\angle(b'_1, b'_2) = 2\pi/3$, the angles between b'_1 and b'_3 and between b'_2 and b'_3 have to be $\angle(b'_1, b'_3) = \angle(b'_2, b'_3) = \pi/2$. To obtain orthogonal fundamental cells, we need to apply a coordinate transformation between

$$\mathcal{B}' = (b'_1, b'_2, b'_3) \quad \text{and} \quad \mathcal{B}'' = (b''_1, b''_2, b''_3) = (2b'_1 + b'_2, b'_2, b'_3).$$

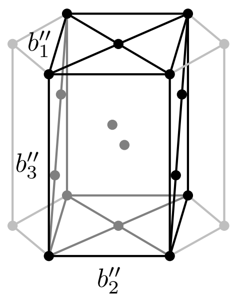
We get the new sublattice $L'' = \langle b''_1, b''_2, b''_3 \rangle$. Of course we have to apply this transformation to the trigonal and hexagonal groups of the IT accordingly. The basis exchange matrix $X = X_{\mathcal{B}'' \to \mathcal{B}'}$ is

$$X = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \text{and} \qquad X^{-1} = \begin{bmatrix} 1/2 & 0 & 0 \\ -1/2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and thus, if Γ is a trigonal or hexagonal group from the IT and $(A, a) \in \Gamma$ is an isometry, we have to work with the isometry $(X^{-1}AX, X^{-1}a)$ instead. After the coordinate transformation we have the following two orthogonal fundamental parallelepiped types for sublattices:



transformed
primitive



transformed
rhombohedral

Here we need to have $\|b''_1\| = \sqrt{3}\|b''_2\|$, the length of b''_3 can be freely chosen, and the angles between all pairs of vectors have to be $\pi/2$.

Space group type $(3, 5, 1, 2, 1)$**;** IT(143) $= P3$

Normalizer: IT(191) $= P^1 6/mmm$ with basis $\frac{2}{3}b'_1 + \frac{1}{3}b'_2, -\frac{1}{3}b'_1 + \frac{1}{3}b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{143} = \text{conv}\left\{(0,0,0),(1/6,0,0),(1/6,1/6,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 30$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $^1/_2, \ldots, ^7/_2$ in 1001 steps of $^3/_{1000}$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $^{\|b_3'\|}/_{\|b_1'\|}$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8,12,6)$	3497/1000	$(1/6,0,0)$
$(12,18,8)$	3497/1000	$(0,0,0)$

Space group type $(3,5,1,2,2)$**;** IT(144) $= P3_1$**,** IT(145) $= P3_2$

Normalizer: IT(177) $= P^1622$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{144} = \text{conv}\left\{(0,0,0),(1/6,0,0),(1/6,1/6,0),(1/12,1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 30$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $^1/_2, \ldots, ^7/_2$ in 1001 steps of $^3/_{1000}$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $^{\|b_3'\|}/_{\|b_1'\|}$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(12,18,8)$	3497/1000	$(0,0,0)$
$(14,24,12)$	3497/1000	$(1/6,1/6,0)$
$(18,28,12)$	3497/1000	$(1997/11988,1997/11988,0)$
$(24,36,14)$	3497/1000	$(1/6,0,0)$
$(25,39,16)$	1/2	$(29/324,25/108,0)$
$(26,40,16)$	797/1000	$(35/666,35/666,0)$
$(28,42,16)$	797/1000	$(1/6,0,0)$
$(32,48,18)$	797/1000	$(11/111,15/74,0)$
$(36,54,20)$	797/1000	$(9/148,1/12,0)$

Space group type $(3,5,1,1,1)$**;** IT(146) $= R3$

Normalizer: IT(162) $= P^1\bar{3}1m$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{146} = \text{conv}\left\{(0,0,0),(1/6,0,0),(1/6,1/6,0),(1/12,1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 30$ (Theorem 1.2.6)

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	**b-ratio**	**generating grid point**
$(12, 18, 8)$	3497/1000	$(1/6, 1/6, 0)$
$(8, 14, 8)$	3497/1000	$(1/6, 0, 0)$
$(12, 22, 12)$	1/2	$(5/36, 5/36, 0)$
$(14, 24, 12)$	3497/1000	$(0, 0, 0)$
$(15, 25, 12)$	3497/1000	$(5/37, 6/37, 0)$
$(19, 29, 12)$	797/1000	$(7/162, 7/54, 0)$
$(17, 29, 14)$	1/2	$(1769/11988, 659/3996, 0)$
$(18, 30, 14)$	3497/1000	$(250/2997, 749/2997, 0)$
$(19, 31, 14)$	1/2	$(1/9, 1/6, 0)$
$(20, 32, 14)$	797/1000	$(227/1998, 53/333, 0)$
$(21, 33, 14)$	797/1000	$(575/11988, 575/3996, 0)$
$(23, 35, 14)$	797/1000	$(941/11988, 421/3996, 0)$
$(24, 36, 14)$	797/1000	$(0, 0, 0)$
$(22, 36, 16)$	797/1000	$(461/3996, 205/1332, 0)$
$(23, 37, 16)$	1/2	$(1573/11988, 1757/11988, 0)$
$(24, 38, 16)$	797/1000	$(250/2997, 749/2997, 0)$
$(27, 41, 16)$	797/1000	$(575/5994, 32/333, 0)$
$(28, 44, 18)$	527/1000	$(1529/11988, 577/3996, 0)$
$(31, 47, 18)$	797/1000	$(31/324, 385/3996, 0)$

Space group type $(3, 5, 2, 2, 1)$**;** IT(147) $= P\bar{3}$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{147} = \operatorname{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	**b-ratio**	**generating grid point**
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(7, 11, 6)$	4/5	$(29/100, -13/100, 1/4)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(10, 15, 7)$	3497/1000	$(33/100, -1/500, 0)$

f-vector	b-ratio	generating grid point
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(6, 12, 8)$	$4/5$	$(4/25, 0, 1/4)$
$(8, 14, 8)$	$3497/1000$	$(124/375, 0, 1/4)$
$(14, 22, 10)$	$3497/1000$	$(124/375, 0, 3/250)$
$(13, 23, 12)$	$4/5$	$(36/125, -16/125, 1/4)$
$(14, 24, 12)$	$3497/1000$	$(1/3, 0, 1/4)$
$(17, 27, 12)$	$3497/1000$	$(33/100, -1/500, 1/125)$
$(18, 30, 14)$	$3497/1000$	$(1/3, 0, 7/500)$
$(21, 33, 14)$	$3497/1000$	$(33/100, -1/500, 3/250)$

Space group type $(3, 5, 2, 1, 1)$**;** IT(148) $= R\bar{3}$

Normalizer: IT(166) $= R\bar{3}m$ with basis $-b'_1, -b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{148} = \text{conv}\,\big\{(0,0,0), (-1/3,0,0), (-1/6,-1/2,0), (0,0,1/12), (-1/3,0,1/12), (-1/6,-1/2,1/12)\big\}$$

Upper bound on number of facets: $f_2 \leq 48$ [BS06, Proposition 2.7] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(-1/250, -1/250, 0)$
$(10, 15, 7)$	$797/1000$	$(-51/250, -51/250, 0)$
$(6, 11, 7)$	$7/2$	$(-49/375, -49/125, 4/125)$
$(7, 12, 7)$	$7/2$	$(-163/750, -87/250, 2/125)$
$(8, 13, 7)$	$3497/1000$	$(-1/750, -1/250, 1/12)$
$(12, 18, 8)$	$797/1000$	$(-1/250, -1/250, 0)$
$(6, 12, 8)$	$13/5$	$(-88/375, 0, 1/15)$
$(8, 14, 8)$	$3497/1000$	$(-1/375, 0, 1/12)$
$(11, 18, 9)$	$797/1000$	$(-1/15, -1/5, 1/12)$
$(14, 21, 9)$	$527/1000$	$(-29/125, -29/125, 0)$
$(13, 21, 10)$	$3497/1000$	$(-1/3, 0, 1/12)$
$(15, 23, 10)$	$797/1000$	$(-1/150, -1/250, 0)$
$(12, 21, 11)$	$5/4$	$(-4/15, -1/5, 19/750)$
$(13, 22, 11)$	$3497/1000$	$(-1/750, -1/250, 0)$
$(14, 23, 11)$	$3497/1000$	$(-83/250, -1/250, 0)$
$(16, 25, 11)$	$3497/1000$	$(-63/250, -61/250, 1/1500)$
$(11, 21, 12)$	$17/10$	$(-63/250, -9/50, 1/15)$
$(12, 22, 12)$	$7/2$	$(-49/375, 0, 1/125)$
$(13, 23, 12)$	$7/2$	$(-11/50, -1/50, 2/75)$
$(14, 24, 12)$	$3497/1000$	$(-1/6, -1/2, 1/12)$
$(15, 25, 12)$	$4/5$	$(-17/150, -37/250, 1/12)$
$(16, 26, 12)$	$3497/1000$	$(-1/150, -1/250, 0)$

f-vector	b-ratio	generating grid point
$(19, 29, 12)$	$797/1000$	$(-7/750, -1/250, 0)$
$(15, 26, 13)$	$4/5$	$(-77/375, 0, 1/60)$
$(16, 27, 13)$	$4/5$	$(-91/375, -1/5, 1/20)$
$(17, 28, 13)$	$3497/1000$	$(-101/375, 0, 2/125)$
$(18, 29, 13)$	$3497/1000$	$(-14/125, -42/125, 41/1500)$
$(19, 30, 13)$	$3497/1000$	$(-1/6, -1/2, 0)$
$(20, 31, 13)$	$3497/1000$	$(-83/250, -1/250, 1/1500)$
$(17, 29, 14)$	$3497/1000$	$(-29/150, -17/50, 1/150)$
$(18, 30, 14)$	$3497/1000$	$(-59/250, -29/250, 11/750)$
$(19, 31, 14)$	$797/1000$	$(-29/150, -17/50, 1/150)$
$(20, 32, 14)$	$3497/1000$	$(-163/750, -1/250, 43/1500)$
$(21, 33, 14)$	$797/1000$	$(-23/375, -23/125, 79/1500)$
$(22, 34, 14)$	$797/1000$	$(-9/125, 0, 1/12)$
$(23, 35, 14)$	$797/1000$	$(-13/750, -1/250, 0)$
$(24, 36, 14)$	$797/1000$	$(-1/3, 0, 1/12)$
$(20, 33, 15)$	$4/5$	$(-97/375, -27/125, 1/20)$
$(21, 34, 15)$	$7/2$	$(-97/375, -16/125, 1/125)$
$(23, 36, 15)$	$527/1000$	$(-97/375, -1/5, 0)$
$(16, 30, 16)$	$5/4$	$(0, 0, 1/150)$
$(21, 35, 16)$	$3497/1000$	$(-9/50, -19/50, 1/50)$
$(22, 36, 16)$	$3497/1000$	$(-1/3, 0, 31/1500)$
$(23, 37, 16)$	$797/1000$	$(-21/250, -37/250, 77/1500)$
$(24, 38, 16)$	$3497/1000$	$(-83/375, -2/125, 2/75)$
$(26, 40, 16)$	$797/1000$	$(-1/250, -1/250, 1/12)$
$(25, 40, 17)$	$7/2$	$(-4/15, -17/125, 1/125)$
$(27, 42, 17)$	$797/1000$	$(-11/375, -11/125, 1/12)$
$(25, 41, 18)$	$68/25$	$(-104/375, -16/125, 1/60)$
$(27, 43, 18)$	$1/2$	$(-4/15, -4/25, 11/150)$
$(28, 44, 18)$	$3497/1000$	$(-41/125, -1/125, 1/1500)$
$(29, 45, 18)$	$797/1000$	$(-3/50, -9/50, 4/75)$
$(30, 46, 18)$	$797/1000$	$(-7/125, -21/125, 83/1500)$
$(29, 46, 19)$	$7/2$	$(-203/750, -7/50, 1/125)$
$(31, 48, 19)$	$3497/1000$	$(-1/6, -1/2, 1/1500)$
$(29, 47, 20)$	$47/25$	$(-217/750, -1/10, 1/30)$
$(32, 50, 20)$	$3497/1000$	$(-104/375, -4/25, 1/750)$
$(34, 52, 20)$	$797/1000$	$(-19/375, -19/125, 29/500)$
$(34, 53, 21)$	$797/1000$	$(-49/750, -49/250, 1/12)$
$(36, 56, 22)$	$3497/1000$	$(-199/750, -49/250, 1/250)$
$(38, 58, 22)$	$797/1000$	$(-13/50, -53/250, 6/125)$
$(42, 64, 24)$	$4/5$	$(-98/375, -26/125, 89/1500)$
$(46, 70, 26)$	$821/1000$	$(-98/375, -26/125, 7/125)$

Space group type $(3, 5, 3, 2, 1)$**;** IT(149) $= P312$

Normalizer: IT(191) $= P6/mmm$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{149} = \text{conv}\left\{(0,0,0),(1/6,0,0),(1/6,1/6,0),(0,0,1/4),\right.$$
$$\left.(1/6,0,1/4),(1/6,1/6,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f**-vector**	**b-ratio**	**generating grid point**
$(6,9,5)$	3497/1000	$(1/6,1/6,0)$
$(8,12,6)$	3497/1000	$(1/6,0,0)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(14,24,12)$	3497/1000	$(1/6,1/6,1/4)$
$(18,30,14)$	3497/1000	$(1/6,1/6,1/250)$

Space group type $(3,5,3,3,1)$**;** IT(150) $=$ $P321$

Normalizer: IT(191) $=$ $P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{150} = \text{conv}\left\{(0,0,0),(1/3,0,0),(1/4,-1/4,0),(0,0,1/4),\right.$$
$$\left.(1/3,0,1/4),(1/4,-1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f**-vector**	**b-ratio**	**generating grid point**
$(6,9,5)$	3497/1000	$(1/3,0,0)$
$(7,11,6)$	4/5	$(29/100,-13/100,1/4)$
$(8,12,6)$	3497/1000	$(1/4,-1/4,0)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(6,12,8)$	4/5	$(4/25,0,1/4)$
$(8,14,8)$	3497/1000	$(124/375,0,1/4)$
$(14,22,10)$	3497/1000	$(124/375,0,3/250)$
$(14,24,12)$	3497/1000	$(1/3,0,1/4)$
$(17,29,14)$	4/5	$(36/125,-16/125,1/4)$
$(18,30,14)$	3497/1000	$(1/3,0,7/500)$
$(21,33,14)$	3497/1000	$(33/100,-1/500,1/125)$
$(22,36,16)$	3497/1000	$(81/500,-57/500,1/500)$
$(25,39,16)$	3497/1000	$(33/100,-1/500,3/250)$

Space group type $(3,5,3,2,2)$**;** IT(151) $= P3_112$**,** IT(153) $= P3_212$

Normalizer: IT(180) $= P6_222$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \frac{1}{2}b_3'$ (only the normalizer for IT(151) but not for IT(153))

Reduced fundamental domain:

$$R_{151} = \operatorname{conv}\{(0,0,0),(1/3,0,0),(1/6,1/2,0),(0,0,1/12),(1/3,0,1/12),(1/6,1/2,1/12)\}$$

Upper bound on number of facets: $f_2 \leq 48$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from 1/2, ..., 7/2 in 1001 steps of 3/1000. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
(12, 18, 8)	3497/1000	(0, 0, 0)
(12, 19, 9)	4/5	(1/75, 0, 23/300)
(13, 22, 11)	3497/1000	(62/375, 62/125, 0)
(18, 27, 11)	3497/1000	(62/375, 62/125, 1/12)
(16, 26, 12)	797/1000	(23/150, 23/50, 0)
(18, 30, 14)	4/5	(133/750, 53/250, 0)
(20, 32, 14)	797/1000	(109/750, 109/250, 1/12)
(22, 34, 14)	3497/1000	(1/6, 123/250, 0)
(24, 36, 14)	3497/1000	(21/125, 62/125, 31/375)
(22, 35, 15)	3497/1000	(4/75, 4/25, 2/75)
(23, 36, 15)	4/5	(13/75, 12/25, 23/300)
(25, 38, 15)	797/1000	(67/375, 57/125, 0)
(24, 38, 16)	797/1000	(193/750, 13/250, 0)
(25, 39, 16)	4/5	(169/750, 13/50, 39/500)
(27, 41, 16)	797/1000	(6/25, 18/125, 1/12)
(28, 42, 16)	797/1000	(13/75, 12/25, 2/25)
(27, 42, 17)	4/5	(7/30, 11/50, 23/300)
(29, 44, 17)	797/1000	(13/50, 39/250, 1/12)
(30, 45, 17)	3497/1000	(7/25, 4/25, 2/75)
(29, 45, 18)	4/5	(1/6, 23/50, 23/300)
(31, 47, 18)	797/1000	(2/75, 2/125, 1/12)
(32, 48, 18)	3497/1000	(19/75, 6/25, 1/25)
(31, 48, 19)	4/5	(4/15, 9/125, 6/125)
(34, 51, 19)	797/1000	(47/150, 1/50, 2/25)
(33, 51, 20)	4/5	(34/125, 8/125, 9/250)
(35, 53, 20)	797/1000	(101/375, 8/125, 16/375)
(36, 54, 20)	3497/1000	(6/125, 16/125, 17/750)
(38, 57, 21)	797/1000	(223/750, 7/250, 2/375)
(40, 60, 22)	797/1000	(113/375, 1/125, 1/300)

Space group type $(3, 5, 3, 3, 2)$**;** IT(152) $= P3_121$**,** IT(154) $= P3_221$

Normalizer: IT(180) $= P6_222$ with basis $b'_1 + b'_2, -b'_1, \frac{1}{2}b'_3$ (only the normalizer for IT(152) but not for IT(154))

Reduced fundamental domain:

$$R_{152} = \text{conv}\{(0,0,0),(1/2,1/2,0),(0,1,0),(0,0,1/12),\\ (1/2,1/2,1/12),(0,1,1/12)\}$$

Upper bound on number of facets: $f_2 \leq 48$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Lemma 4.2 in [BS06] implies that there exists a stereohedron with at least 13 facets for this group.

Metrical parameters: The b-ratio varies from 1/2, ..., 7/2 in 1001 steps of 3/1000. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(12,18,8)$	3497/1000	$(0,0,0)$
$(15,23,10)$	3497/1000	$(62/125,62/125,1/12)$
$(13,22,11)$	3497/1000	$(31/125,93/125,0)$
$(15,24,11)$	2	$(1/5,1/5,7/150)$
$(18,27,11)$	3497/1000	$(83/250,83/250,1/12)$
$(15,25,12)$	7/5	$(3/50,1/10,3/50)$
$(16,26,12)$	797/1000	$(31/125,93/125,0)$
$(18,28,12)$	3497/1000	$(62/125,63/125,1/12)$
$(18,29,13)$	3497/1000	$(21/125,62/125,0)$
$(19,30,13)$	797/1000	$(3/125,6/125,1/12)$
$(21,32,13)$	3497/1000	$(83/250,33/50,1/12)$
$(19,31,14)$	17/10	$(111/250,113/250,4/375)$
$(20,32,14)$	797/1000	$(59/250,177/250,0)$
$(21,33,14)$	7/2	$(9/50,31/50,22/375)$
$(22,34,14)$	3497/1000	$(83/250,167/250,0)$
$(23,35,14)$	3497/1000	$(71/250,121/250,19/1500)$
$(24,36,14)$	3497/1000	$(83/250,167/250,1/12)$
$(18,31,15)$	797/1000	$(27/125,44/125,0)$
$(22,35,15)$	3497/1000	$(1/250,247/250,0)$
$(23,36,15)$	4/5	$(3/125,121/125,7/1500)$
$(25,38,15)$	3497/1000	$(62/125,63/125,0)$
$(26,39,15)$	797/1000	$(54/125,61/125,1/12)$
$(24,38,16)$	3497/1000	$(0,41/125,41/1500)$
$(25,39,16)$	4/5	$(28/125,89/125,61/1500)$
$(26,40,16)$	3497/1000	$(4/25,21/25,31/750)$
$(27,41,16)$	3497/1000	$(7/25,53/125,0)$
$(28,42,16)$	3497/1000	$(61/250,189/250,61/1500)$
$(23,38,17)$	2	$(0,3/5,7/100)$
$(26,41,17)$	4/5	$(22/125,54/125,9/125)$
$(27,42,17)$	3497/1000	$(0,11/25,11/300)$

f-vector	b-ratio	generating grid point
$(28, 43, 17)$	$797/1000$	$(23/125, 46/125, 1/30)$
$(29, 44, 17)$	$3497/1000$	$(0, 3/5, 1/60)$
$(30, 45, 17)$	$3497/1000$	$(49/250, 187/250, 49/1500)$
$(25, 41, 18)$	$4/5$	$(37/250, 117/250, 9/125)$
$(27, 43, 18)$	$797/1000$	$(59/250, 19/50, 0)$
$(28, 44, 18)$	$4/5$	$(41/250, 121/250, 9/250)$
$(29, 45, 18)$	$4/5$	$(11/50, 101/250, 61/1500)$
$(30, 46, 18)$	$3497/1000$	$(12/125, 53/125, 2/125)$
$(31, 47, 18)$	$3497/1000$	$(41/125, 16/25, 59/1500)$
$(32, 48, 18)$	$3497/1000$	$(0, 83/125, 1/1500)$
$(28, 45, 19)$	$4/5$	$(4/25, 11/25, 23/300)$
$(30, 47, 19)$	$797/1000$	$(57/250, 119/250, 0)$
$(31, 48, 19)$	$3497/1000$	$(0, 13/25, 43/1500)$
$(32, 49, 19)$	$797/1000$	$(27/125, 39/125, 1/60)$
$(33, 50, 19)$	$3497/1000$	$(41/250, 209/250, 41/1500)$
$(34, 51, 19)$	$3497/1000$	$(1/5, 4/5, 1/30)$
$(30, 48, 20)$	$4/5$	$(4/25, 53/125, 22/375)$
$(33, 51, 20)$	$1/2$	$(4/125, 2/5, 16/375)$
$(35, 53, 20)$	$797/1000$	$(22/125, 11/25, 1/12)$
$(36, 54, 20)$	$3497/1000$	$(24/125, 101/125, 4/125)$
$(32, 51, 21)$	$29/25$	$(29/250, 21/50, 23/300)$
$(35, 54, 21)$	$4/5$	$(9/50, 83/250, 7/1500)$
$(37, 56, 21)$	$3497/1000$	$(6/125, 98/125, 1/125)$
$(38, 57, 21)$	$797/1000$	$(109/250, 23/50, 1/12)$
$(34, 54, 22)$	$14/25$	$(49/250, 19/50, 23/300)$
$(37, 57, 22)$	$136/125$	$(7/50, 101/250, 1/12)$
$(39, 59, 22)$	$797/1000$	$(43/250, 109/250, 1/12)$
$(40, 60, 22)$	$3497/1000$	$(13/250, 177/250, 13/1500)$
$(41, 62, 23)$	$797/1000$	$(53/250, 73/250, 61/1500)$
$(42, 63, 23)$	$797/1000$	$(21/125, 53/125, 1/12)$
$(43, 65, 24)$	$1037/1000$	$(51/250, 73/250, 53/1500)$
$(44, 66, 24)$	$797/1000$	$(41/250, 109/250, 1/12)$
$(45, 68, 25)$	$527/1000$	$(57/250, 71/250, 43/1500)$
$(46, 69, 25)$	$797/1000$	$(1/5, 37/125, 1/50)$

Space group type $(3, 5, 3, 1, 1)$**;** IT(155) $= R32$

Normalizer: IT(166) $= R\bar{3}m$ with basis $-b_1', -b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{155} = \operatorname{conv}\big\{(0,0,0), (-1/3,0,0), (-1/6,-1/2,0), (0,0,1/12), (-1/3,0,1/12), (-1/6,-1/2,1/12)\big\}$$

Upper bound on number of facets: $f_2 \le 42$ [BS06, Proposition 2.7] for points with trivial stabilizer and $f_2 \le 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 11, 7)$	$7/2$	$(-49/375, -49/125, 4/125)$
$(7, 12, 7)$	$7/2$	$(-163/750, -87/250, 2/125)$
$(8, 13, 7)$	$3497/1000$	$(-1/750, -1/250, 1/12)$
$(10, 16, 8)$	$3497/1000$	$(-247/750, -1/250, 0)$
$(6, 12, 8)$	$13/5$	$(-88/375, 0, 1/15)$
$(8, 14, 8)$	$3497/1000$	$(-1/375, 0, 1/12)$
$(11, 18, 9)$	$7/2$	$(-38/375, -29/125, 2/125)$
$(13, 20, 9)$	$797/1000$	$(-247/750, -1/250, 0)$
$(13, 21, 10)$	$3497/1000$	$(-1/3, 0, 1/12)$
$(11, 20, 11)$	$4/5$	$(-71/375, -2/125, 0)$
$(12, 21, 11)$	$5/4$	$(-4/15, -1/5, 19/750)$
$(13, 22, 11)$	$3497/1000$	$(-1/750, -1/250, 0)$
$(14, 23, 11)$	$3497/1000$	$(-83/250, -1/250, 0)$
$(15, 24, 11)$	$3497/1000$	$(-1/250, -1/250, 1/12)$
$(16, 25, 11)$	$3497/1000$	$(-63/250, -61/250, 1/1500)$
$(12, 22, 12)$	$7/2$	$(-49/375, 0, 1/125)$
$(14, 24, 12)$	$3497/1000$	$(-1/6, -1/2, 1/12)$
$(15, 25, 12)$	$4/5$	$(-17/150, -17/250, 1/12)$
$(16, 26, 12)$	$797/1000$	$(-1/750, -1/250, 0)$
$(14, 25, 13)$	$7/2$	$(-26/375, -1/5, 2/125)$
$(15, 26, 13)$	$4/5$	$(-77/375, 0, 1/60)$
$(16, 27, 13)$	$4/5$	$(-61/750, -61/250, 1/30)$
$(17, 28, 13)$	$3497/1000$	$(-101/375, 0, 2/125)$
$(18, 29, 13)$	$3497/1000$	$(-14/125, -42/125, 41/1500)$
$(19, 30, 13)$	$3497/1000$	$(-1/6, -1/2, 0)$
$(20, 31, 13)$	$3497/1000$	$(-83/250, -1/250, 1/1500)$
$(15, 27, 14)$	$7/5$	$(-67/375, -29/125, 1/15)$
$(16, 28, 14)$	$4/5$	$(-77/375, -24/125, 1/60)$
$(17, 29, 14)$	$7/2$	$(-11/50, -1/50, 2/75)$
$(18, 30, 14)$	$3497/1000$	$(-2/375, -1/125, 1/12)$
$(19, 31, 14)$	$3497/1000$	$(-247/750, -1/250, 1/1500)$
$(20, 32, 14)$	$797/1000$	$(-43/375, 0, 1/12)$
$(21, 33, 14)$	$797/1000$	$(-23/375, -23/125, 79/1500)$
$(22, 34, 14)$	$797/1000$	$(-9/125, 0, 1/12)$
$(24, 36, 14)$	$797/1000$	$(-1/3, 0, 1/12)$
$(19, 32, 15)$	$7/2$	$(-49/375, -31/125, 4/375)$
$(20, 33, 15)$	$527/1000$	$(-203/750, -47/250, 0)$
$(21, 34, 15)$	$3497/1000$	$(-32/125, -11/125, 3/250)$
$(22, 35, 15)$	$3497/1000$	$(-67/250, -1/250, 2/125)$
$(23, 36, 15)$	$3497/1000$	$(-121/750, -43/250, 1/1500)$
$(24, 37, 15)$	$797/1000$	$(-1/150, -3/250, 1/12)$
$(16, 30, 16)$	$5/4$	$(0, 0, 1/150)$
$(19, 33, 16)$	$4/5$	$(-76/375, -22/125, 1/20)$
$(21, 35, 16)$	$4/5$	$(-103/750, -7/50, 1/20)$
$(22, 36, 16)$	$3497/1000$	$(-1/3, 0, 31/1500)$
$(23, 37, 16)$	$797/1000$	$(-2/25, -4/25, 1/20)$
$(24, 38, 16)$	$3497/1000$	$(-163/750, -1/250, 43/1500)$
$(25, 39, 16)$	$797/1000$	$(-81/250, -3/250, 0)$
$(26, 40, 16)$	$797/1000$	$(-2/375, 0, 1/1500)$

f-vector	b-ratio	generating grid point
$(23, 38, 17)$	797/1000	$(-46/375, -19/125, 1/12)$
$(24, 39, 17)$	4/5	$(-163/750, -9/50, 1/60)$
$(25, 40, 17)$	3497/1000	$(-1/6, -77/250, 2/125)$
$(26, 41, 17)$	3497/1000	$(-77/250, -7/250, 1/250)$
$(27, 42, 17)$	797/1000	$(-11/375, -11/125, 1/12)$
$(28, 43, 17)$	797/1000	$(-4/125, -11/125, 1/12)$
$(25, 41, 18)$	4/5	$(-13/150, -9/50, 1/12)$
$(27, 43, 18)$	4/5	$(-91/375, -1/5, 1/20)$
$(28, 44, 18)$	3497/1000	$(-82/375, -1/125, 7/250)$
$(29, 45, 18)$	797/1000	$(-3/50, -9/50, 4/75)$
$(30, 46, 18)$	797/1000	$(-7/125, -21/125, 83/1500)$
$(26, 43, 19)$	2	$(-32/125, -24/125, 3/250)$
$(27, 44, 19)$	7/2	$(-181/750, -37/250, 1/375)$
$(28, 45, 19)$	797/1000	$(-44/375, -19/125, 1/12)$
$(29, 46, 19)$	3497/1000	$(-191/750, -31/250, 7/750)$
$(30, 47, 19)$	3497/1000	$(-39/125, -3/125, 1/300)$
$(31, 48, 19)$	3497/1000	$(-1/6, -1/2, 1/1500)$
$(32, 49, 19)$	797/1000	$(-1/30, -23/250, 1/12)$
$(29, 47, 20)$	44/25	$(-33/125, -1/5, 1/60)$
$(31, 49, 20)$	4/5	$(-76/375, -24/125, 1/300)$
$(32, 50, 20)$	3497/1000	$(-41/125, -1/125, 1/1500)$
$(33, 51, 20)$	797/1000	$(-28/375, -23/125, 1/12)$
$(34, 52, 20)$	797/1000	$(-19/375, -19/125, 29/500)$
$(31, 50, 21)$	7/2	$(-101/375, -22/125, 2/375)$
$(32, 51, 21)$	7/5	$(-103/375, -18/125, 1/20)$
$(33, 52, 21)$	3497/1000	$(-19/75, -4/25, 1/150)$
$(34, 53, 21)$	3497/1000	$(-79/250, -1/50, 1/375)$
$(35, 54, 21)$	797/1000	$(-13/150, -7/50, 1/12)$
$(36, 55, 21)$	797/1000	$(-17/375, -16/125, 1/12)$
$(33, 53, 22)$	7/2	$(-197/750, -47/250, 1/250)$
$(35, 55, 22)$	4/5	$(-86/375, -26/125, 1/60)$
$(36, 56, 22)$	3497/1000	$(-199/750, -37/250, 7/1500)$
$(38, 58, 22)$	797/1000	$(-26/375, -24/125, 1/12)$
$(38, 59, 23)$	3497/1000	$(-98/375, -16/125, 11/1500)$
$(40, 61, 23)$	797/1000	$(-53/750, -43/250, 1/12)$
$(39, 61, 24)$	7/8	$(-8/125, -22/125, 61/750)$
$(40, 62, 24)$	3497/1000	$(-33/125, -22/125, 7/1500)$
$(42, 64, 24)$	797/1000	$(-19/250, -39/250, 1/12)$
$(44, 67, 25)$	797/1000	$(-1/15, -24/125, 1/12)$
$(48, 73, 27)$	797/1000	$(-193/750, -53/250, 6/125)$

Space group type $(3, 5, 4, 2, 1)$**;** IT(156) $= P3m1$

Normalizer: IT(191) $= P^16/mmm$ with basis $\frac{2}{3}b'_1 + \frac{1}{3}b'_2, -\frac{1}{3}b'_1 + \frac{1}{3}b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{156} = \text{conv}\left\{(0,0,0),(1/6,0,0),(1/6,1/6,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/6, 1/6, 0)$
$(8, 12, 6)$	3497/1000	$(1/6, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 5, 4, 3, 1)$**;** IT(157) $= P31m$

Normalizer: IT(191) $= P^1 6/mmm$ with basis $b_1', b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{157} = \text{conv}\left\{(0,0,0), (1/3,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 5, 4, 2, 2)$**;** IT(158) $= P3c1$

Normalizer: IT(191) $= P^1 6/mmm$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{158} = \text{conv}\left\{(0,0,0), (1/6,0,0), (1/6,1/6,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/6, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(14, 24, 12)$	3497/1000	$(1/6, 1/6, 0)$
$(18, 30, 14)$	527/1000	$(1/6, 1/6, 0)$

Space group type $(3, 5, 4, 3, 2)$**;** IT(159) $= P31c$

Normalizer: IT(191) $= P^1 6/mmm$ with basis $b'_1, b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{159} = \operatorname{conv}\left\{(0, 0, 0), (1/3, 0, 0), (1/4, -1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(8, 14, 8)$	3497/1000	$(1412/4239, 0, 0)$
$(14, 22, 10)$	797/1000	$(1412/4239, 0, 0)$
$(14, 24, 12)$	3497/1000	$(1/3, 0, 0)$
$(18, 30, 14)$	3497/1000	$(5647/16956, -1/5652, 0)$
$(21, 33, 14)$	797/1000	$(5647/16956, -1/5652, 0)$
$(22, 36, 16)$	797/1000	$(703/4239, -10/1413, 0)$
$(25, 39, 16)$	797/1000	$(5645/16956, -1/1884, 0)$

Space group type $(3, 5, 4, 1, 1)$**;** IT(160) $= R3m$

Normalizer: IT(162) $= P^1\bar{3}1m$ with basis $\frac{2}{3}b'_1 + \frac{1}{3}b'_2, -\frac{1}{3}b'_1 + \frac{1}{3}b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{160} = \operatorname{conv}\left\{(0, 0, 0), (1/6, 0, 0), (1/6, 1/6, 0), (1/12, 1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(4, 6, 4)$	$1/2$	$(5/36, 5/36, 0)$
$(5, 8, 5)$	$1/2$	$(1831/11988, 721/3996, 0)$
$(6, 9, 5)$	$3497/1000$	$(1/6, 1/6, 0)$
$(7, 11, 6)$	$1/2$	$(1/9, 1/6, 0)$
$(10, 15, 7)$	$797/1000$	$(250/2997, 749/2997, 0)$
$(8, 13, 7)$	$1/2$	$(1/9, 2/9, 0)$
$(9, 14, 7)$	$1/2$	$(1333/11988, 1997/11988, 0)$
$(10, 16, 8)$	$1/2$	$(443/3996, 667/3996, 0)$
$(12, 18, 8)$	$797/1000$	$(383/3996, 383/3996, 0)$
$(8, 14, 8)$	$3497/1000$	$(1/6, 0, 0)$
$(9, 15, 8)$	$1/2$	$(38/333, 53/333, 0)$
$(14, 21, 9)$	$797/1000$	$(575/5994, 32/333, 0)$
$(14, 24, 12)$	$3497/1000$	$(0, 0, 0)$
$(19, 29, 12)$	$797/1000$	$(7/162, 7/54, 0)$
$(20, 32, 14)$	$527/1000$	$(1/6, 0, 0)$
$(21, 33, 14)$	$797/1000$	$(575/11988, 575/3996, 0)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 0)$

Space group type $(3, 5, 4, 1, 2)$**;** IT(161) $= R3c$

Normalizer: IT(162) $= P^1\bar{3}1m$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{161} = \operatorname{conv}\big\{(0, 0, 0), (1/6, 0, 0), (1/6, 1/6, 0), (1/12, 1/4, 0)\big\}$$

Upper bound on number of facets: $f_2 \leq 42$ [BS06, Proposition 2.7] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 14, 8)$	$3497/1000$	$(1/6, 0, 0)$
$(8, 16, 10)$	2	$(1/18, 1/18, 0)$
$(11, 21, 12)$	2	$(1/6, 1/6, 0)$
$(13, 23, 12)$	2	$(1/9, 2/9, 0)$
$(14, 24, 12)$	$3497/1000$	$(0, 0, 0)$
$(19, 29, 12)$	$797/1000$	$(893/11988, 893/3996, 0)$
$(18, 30, 14)$	$797/1000$	$(1/6, 1/6, 0)$
$(19, 31, 14)$	2	$(221/3996, 223/3996, 0)$
$(20, 32, 14)$	$797/1000$	$(1/6, 0, 0)$

f-vector	b-ratio	generating grid point
$(21, 33, 14)$	$709/500$	$(166/2997, 166/999, 0)$
$(22, 34, 14)$	$797/1000$	$(1211/11988, 787/3996, 0)$
$(24, 36, 14)$	$797/1000$	$(0, 0, 0)$
$(24, 38, 16)$	$797/1000$	$(787/5994, 605/2997, 0)$
$(26, 40, 16)$	$797/1000$	$(1271/11988, 727/3996, 0)$
$(28, 44, 18)$	$797/1000$	$(565/3996, 211/1332, 0)$
$(30, 46, 18)$	$1397/1000$	$(1331/11988, 455/3996, 0)$
$(32, 50, 20)$	$527/1000$	$(428/2997, 1081/5994, 0)$

Space group type $(3, 5, 5, 2, 1)$**;** IT(162) $= P\bar{3}1m$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{162} = \operatorname{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), \\ (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(1/3, 0, 0)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 16, 8)$	$3497/1000$	$(33/100, -1/500, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(8, 14, 8)$	$4/5$	$(3/25, -8/125, 1/20)$
$(14, 22, 10)$	$3497/1000$	$(88/375, -29/125, 1/500)$
$(14, 24, 12)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(18, 30, 14)$	$3497/1000$	$(117/500, -117/500, 1/500)$

Space group type $(3, 5, 5, 2, 2)$**;** IT(163) $= P\bar{3}1c$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{163} = \operatorname{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), \\ (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(36/125, -16/125, 1/4)$
$(6, 9, 5)$	$3497/1000$	$(1/3, 0, 0)$
$(7, 11, 6)$	$4/5$	$(29/100, -13/100, 1/4)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$3497/1000$	$(499/1500, -1/500, 13/500)$
$(6, 11, 7)$	$4/5$	$(16/125, 0, 1/5)$
$(8, 13, 7)$	$3497/1000$	$(124/375, 0, 31/125)$
$(11, 17, 8)$	$3497/1000$	$(124/375, 0, 13/500)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(6, 12, 8)$	$4/5$	$(4/25, 0, 1/4)$
$(8, 14, 8)$	$3497/1000$	$(124/375, 0, 1/4)$
$(10, 18, 10)$	2	$(11/50, -1/50, 1/20)$
$(13, 21, 10)$	$3497/1000$	$(1/3, 0, 31/125)$
$(14, 22, 10)$	$797/1000$	$(124/375, 0, 1/4)$
$(14, 23, 11)$	$3497/1000$	$(33/100, -1/500, 0)$
$(15, 24, 11)$	$3497/1000$	$(1/3, 0, 13/500)$
$(11, 21, 12)$	$5/4$	$(3/25, -3/25, 3/25)$
$(13, 23, 12)$	$4/5$	$(29/125, -13/125, 1/5)$
$(14, 24, 12)$	$3497/1000$	$(1/3, 0, 1/4)$
$(18, 30, 14)$	$3497/1000$	$(121/500, -121/500, 1/500)$
$(20, 32, 14)$	$3497/1000$	$(33/100, -1/500, 2/125)$
$(24, 38, 16)$	$3497/1000$	$(33/100, -1/500, 13/500)$

Space group type $(3, 5, 5, 3, 1)$**;** IT(164) $= P\bar{3}m1$

Normalizer: IT(191) $= P6/mmm$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{164} = \operatorname{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5, 8, 5)$	$4/5$	$(36/125, -16/125, 1/4)$
$(6, 9, 5)$	$3497/1000$	$(1/3, 0, 0)$
$(7, 11, 6)$	$4/5$	$(29/100, -13/100, 1/4)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$3497/1000$	$(33/100, -1/500, 3/250)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(6, 12, 8)$	$4/5$	$(4/25, 0, 1/4)$
$(8, 14, 8)$	$3497/1000$	$(124/375, 0, 1/4)$
$(14, 22, 10)$	$3497/1000$	$(124/375, 0, 3/250)$

f-vector	b-ratio	generating grid point
$(14, 24, 12)$	$3497/1000$	$(1/3, 0, 1/4)$
$(18, 30, 14)$	$3497/1000$	$(1/3, 0, 7/500)$

Space group type $(3, 5, 5, 3, 2)$**;** IT(165) $= P\bar{3}c1$

Normalizer: IT(191) $= P6/mmm$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{165} = \text{conv}\,\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(1/3, 0, 0)$
$(7, 11, 6)$	2	$(29/100, -13/100, 1/5)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 16, 8)$	$3497/1000$	$(33/100, -1/500, 1/4)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(6, 12, 8)$	2	$(4/25, 0, 1/5)$
$(8, 14, 8)$	$3497/1000$	$(37/125, 0, 111/500)$
$(10, 18, 10)$	$5/4$	$(1/5, -1/5, 8/125)$
$(13, 21, 10)$	$3497/1000$	$(31/125, -31/125, 31/125)$
$(14, 22, 10)$	$3497/1000$	$(124/375, 0, 31/125)$
$(14, 23, 11)$	$3497/1000$	$(33/100, -1/500, 0)$
$(15, 24, 11)$	$3497/1000$	$(121/500, -121/500, 1/500)$
$(14, 24, 12)$	$3497/1000$	$(31/125, -31/125, 1/4)$
$(15, 26, 13)$	$7/2$	$(23/125, -7/125, 1/250)$
$(16, 27, 13)$	$3497/1000$	$(161/500, -13/500, 111/500)$
$(18, 30, 14)$	$3497/1000$	$(1/3, 0, 31/125)$
$(20, 32, 14)$	$3497/1000$	$(36/125, -13/125, 1/500)$
$(17, 30, 15)$	$4/5$	$(6/25, -28/125, 7/100)$
$(20, 33, 15)$	$3497/1000$	$(307/1500, -97/500, 1/125)$
$(22, 35, 15)$	$3497/1000$	$(33/100, -1/500, 123/500)$
$(24, 38, 16)$	$527/1000$	$(59/250, -43/250, 31/125)$
$(26, 41, 17)$	$3497/1000$	$(41/125, -1/125, 6/25)$
$(26, 42, 18)$	$3497/1000$	$(91/375, -6/25, 1/500)$

Space group type $(3, 5, 5, 1, 1)$**;** IT(166) $= R\bar{3}m$

Normalizer: IT(166) $= R\bar{3}m$ with basis $-b'_1, -b'_2, \frac{1}{2}b'_3$; so the normalizer is identical with the group itself but the basis is different.

Reduced fundamental domain:

$$R_{166} = \text{conv}\left\{(0,0,0), (-1/3,0,0), (-1/6,-1/2,0), (0,0,1/12), (-1/3,0,1/12), (-1/6,-1/2,1/12)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: In Dress et al. [DHM93] a stereohedron with 6 facets for this group is presented.

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5,8,5)$	$7/2$	$(-11/50,-1/50,2/75)$
$(6,9,5)$	$3497/1000$	$(-1/250,-1/250,1/12)$
$(8,12,6)$	$797/1000$	$(-59/750,-49/250,1/12)$
$(10,15,7)$	$3497/1000$	$(-163/750,-1/250,43/1500)$
$(6,11,7)$	$7/2$	$(-49/375,-49/125,4/125)$
$(7,12,7)$	$7/2$	$(-163/750,-87/250,2/125)$
$(8,13,7)$	$3497/1000$	$(-1/750,-1/250,1/12)$
$(9,14,7)$	$3497/1000$	$(-1/150,-1/250,0)$
$(10,16,8)$	$4/5$	$(-17/150,-9/250,1/12)$
$(11,17,8)$	$797/1000$	$(-19/375,-16/125,1/12)$
$(12,18,8)$	$3497/1000$	$(-67/250,-1/250,2/125)$
$(6,12,8)$	$13/5$	$(-88/375,0,1/15)$
$(8,14,8)$	$3497/1000$	$(-1/375,0,1/12)$
$(11,18,9)$	$797/1000$	$(-1/15,-1/5,1/12)$
$(12,19,9)$	$797/1000$	$(-1/150,-1/250,0)$
$(13,20,9)$	$797/1000$	$(-17/375,-8/125,1/150)$
$(14,21,9)$	$797/1000$	$(-19/250,-1/250,1/12)$
$(13,21,10)$	$3497/1000$	$(-1/3,0,1/12)$
$(14,22,10)$	$4/5$	$(-32/375,-3/25,1/60)$
$(15,23,10)$	$1/2$	$(-13/375,-2/25,17/250)$
$(16,24,10)$	$797/1000$	$(-1/30,-23/250,1/12)$
$(12,21,11)$	$5/4$	$(-4/15,-1/5,19/750)$
$(13,22,11)$	$3497/1000$	$(-1/750,-1/250,0)$
$(14,23,11)$	$3497/1000$	$(-83/250,-1/250,0)$
$(15,24,11)$	$4/5$	$(-19/250,-39/250,1/20)$
$(16,25,11)$	$3497/1000$	$(-63/250,-61/250,1/1500)$
$(17,26,11)$	$4/5$	$(-7/150,-33/250,1/20)$
$(18,27,11)$	$797/1000$	$(-17/375,-16/125,1/12)$
$(12,22,12)$	$7/2$	$(-49/375,0,1/125)$
$(14,24,12)$	$3497/1000$	$(-1/6,-1/2,1/12)$
$(15,25,12)$	$7/8$	$(-38/375,0,29/375)$
$(16,26,12)$	$797/1000$	$(-1/750,-1/250,0)$
$(18,28,12)$	$1/2$	$(-13/250,-31/250,3/50)$
$(20,30,12)$	$797/1000$	$(-26/375,-24/125,1/12)$

f-vector	b-ratio	generating grid point
$(15, 26, 13)$	$4/5$	$(-77/375, 0, 1/60)$
$(16, 27, 13)$	$4/5$	$(-61/750, -61/250, 1/30)$
$(17, 28, 13)$	$3497/1000$	$(-101/375, 0, 2/125)$
$(18, 29, 13)$	$3497/1000$	$(-14/125, -42/125, 41/1500)$
$(19, 30, 13)$	$3497/1000$	$(-1/6, -1/2, 0)$
$(20, 31, 13)$	$3497/1000$	$(-83/250, -1/250, 1/1500)$
$(22, 33, 13)$	$797/1000$	$(-1/150, -3/250, 1/1500)$
$(20, 32, 14)$	$797/1000$	$(-43/375, 0, 1/12)$
$(21, 33, 14)$	$797/1000$	$(-23/375, -23/125, 79/1500)$
$(22, 34, 14)$	$797/1000$	$(-9/125, 0, 1/12)$
$(24, 36, 14)$	$797/1000$	$(-1/3, 0, 1/12)$
$(20, 33, 15)$	$527/1000$	$(-203/750, -47/250, 0)$
$(16, 30, 16)$	$5/4$	$(0, 0, 1/150)$
$(22, 36, 16)$	$3497/1000$	$(-1/3, 0, 31/1500)$
$(23, 37, 16)$	$7/8$	$(-19/375, -19/125, 29/750)$
$(24, 38, 16)$	$1/2$	$(-94/375, -31/125, 1/750)$
$(26, 40, 16)$	$797/1000$	$(-2/375, 0, 1/1500)$
$(25, 40, 17)$	$1/2$	$(-3/10, -1/10, 1/15)$
$(27, 42, 17)$	$797/1000$	$(-11/375, -11/125, 1/12)$
$(29, 45, 18)$	$797/1000$	$(-3/50, -9/50, 4/75)$
$(30, 46, 18)$	$797/1000$	$(-7/125, -21/125, 83/1500)$
$(29, 46, 19)$	$4/5$	$(-16/375, -16/125, 1/20)$
$(31, 48, 19)$	$3497/1000$	$(-1/6, -1/2, 1/1500)$
$(34, 52, 20)$	$797/1000$	$(-19/375, -19/125, 29/500)$
$(34, 53, 21)$	$797/1000$	$(-49/750, -49/250, 1/12)$
$(38, 58, 22)$	$527/1000$	$(-16/375, -16/125, 31/500)$

Space group type $(3, 5, 5, 1, 2)$**;** IT(167) $= R\bar{3}c$

Normalizer: IT(166) $= R\bar{3}m$ with basis $-b_1', -b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{167} = \operatorname{conv}\big\{(0,0,0), (-1/3,0,0), (-1/6,-1/2,0), (0,0,1/12), (-1/3,0,1/12), (-1/6,-1/2,1/12)\big\}$$

Upper bound on number of facets: $f_2 \leq 79$ [BS06, Corollary 2.8] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(-1/250, -1/250, 0)$
$(10, 15, 7)$	$797/1000$	$(-22/125, -22/125, 0)$
$(6, 11, 7)$	$7/2$	$(-29/125, -38/125, 77/1500)$
$(8, 13, 7)$	$3497/1000$	$(-37/375, 0, 22/375)$
$(12, 18, 8)$	$797/1000$	$(-1/250, -1/250, 0)$

f-vector	b-ratio	generating grid point
$(10, 17, 9)$	3497/1000	$(-1/250, -1/250, 1/12)$
$(14, 21, 9)$	797/1000	$(-51/250, -51/250, 0)$
$(12, 20, 10)$	7/2	$(-1/6, -107/250, 8/125)$
$(13, 21, 10)$	3497/1000	$(-1/6, -1/2, 41/500)$
$(12, 21, 11)$	7/2	$(-223/750, -27/250, 29/1500)$
$(13, 22, 11)$	3497/1000	$(-1/750, -1/250, 0)$
$(14, 23, 11)$	3497/1000	$(-1/375, 0, 1/12)$
$(16, 25, 11)$	3497/1000	$(-31/375, 0, 47/750)$
$(12, 22, 12)$	7/2	$(-49/375, -49/125, 4/125)$
$(13, 23, 12)$	4/5	$(-119/750, -17/250, 0)$
$(14, 24, 12)$	3497/1000	$(-1/6, -1/2, 1/12)$
$(15, 25, 12)$	7/2	$(-223/750, -1/250, 29/1500)$
$(16, 26, 12)$	3497/1000	$(-1/150, -1/250, 0)$
$(18, 28, 12)$	797/1000	$(-7/250, -7/250, 1/12)$
$(19, 29, 12)$	527/1000	$(-4/25, -48/125, 1/12)$
$(13, 24, 13)$	7/2	$(-11/50, -13/50, 3/100)$
$(14, 25, 13)$	1/2	$(-1/6, -43/250, 8/125)$
$(15, 26, 13)$	7/2	$(-14/75, -7/125, 4/125)$
$(16, 27, 13)$	3497/1000	$(-73/750, -1/250, 22/375)$
$(17, 28, 13)$	3497/1000	$(-1/750, -1/250, 31/375)$
$(18, 29, 13)$	3497/1000	$(-64/375, 0, 61/1500)$
$(19, 30, 13)$	3497/1000	$(-1/3, 0, 1/12)$
$(20, 31, 13)$	3497/1000	$(-1/375, 0, 31/375)$
$(21, 32, 13)$	797/1000	$(-8/75, -33/125, 1/12)$
$(17, 29, 14)$	7/2	$(-29/150, -1/50, 1/25)$
$(18, 30, 14)$	797/1000	$(-1/6, -49/250, 1/12)$
$(19, 31, 14)$	3497/1000	$(-247/750, -1/250, 1/1500)$
$(20, 32, 14)$	3497/1000	$(-56/375, -6/25, 13/500)$
$(21, 33, 14)$	3497/1000	$(-1/6, -1/250, 59/1500)$
$(22, 34, 14)$	3497/1000	$(-49/150, -1/250, 2/375)$
$(23, 35, 14)$	797/1000	$(-71/750, -69/250, 1/12)$
$(24, 36, 14)$	3497/1000	$(-1/3, 0, 1/500)$
$(17, 30, 15)$	7/2	$(-16/75, -37/125, 2/125)$
$(19, 32, 15)$	3497/1000	$(-13/50, -1/10, 1/20)$
$(20, 33, 15)$	3497/1000	$(-64/375, -1/125, 1/25)$
$(21, 34, 15)$	3497/1000	$(-88/375, -14/125, 23/1500)$
$(22, 35, 15)$	3497/1000	$(-1/250, -1/250, 41/500)$
$(23, 36, 15)$	797/1000	$(-41/150, -3/50, 1/100)$
$(24, 37, 15)$	3497/1000	$(-39/125, -7/125, 41/1500)$
$(21, 35, 16)$	3497/1000	$(-29/150, -11/50, 1/60)$
$(22, 36, 16)$	3497/1000	$(-1/6, -1/2, 31/750)$
$(23, 37, 16)$	3497/1000	$(-61/750, -1/250, 1/60)$
$(24, 38, 16)$	3497/1000	$(-43/250, -1/250, 1/25)$
$(25, 39, 16)$	3497/1000	$(-247/750, -1/250, 1/250)$
$(26, 40, 16)$	797/1000	$(-13/125, -39/125, 0)$
$(23, 38, 17)$	1/2	$(-1/5, -1/5, 1/15)$
$(24, 39, 17)$	4/5	$(-39/250, -33/250, 1/30)$
$(25, 40, 17)$	797/1000	$(-29/125, -31/125, 7/250)$
$(26, 41, 17)$	3497/1000	$(-7/75, -1/125, 89/1500)$

f-vector	b-ratio	generating grid point
$(27, 42, 17)$	$797/1000$	$(-6/125, 0, 107/1500)$
$(28, 43, 17)$	$3497/1000$	$(-41/125, -1/125, 7/1500)$
$(25, 41, 18)$	$1/2$	$(-37/150, -63/250, 11/300)$
$(26, 42, 18)$	$3497/1000$	$(-149/750, -37/250, 8/375)$
$(27, 43, 18)$	$3497/1000$	$(-57/250, -73/250, 1/100)$
$(28, 44, 18)$	$3497/1000$	$(-86/375, -32/125, 7/1500)$
$(29, 45, 18)$	$797/1000$	$(-4/25, 0, 13/300)$
$(30, 46, 18)$	$797/1000$	$(-22/375, 0, 103/1500)$
$(27, 44, 19)$	$1/2$	$(-161/750, -53/250, 2/25)$
$(29, 46, 19)$	$4/5$	$(-13/75, -59/125, 2/25)$
$(30, 47, 19)$	$3497/1000$	$(-1/150, -1/250, 61/750)$
$(31, 48, 19)$	$3497/1000$	$(-1/6, -1/2, 1/1500)$
$(32, 49, 19)$	$3497/1000$	$(-77/250, -7/250, 7/500)$
$(30, 48, 20)$	$3497/1000$	$(-21/125, -26/125, 3/125)$
$(31, 49, 20)$	$527/1000$	$(-59/250, -59/250, 11/250)$
$(32, 50, 20)$	$3497/1000$	$(-24/125, -44/125, 37/1500)$
$(33, 51, 20)$	$797/1000$	$(-83/375, -41/125, 43/1500)$
$(34, 52, 20)$	$797/1000$	$(-1/15, 0, 1/15)$
$(34, 53, 21)$	$3497/1000$	$(-37/750, -1/250, 53/750)$
$(35, 54, 21)$	$181/200$	$(-139/750, -89/250, 11/300)$
$(36, 55, 21)$	$797/1000$	$(-53/375, -6/125, 11/250)$
$(35, 55, 22)$	2	$(-17/75, -39/125, 7/250)$
$(36, 56, 22)$	$527/1000$	$(-173/750, -57/250, 17/375)$
$(37, 57, 22)$	$769/500$	$(-68/375, -52/125, 1/15)$
$(38, 58, 22)$	$797/1000$	$(-14/125, 0, 83/1500)$
$(39, 60, 23)$	$131/100$	$(-29/125, -7/25, 9/500)$
$(40, 61, 23)$	$797/1000$	$(-127/750, -111/250, 109/1500)$
$(42, 64, 24)$	$299/250$	$(-169/750, -71/250, 19/1500)$
$(44, 67, 25)$	$649/500$	$(-91/375, -33/125, 17/1500)$
$(46, 70, 26)$	$323/250$	$(-41/250, -1/250, 59/750)$

2.2.4 Hexagonal groups

The remarks at the beginning of Subsection 2.2.3 apply here as well.

Space group type $(3, 6, 1, 1, 1)$**;** IT(168) $= P6$

Normalizer: IT(191) $= P^1 6/mmm$ with basis $b_1', b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{168} = \operatorname{conv}\left\{(0,0,0), (1/3, 0, 0), (1/4, -1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(1/3, 0, 0)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$3497/1000$	$(5647/16956, -1/5652, 0)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$

Space group type $(3, 6, 1, 1, 4)$**;** IT(169) $= P6_1$**,** IT(170) $= P6_5$

Normalizer: IT(177) $= P^1622$ with basis $b'_1, b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{169} = \text{conv}\left\{(0, 0, 0), (1/3, 0, 0), (1/4, 1/4, 0), (1/4, -1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 48$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(14, 24, 12)$	$3497/1000$	$(1/3, 0, 0)$
$(18, 28, 12)$	$3497/1000$	$(1997/5994, 0, 0)$
$(18, 30, 14)$	$797/1000$	$(1/3, 0, 0)$
$(22, 34, 14)$	$797/1000$	$(1997/5994, 0, 0)$
$(24, 36, 14)$	$3497/1000$	$(1/4, -1/4, 0)$
$(25, 39, 16)$	2	$(2/9, 1/9, 0)$
$(28, 42, 16)$	$797/1000$	$(1/4, -1/4, 0)$
$(26, 42, 18)$	$1/2$	$(1/27, 0, 0)$
$(29, 45, 18)$	$4/5$	$(2/9, 2/9, 0)$
$(30, 46, 18)$	$797/1000$	$(1885/5994, 0, 0)$
$(32, 48, 18)$	$797/1000$	$(1595/5994, 403/1998, 0)$
$(36, 54, 20)$	$797/1000$	$(1/4, 715/3996, 0)$
$(40, 60, 22)$	$797/1000$	$(1/4, 685/3996, 0)$
$(44, 66, 24)$	$797/1000$	$(1/4, 5/148, 0)$
$(48, 72, 26)$	$797/1000$	$(55/1998, 5/1998, 0)$

Space group type $(3, 6, 1, 1, 2)$**;** IT(171) $= P6_2$**,** IT(172) $= P6_4$

Normalizer: IT(177) $= P^1622$ with basis $b'_1, b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{171} = \text{conv}\left\{(0, 0, 0), (1/3, 0, 0), (1/4, 1/4, 0), (1/4, -1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 36$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $^1/_2, \dots, ^7/_2$ in 1001 steps of $^3/_{1000}$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 000 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(12, 19, 9)$	3497/1000	$(1/6, 0, 0)$
$(12, 23, 13)$	1/2	$(17/54, 1/18, 0)$
$(18, 29, 13)$	3497/1000	$(1499/5994, 499/1998, 0)$
$(20, 31, 13)$	797/1000	$(1/6, 0, 0)$
$(18, 30, 14)$	1/2	$(1/18, 1/18, 0)$
$(20, 32, 14)$	1/2	$(5/27, 4/27, 0)$
$(21, 33, 14)$	1/2	$(293/999, 1/18, 0)$
$(22, 34, 14)$	3497/1000	$(1/4, 997/3996, 0)$
$(23, 35, 14)$	3497/1000	$(28/111, 15/74, 0)$
$(24, 36, 14)$	3497/1000	$(1/4, -1/4, 0)$
$(18, 31, 15)$	797/1000	$(1499/5994, 499/1998, 0)$
$(20, 33, 15)$	1/2	$(1/54, 0, 0)$
$(22, 35, 15)$	3497/1000	$(166/999, 0, 0)$
$(23, 36, 15)$	1/2	$(17/54, 19/666, 0)$
$(26, 39, 15)$	797/1000	$(1/4, 467/3996, 0)$
$(24, 38, 16)$	797/1000	$(499/1998, 499/1998, 0)$
$(25, 39, 16)$	7/8	$(104/333, 35/666, 0)$
$(27, 41, 16)$	797/1000	$(1/4, 997/3996, 0)$
$(28, 42, 16)$	3497/1000	$(1499/5994, 83/333, 0)$
$(27, 42, 17)$	1/2	$(17/54, 55/999, 0)$
$(30, 45, 17)$	797/1000	$(1/4, 563/3996, 0)$
$(28, 44, 18)$	1/2	$(383/1332, 19/148, 0)$
$(29, 45, 18)$	1/2	$(619/1998, 1/18, 0)$
$(31, 47, 18)$	797/1000	$(3001/11988, 331/1332, 0)$
$(32, 48, 18)$	3497/1000	$(665/3996, 1/3996, 0)$
$(31, 48, 19)$	1/2	$(47/1998, 5/666, 0)$
$(34, 51, 19)$	797/1000	$(3431/11988, 563/3996, 0)$
$(33, 51, 20)$	1/2	$(943/2997, 1/18, 0)$
$(35, 53, 20)$	797/1000	$(3005/11988, 989/3996, 0)$
$(36, 54, 20)$	797/1000	$(286/999, 227/1998, 0)$
$(38, 57, 21)$	797/1000	$(1715/5994, 47/333, 0)$
$(40, 60, 22)$	797/1000	$(52/999, 5/666, 0)$

Space group type $(3, 6, 1, 1, 3)$**;** IT(173) $= P6_3$

Normalizer: IT(191) $= P^16/mmm$ with basis $b_1', b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{173} = \operatorname{conv}\left\{(0,0,0), (1/3,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(8, 14, 8)$	3497/1000	$(1412/4239, 0, 0)$
$(14, 22, 10)$	797/1000	$(1412/4239, 0, 0)$
$(14, 24, 12)$	3497/1000	$(1/3, 0, 0)$
$(17, 27, 12)$	797/1000	$(5647/16956, -1/5652, 0)$
$(18, 30, 14)$	797/1000	$(1/3, 0, 0)$
$(21, 33, 14)$	797/1000	$(5645/16956, -1/1884, 0)$

Space group type $(3, 6, 2, 1, 1)$**;** IT(174) $= P\bar{6}$

Normalizer: IT(191) $= P6/mmm$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{174} = \text{conv}\big\{(0,0,0), (1/6,0,0), (1/6,1/6,0), (0,0,1/4), (1/6,0,1/4), (1/6,1/6,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 54$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/6, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 3, 1, 1)$**;** IT(175) $= P6/m$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{175} = \text{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(10, 15, 7)$	3497/1000	$(33/100, -1/500, 1/4)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 3, 1, 2)$; IT(176) $= P6_3/m$

Normalizer: IT(191) $= P6/mmm$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{176} = \text{conv}\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(7, 11, 6)$	4/5	$(29/100, -13/100, 1/4)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(10, 15, 7)$	3497/1000	$(33/100, -1/500, 0)$
$(6, 11, 7)$	4/5	$(16/125, 0, 1/5)$
$(8, 13, 7)$	3497/1000	$(124/375, 0, 31/125)$
$(11, 17, 8)$	3497/1000	$(124/375, 0, 13/500)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(6, 12, 8)$	4/5	$(4/25, 0, 1/4)$
$(8, 14, 8)$	3497/1000	$(124/375, 0, 1/4)$
$(11, 18, 9)$	4/5	$(87/500, -39/500, 3/20)$
$(13, 20, 9)$	3497/1000	$(33/100, -1/500, 2/125)$
$(10, 18, 10)$	5/4	$(1/5, -1/5, 8/125)$
$(12, 20, 10)$	4/5	$(29/125, -13/125, 1/5)$
$(13, 21, 10)$	3497/1000	$(1/3, 0, 31/125)$
$(14, 22, 10)$	797/1000	$(124/375, 0, 1/4)$
$(15, 24, 11)$	3497/1000	$(1/3, 0, 13/500)$
$(17, 26, 11)$	3497/1000	$(33/100, -1/500, 13/500)$
$(13, 23, 12)$	4/5	$(36/125, -16/125, 1/4)$
$(14, 24, 12)$	3497/1000	$(1/3, 0, 1/4)$
$(17, 27, 12)$	797/1000	$(33/100, -1/500, 1/4)$
$(18, 30, 14)$	797/1000	$(1/3, 0, 1/4)$
$(21, 33, 14)$	797/1000	$(493/1500, -3/500, 1/4)$

Space group type $(3,6,4,1,1)$**;** IT(177) $=$ $P622$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{177} = \operatorname{conv}\big\{(0,0,0),(1/3,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/3,0,1/4),(1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	$3497/1000$	$(1/3,0,0)$
$(8,12,6)$	$3497/1000$	$(1/4,-1/4,0)$
$(12,18,8)$	$3497/1000$	$(0,0,0)$
$(14,23,11)$	$3497/1000$	$(33/100,-1/500,1/4)$
$(18,29,13)$	$797/1000$	$(88/375,-29/125,1/500)$

Space group type $(3,6,4,1,4)$**;** IT(178) $=$ $P6_122$**,** IT(179) $=$ $P6_522$

Normalizer: IT(180) $= P6_222$ with basis $b_1', b_2', \frac{1}{2}b_3'$ (only the normalizer for IT(178) but not for IT(179))

Reduced fundamental domain:

$$R_{178} = \operatorname{conv}\big\{(0,0,0),(1/2,1/2,0),(1/2,-1/2,0),(0,0,1/12),\\ (1/2,1/2,1/12),(1/2,-1/2,1/12)\big\}$$

Upper bound on number of facets: $f_2 \leq 78$ [BS06, Proposition 4.1] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: In [BS06, Example 4.4] a stereohedron with 32 facets is constructed for this group.

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(12,18,8)$	$3497/1000$	$(0,0,0)$
$(12,19,9)$	$44/25$	$(121/250,-121/250,4/75)$
$(15,23,10)$	$3497/1000$	$(41/125,0,31/375)$
$(11,20,11)$	$4/5$	$(8/25,0,3/50)$
$(13,22,11)$	$3497/1000$	$(62/125,0,0)$
$(18,27,11)$	$3497/1000$	$(21/125,-21/125,7/250)$
$(15,25,12)$	$3497/1000$	$(62/125,61/125,1/12)$

f-vector	b-ratio	generating grid point
$(16, 26, 12)$	$797/1000$	$(62/125, 0, 0)$
$(18, 28, 12)$	$3497/1000$	$(41/125, 0, 1/12)$
$(15, 26, 13)$	2	$(2/5, 0, 11/300)$
$(16, 27, 13)$	$4/5$	$(17/50, 1/50, 0)$
$(18, 29, 13)$	$3497/1000$	$(83/250, -1/250, 0)$
$(20, 31, 13)$	$16/5$	$(1/2, 9/50, 3/100)$
$(21, 32, 13)$	$3497/1000$	$(1/250, 1/250, 121/1500)$
$(18, 30, 14)$	$4/5$	$(8/25, 0, 1/150)$
$(20, 32, 14)$	$797/1000$	$(62/125, 0, 31/375)$
$(21, 33, 14)$	$4/5$	$(69/250, 61/250, 1/15)$
$(22, 34, 14)$	$3497/1000$	$(62/125, -62/125, 1/12)$
$(23, 35, 14)$	$3497/1000$	$(1/2, -43/250, 41/1500)$
$(24, 36, 14)$	$3497/1000$	$(62/125, -62/125, 0)$
$(18, 31, 15)$	$797/1000$	$(8/25, -1/25, 0)$
$(22, 35, 15)$	$3497/1000$	$(62/125, 61/125, 0)$
$(23, 36, 15)$	$797/1000$	$(1/2, 23/50, 1/150)$
$(24, 37, 15)$	$3497/1000$	$(119/250, 67/250, 1/60)$
$(25, 38, 15)$	$3497/1000$	$(1/250, 1/250, 41/500)$
$(26, 39, 15)$	$3497/1000$	$(53/125, -6/125, 53/750)$
$(22, 36, 16)$	$4/5$	$(59/250, 9/250, 1/12)$
$(23, 37, 16)$	$797/1000$	$(3/10, 1/10, 1/12)$
$(24, 38, 16)$	$797/1000$	$(1/2, 107/250, 1/12)$
$(25, 39, 16)$	$3497/1000$	$(11/25, 0, 11/150)$
$(26, 40, 16)$	$3497/1000$	$(67/250, 1/250, 23/300)$
$(27, 41, 16)$	$3497/1000$	$(44/125, -11/125, 0)$
$(28, 42, 16)$	$3497/1000$	$(62/125, 62/125, 31/375)$
$(26, 41, 17)$	$797/1000$	$(58/125, 0, 29/375)$
$(27, 42, 17)$	$4/5$	$(23/50, -13/50, 1/60)$
$(29, 44, 17)$	$3497/1000$	$(41/250, 41/250, 41/1500)$
$(30, 45, 17)$	$3497/1000$	$(41/125, 41/125, 41/750)$
$(27, 43, 18)$	$527/1000$	$(56/125, 0, 28/375)$
$(28, 44, 18)$	$797/1000$	$(13/50, 1/250, 1/12)$
$(29, 45, 18)$	$7/2$	$(9/50, 7/50, 53/1500)$
$(30, 46, 18)$	$797/1000$	$(81/250, -17/250, 0)$
$(31, 47, 18)$	$3497/1000$	$(31/250, 31/250, 17/375)$
$(32, 48, 18)$	$3497/1000$	$(19/50, 19/50, 19/300)$
$(30, 47, 19)$	$4/5$	$(36/125, -16/125, 3/500)$
$(31, 48, 19)$	$797/1000$	$(57/250, -3/50, 7/100)$
$(32, 49, 19)$	$3497/1000$	$(29/125, 12/125, 1/300)$
$(33, 50, 19)$	$3497/1000$	$(91/250, -3/10, 91/1500)$
$(34, 51, 19)$	$3497/1000$	$(7/50, 7/50, 37/750)$
$(32, 50, 20)$	2	$(1/10, -9/250, 47/750)$
$(33, 51, 20)$	$797/1000$	$(69/250, -1/50, 2/25)$
$(34, 52, 20)$	$797/1000$	$(81/250, -11/250, 0)$
$(35, 53, 20)$	$3497/1000$	$(77/250, -1/250, 77/1500)$
$(36, 54, 20)$	$3497/1000$	$(1/2, 27/250, 19/375)$
$(35, 54, 21)$	$4/5$	$(34/125, 18/125, 39/500)$
$(36, 55, 21)$	$163/200$	$(3/125, -1/125, 1/20)$
$(37, 56, 21)$	$3497/1000$	$(1/2, 43/250, 37/1500)$

f-vector	b-ratio	generating grid point
$(38, 57, 21)$	3497/1000	$(1/2, 21/250, 73/1500)$
$(37, 57, 22)$	797/1000	$(57/250, -3/250, 2/25)$
$(38, 58, 22)$	797/1000	$(3/10, -9/250, 11/150)$
$(39, 59, 22)$	797/1000	$(38/125, -6/125, 19/375)$
$(40, 60, 22)$	3497/1000	$(1/2, 41/250, 13/500)$
$(39, 60, 23)$	797/1000	$(27/125, -1/125, 39/500)$
$(40, 61, 23)$	977/1000	$(4/125, -3/125, 1/60)$
$(41, 62, 23)$	797/1000	$(38/125, -2/125, 29/375)$
$(42, 63, 23)$	797/1000	$(113/250, -7/50, 0)$
$(41, 63, 24)$	797/1000	$(19/250, -1/250, 2/25)$
$(42, 64, 24)$	833/1000	$(69/250, -23/250, 1/20)$
$(43, 65, 24)$	797/1000	$(3/10, -9/250, 1/20)$
$(44, 66, 24)$	797/1000	$(56/125, -14/125, 0)$
$(40, 63, 25)$	7/5	$(53/250, -21/250, 71/1500)$
$(43, 66, 25)$	797/1000	$(28/125, -2/125, 39/500)$
$(44, 67, 25)$	827/1000	$(6/25, -24/125, 1/60)$
$(45, 68, 25)$	797/1000	$(77/250, -3/250, 119/1500)$
$(46, 69, 25)$	797/1000	$(3/10, -7/250, 1/20)$
$(45, 69, 26)$	797/1000	$(67/250, -3/250, 2/25)$
$(46, 70, 26)$	163/200	$(69/250, -23/250, 1/20)$
$(47, 71, 26)$	797/1000	$(69/250, -27/250, 23/500)$
$(48, 72, 26)$	797/1000	$(34/125, -12/125, 17/375)$
$(46, 71, 27)$	4/5	$(1/25, -2/125, 1/20)$
$(47, 72, 27)$	797/1000	$(37/125, -1/125, 2/25)$
$(48, 73, 27)$	797/1000	$(6/25, -24/125, 1/60)$
$(49, 74, 27)$	797/1000	$(3/10, -3/250, 2/25)$
$(50, 75, 27)$	797/1000	$(33/125, -16/125, 11/250)$
$(46, 72, 28)$	4/5	$(73/250, -3/50, 49/750)$
$(49, 75, 28)$	797/1000	$(11/250, -3/250, 4/75)$
$(51, 77, 28)$	797/1000	$(69/250, -1/10, 23/500)$
$(52, 78, 28)$	797/1000	$(34/125, -13/125, 17/375)$
$(51, 78, 29)$	4/5	$(29/125, -14/125, 1/25)$
$(53, 80, 29)$	797/1000	$(6/125, -2/125, 1/20)$
$(54, 81, 29)$	797/1000	$(67/250, -1/10, 67/1500)$
$(55, 83, 30)$	797/1000	$(33/125, -17/125, 13/375)$
$(56, 84, 30)$	797/1000	$(67/250, -27/250, 67/1500)$
$(57, 86, 31)$	1031/1000	$(51/250, -49/250, 1/300)$
$(58, 87, 31)$	797/1000	$(32/125, -3/25, 16/375)$
$(60, 90, 32)$	797/1000	$(34/125, -14/125, 17/375)$
$(62, 93, 33)$	103/125	$(57/250, -51/250, 7/750)$
$(64, 96, 34)$	163/200	$(32/125, -19/125, 43/1500)$

Space group type $(3, 6, 4, 1, 2)$**;** IT(180) $= P6_222$**,** IT(181) $= P6_422$

Normalizer: IT(180) $= P6_222$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$ (only the normalizer for IT(181) but not for IT(180))

Reduced fundamental domain:

$$R_{180} = \text{conv}\big\{(0,0,0),(1/2,1/2,0),(1/2,-1/2,0),(0,0,1/12),\\ (1/2,1/2,1/12),(1/2,-1/2,1/12)\big\}$$

Upper bound on number of facets: $f_2 \leq 78$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(9,14,7)$	3497/1000	$(62/125,0,0)$
$(11,17,8)$	797/1000	$(62/125,0,0)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(9,15,8)$	3497/1000	$(62/125,62/125,0)$
$(11,18,9)$	797/1000	$(107/250,107/250,0)$
$(11,19,10)$	4/5	$(12/25,-12/25,23/300)$
$(14,22,10)$	3497/1000	$(83/250,1/250,83/1500)$
$(15,23,10)$	3497/1000	$(62/125,-62/125,1/12)$
$(13,22,11)$	3497/1000	$(62/125,-1/125,0)$
$(14,23,11)$	1/2	$(123/250,119/250,17/750)$
$(16,25,11)$	3497/1000	$(62/125,61/125,31/375)$
$(16,26,12)$	797/1000	$(23/50,-3/10,0)$
$(15,26,13)$	4/5	$(93/250,-93/250,1/30)$
$(16,27,13)$	797/1000	$(44/125,-43/125,0)$
$(18,29,13)$	3497/1000	$(83/250,-1/250,0)$
$(19,30,13)$	797/1000	$(62/125,-1/125,0)$
$(15,27,14)$	4/5	$(47/125,0,1/60)$
$(17,29,14)$	7/2	$(38/125,38/125,3/125)$
$(18,30,14)$	797/1000	$(49/125,-49/125,1/12)$
$(19,31,14)$	3497/1000	$(62/125,12/25,0)$
$(20,32,14)$	3497/1000	$(123/250,123/250,1/1500)$
$(21,33,14)$	797/1000	$(109/250,-77/250,109/1500)$
$(22,34,14)$	3497/1000	$(62/125,-62/125,0)$
$(18,31,15)$	797/1000	$(71/250,-37/250,0)$
$(20,33,15)$	3497/1000	$(62/125,0,11/375)$
$(21,34,15)$	3497/1000	$(4/25,4/25,2/75)$
$(22,35,15)$	3497/1000	$(62/125,61/125,0)$
$(23,36,15)$	3497/1000	$(62/125,-61/125,1/1500)$
$(24,37,15)$	797/1000	$(62/125,4/125,0)$
$(26,39,15)$	797/1000	$(79/250,-3/250,79/1500)$
$(24,38,16)$	797/1000	$(89/250,-89/250,0)$
$(25,39,16)$	7/2	$(34/125,-3/125,4/375)$
$(26,40,16)$	3497/1000	$(1/2,121/250,1/1500)$
$(28,42,16)$	3497/1000	$(1/2,-1/50,1/25)$
$(27,42,17)$	7/2	$(21/50,-33/250,3/125)$
$(29,44,17)$	1037/1000	$(46/125,26/125,1/15)$
$(30,45,17)$	3497/1000	$(51/250,27/250,17/500)$

f-vector	b-ratio	generating grid point
$(29,45,18)$	$4/5$	$(62/125,48/125,1/60)$
$(31,47,18)$	$239/250$	$(44/125,19/125,2/25)$
$(32,48,18)$	$3497/1000$	$(62/125,1/125,31/375)$
$(31,48,19)$	$7/2$	$(12/25,6/125,3/125)$
$(33,50,19)$	$797/1000$	$(91/250,69/250,1/12)$
$(34,51,19)$	$3497/1000$	$(51/250,29/250,17/500)$
$(33,51,20)$	$7/2$	$(38/125,16/125,2/125)$
$(35,53,20)$	$797/1000$	$(17/50,3/50,1/30)$
$(36,54,20)$	$3497/1000$	$(51/250,33/250,17/500)$
$(34,53,21)$	$4/5$	$(38/125,-17/125,1/20)$
$(35,54,21)$	$797/1000$	$(89/250,41/250,1/12)$
$(37,56,21)$	$797/1000$	$(17/50,13/50,1/20)$
$(38,57,21)$	$3497/1000$	$(11/125,-2/125,11/750)$
$(37,57,22)$	$797/1000$	$(52/125,49/125,1/12)$
$(39,59,22)$	$3497/1000$	$(91/250,73/250,1/150)$
$(40,60,22)$	$3497/1000$	$(51/250,31/250,17/500)$
$(39,60,23)$	$797/1000$	$(2/5,9/25,1/15)$
$(41,62,23)$	$797/1000$	$(37/125,-18/125,1/30)$
$(42,63,23)$	$3497/1000$	$(19/50,-37/250,29/1500)$
$(41,63,24)$	$7/2$	$(38/125,31/125,4/375)$
$(43,65,24)$	$5/4$	$(87/250,33/250,1/30)$
$(44,66,24)$	$3497/1000$	$(11/25,49/125,1/1500)$
$(43,66,25)$	$797/1000$	$(9/25,8/25,1/12)$
$(45,68,25)$	$797/1000$	$(49/125,44/125,1/15)$
$(46,69,25)$	$3497/1000$	$(99/250,63/250,1/1500)$
$(45,69,26)$	2	$(33/125,6/25,9/125)$
$(47,71,26)$	$1289/1000$	$(37/125,-28/125,1/15)$
$(48,72,26)$	$3497/1000$	$(47/125,19/125,1/750)$
$(50,75,27)$	$3497/1000$	$(51/125,31/125,1/1500)$
$(52,78,28)$	$3497/1000$	$(9/25,17/125,1/300)$
$(54,81,29)$	$3497/1000$	$(87/250,23/250,1/500)$
$(56,84,30)$	$607/500$	$(34/125,-31/125,67/1500)$

Space group type $(3,6,4,1,3)$**;** $\mathrm{IT}(182) = P6_322$

Normalizer: $\mathrm{IT}(191) = P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{182} = \operatorname{conv}\{(0,0,0),(1/3,0,0),(1/4,-1/4,0),(0,0,1/4),(1/3,0,1/4),(1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 32$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5,8,5)$	$4/5$	$(36/125,-16/125,1/4)$
$(6,9,5)$	$3497/1000$	$(1/3,0,0)$
$(7,11,6)$	$4/5$	$(29/100,-13/100,1/4)$
$(8,12,6)$	$3497/1000$	$(1/4,-1/4,0)$
$(10,15,7)$	$3497/1000$	$(499/1500,-1/500,13/500)$
$(6,11,7)$	$4/5$	$(16/125,0,1/5)$
$(8,13,7)$	$3497/1000$	$(124/375,0,31/125)$
$(10,16,8)$	$3497/1000$	$(33/100,-1/500,0)$
$(11,17,8)$	$3497/1000$	$(124/375,0,13/500)$
$(12,18,8)$	$3497/1000$	$(0,0,0)$
$(6,12,8)$	$4/5$	$(4/25,0,1/4)$
$(8,14,8)$	$3497/1000$	$(124/375,0,1/4)$
$(10,18,10)$	$5/4$	$(1/5,-1/5,93/500)$
$(13,21,10)$	$3497/1000$	$(1/3,0,31/125)$
$(14,22,10)$	$797/1000$	$(124/375,0,1/4)$
$(15,24,11)$	$3497/1000$	$(1/3,0,13/500)$
$(14,24,12)$	$3497/1000$	$(1/3,0,1/4)$
$(15,26,13)$	$4/5$	$(29/250,-13/250,1/10)$
$(16,27,13)$	$3497/1000$	$(33/100,-1/500,123/500)$
$(17,29,14)$	$4/5$	$(29/125,-13/125,1/5)$
$(18,30,14)$	$797/1000$	$(1/3,0,1/4)$
$(17,30,15)$	$7/2$	$(23/125,-7/125,123/500)$
$(19,32,15)$	$4/5$	$(4/15,-4/125,26/125)$
$(20,33,15)$	$3497/1000$	$(17/100,-73/500,1/500)$
$(21,35,16)$	$1/2$	$(7/25,-1/25,1/5)$
$(24,38,16)$	$797/1000$	$(33/100,-1/500,31/125)$
$(26,41,17)$	$3497/1000$	$(33/100,-1/500,2/125)$
$(26,42,18)$	$3497/1000$	$(36/125,-13/125,31/125)$
$(28,44,18)$	$797/1000$	$(122/375,-2/125,31/125)$
$(30,47,19)$	$3497/1000$	$(33/100,-1/500,13/500)$

Space group type $(3,6,5,1,1)$**;** IT(183) $=$ $P6mm$

Normalizer: IT(191) $= P^16/mmm$ with basis $b_1', b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{183} = \text{conv}\left\{(0,0,0),(1/3,0,0),(1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 5, 1, 2)$; IT(184) $= P6cc$

Normalizer: IT(191) $= P^16/mmm$ with basis $b'_1, b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{184} = \text{conv}\left\{(0,0,0), (1/3,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 16$ [BS06, Corollary 1.6] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(14, 23, 11)$	3497/1000	$(5647/16956, -1/5652, 0)$

Space group type $(3, 6, 5, 1, 4)$; IT(185) $= P6_3cm$

Normalizer: IT(191) $= P^16/mmm$ with basis $b'_1, b'_2, \varepsilon b'_3$

Reduced fundamental domain:

$$R_{185} = \text{conv}\left\{(0,0,0), (1/3,0,0), (1/4,-1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b'_3\|/\|b'_1\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(10, 16, 8)$	3497/1000	$(5647/16956, -1/5652, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

f-vector	b-ratio	generating grid point
$(14, 22, 10)$	$527/1000$	$(1907/8478, -635/2826, 0)$
$(14, 24, 12)$	$3497/1000$	$(353/1413, -353/1413, 0)$
$(18, 30, 14)$	$527/1000$	$(1271/5652, -1271/5652, 0)$

Space group type $(3, 6, 5, 1, 3)$**;** IT(186) $= P6_3mc$

Normalizer: IT(191) $= P^16/mmm$ with basis $b_1', b_2', \varepsilon b_3'$

Reduced fundamental domain:

$$R_{186} = \operatorname{conv}\left\{(0, 0, 0), (1/3, 0, 0), (1/4, -1/4, 0)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. Since the fundamental domain was reduced by the normalizer to a 2-dimensional polytope, the approximation is already similarly good for each value $\|b_3'\|/\|b_1'\|$ as our approximation in the case of cubic groups. Our grid uses 1 000 405 points for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(353/1413, -353/1413, 0)$
$(8, 12, 6)$	$3497/1000$	$(1/4, -1/4, 0)$
$(10, 15, 7)$	$797/1000$	$(5647/16956, -1/5652, 0)$
$(12, 18, 8)$	$3497/1000$	$(0, 0, 0)$
$(8, 14, 8)$	$3497/1000$	$(1412/4239, 0, 0)$
$(14, 22, 10)$	$797/1000$	$(1412/4239, 0, 0)$
$(14, 24, 12)$	$3497/1000$	$(1/3, 0, 0)$
$(18, 30, 14)$	$797/1000$	$(1/3, 0, 0)$

Space group type $(3, 6, 6, 1, 1)$**;** IT(187) $= P\bar{6}m2$

Normalizer: IT(191) $= P6/mmm$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{187} = \operatorname{conv}\left\{(0, 0, 0), (1/6, 0, 0), (1/6, 1/6, 0), (0, 0, 1/4), (1/6, 0, 1/4), (1/6, 1/6, 1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	$3497/1000$	$(1/6, 1/6, 0)$

f-vector	b-ratio	generating grid point
$(8, 12, 6)$	3497/1000	$(1/6, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 6, 1, 2)$**;** IT(188) $= P\bar{6}c2$

Normalizer: IT(191) $= P6/mmm$ with basis $\frac{2}{3}b_1' + \frac{1}{3}b_2', -\frac{1}{3}b_1' + \frac{1}{3}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{188} = \text{conv}\{(0,0,0), (1/6,0,0), (1/6,1/6,0), (0,0,1/4), (1/6,0,1/4), (1/6,1/6,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/6, 1/6, 0)$
$(8, 12, 6)$	3497/1000	$(1/6, 0, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(10, 18, 10)$	1/2	$(46/375, 2/125, 14/125)$
$(13, 21, 10)$	3497/1000	$(62/375, 62/375, 31/125)$
$(15, 24, 11)$	3497/1000	$(1/6, 1/6, 1/125)$
$(14, 24, 12)$	3497/1000	$(1/6, 1/6, 1/4)$
$(18, 30, 14)$	527/1000	$(1/6, 1/6, 1/4)$

Space group type $(3, 6, 6, 2, 1)$**;** IT(189) $= P\bar{6}2m$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{189} = \text{conv}\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 18$ [BS01, Theorem 2.7] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 6, 2, 2)$; IT(190) $= P\bar{6}2c$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{190} = \text{conv}\,\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 15$ [BS01, Theorem 2.12] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(7, 11, 6)$	4/5	$(29/100, -13/100, 1/4)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(10, 15, 7)$	3497/1000	$(499/1500, -1/500, 13/500)$
$(6, 11, 7)$	4/5	$(16/125, 0, 1/5)$
$(8, 13, 7)$	3497/1000	$(124/375, 0, 31/125)$
$(11, 17, 8)$	3497/1000	$(124/375, 0, 13/500)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(6, 12, 8)$	4/5	$(4/25, 0, 1/4)$
$(8, 14, 8)$	3497/1000	$(124/375, 0, 1/4)$
$(13, 21, 10)$	3497/1000	$(1/3, 0, 31/125)$
$(14, 22, 10)$	797/1000	$(124/375, 0, 1/4)$
$(15, 23, 10)$	3497/1000	$(33/100, -1/500, 2/125)$
$(14, 23, 11)$	4/5	$(29/125, -13/125, 1/5)$
$(15, 24, 11)$	3497/1000	$(1/3, 0, 13/500)$
$(14, 24, 12)$	3497/1000	$(1/3, 0, 1/4)$
$(17, 27, 12)$	3497/1000	$(81/500, -69/500, 1/500)$
$(19, 29, 12)$	3497/1000	$(33/100, -1/500, 13/500)$
$(17, 29, 14)$	4/5	$(36/125, -16/125, 1/4)$
$(18, 30, 14)$	3497/1000	$(33/100, -1/500, 1/4)$
$(21, 33, 14)$	797/1000	$(33/100, -1/500, 1/4)$
$(22, 36, 16)$	527/1000	$(62/375, -12/125, 1/4)$
$(25, 39, 16)$	797/1000	$(493/1500, -3/500, 1/4)$

Space group type $(3, 6, 7, 1, 1)$; IT(191) $= P6/mmm$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$; so the normalizer is identical with the group itself but the basis is different.

Reduced fundamental domain:

$$R_{191} = \text{conv}\,\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$

Space group type $(3, 6, 7, 1, 2)$**;** IT(192) $= P6/mcc$

Normalizer: IT(191) $= P6/mmm$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{192} = \text{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6, 9, 5)$	3497/1000	$(1/3, 0, 0)$
$(8, 12, 6)$	3497/1000	$(1/4, -1/4, 0)$
$(12, 18, 8)$	3497/1000	$(0, 0, 0)$
$(12, 19, 9)$	3497/1000	$(33/100, -1/500, 123/500)$
$(9, 16, 9)$	1/2	$(3/20, -11/100, 7/50)$
$(14, 22, 10)$	3497/1000	$(433/1500, -47/500, 31/125)$
$(14, 23, 11)$	3497/1000	$(33/100, -1/500, 0)$

Space group type $(3, 6, 7, 1, 4)$**;** IT(193) $= P6_3/mcm$

Normalizer: IT(191) $= P6/mmm$ with basis $b'_1, b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{193} = \text{conv}\big\{(0,0,0), (1/3,0,0), (1/4,-1/4,0), (0,0,1/4), (1/3,0,1/4), (1/4,-1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(6,9,5)$	3497/1000	$(1/3,0,0)$
$(8,12,6)$	3497/1000	$(1/4,-1/4,0)$
$(7,12,7)$	7/2	$(23/125,-7/125,1/250)$
$(9,14,7)$	3497/1000	$(33/100,-1/500,123/500)$
$(10,16,8)$	3497/1000	$(33/100,-1/500,1/4)$
$(11,17,8)$	3497/1000	$(91/375,-6/25,1/500)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(8,14,8)$	14/25	$(17/100,-49/500,1/4)$
$(10,18,10)$	5/4	$(1/5,-1/5,8/125)$
$(13,21,10)$	3497/1000	$(31/125,-31/125,31/125)$
$(14,22,10)$	527/1000	$(343/1500,-21/100,1/4)$
$(15,24,11)$	3497/1000	$(121/500,-121/500,1/500)$
$(14,24,12)$	3497/1000	$(31/125,-31/125,1/4)$
$(18,30,14)$	527/1000	$(28/125,-28/125,1/4)$

Space group type $(3,6,7,1,3)$**;** IT(194) $= P6_3/mmc$

Normalizer: IT(191) $= P6/mmm$ with basis $b_1', b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{194} = \operatorname{conv}\big\{(0,0,0),(1/3,0,0),(1/4,-1/4,0),(0,0,1/4),\\ (1/3,0,1/4),(1/4,-1/4,1/4)\big\}$$

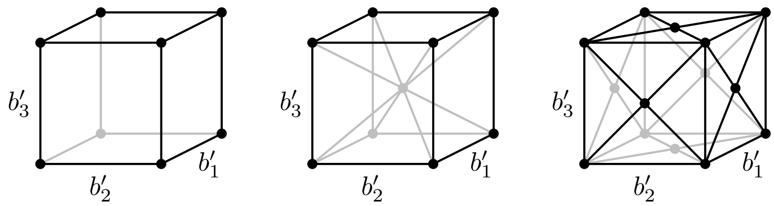
Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: The b-ratio varies from $1/2, \ldots, 7/2$ in 1001 steps of $3/1000$. We used 1 008 126 grid points in the approximating grid for each b-ratio.

f-vector	b-ratio	generating grid point
$(5,8,5)$	4/5	$(36/125,-16/125,1/4)$
$(6,9,5)$	3497/1000	$(1/3,0,0)$
$(7,11,6)$	4/5	$(29/100,-13/100,1/4)$
$(8,12,6)$	3497/1000	$(1/4,-1/4,0)$
$(10,15,7)$	3497/1000	$(499/1500,-1/500,13/500)$
$(6,11,7)$	4/5	$(16/125,0,1/5)$
$(8,13,7)$	3497/1000	$(124/375,0,31/125)$
$(11,17,8)$	3497/1000	$(124/375,0,13/500)$
$(12,18,8)$	3497/1000	$(0,0,0)$
$(6,12,8)$	4/5	$(4/25,0,1/4)$
$(8,14,8)$	3497/1000	$(124/375,0,1/4)$
$(13,21,10)$	3497/1000	$(1/3,0,31/125)$
$(14,22,10)$	797/1000	$(124/375,0,1/4)$
$(15,24,11)$	3497/1000	$(1/3,0,13/500)$
$(14,24,12)$	3497/1000	$(1/3,0,1/4)$
$(18,30,14)$	797/1000	$(1/3,0,1/4)$

2.2.5 Cubic groups

The metrical parameters for cubic groups do not allow for great variation. All angles have to be right angles and the length of the basis vectors are all the same. We therefore list under *Metrical parameters* only the number of grid points used in the approximating grid. The possible types of fundamental parallelepipeds of the sublattice $L' \leq L$ of the space group Γ are



primitive (P) body-centered (I) face-centered (F)

The lengths of b_1', b_2', and b_3' have to be the same and the angles between all pairs of vectors have to be $\pi/2$.

Space group type $(3, 7, 1, 1, 1)$**;** IT(195) $= P23$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{195} = \operatorname{conv}\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 15$ [SS08, Section 5] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 13 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f**-vector**	**generating grid point**	**frequency**
$(5, 8, 5)$	$(1815/3632, 0, 0)$	1815
$(5, 9, 6)$	$(1815/3632, 1815/3632, 0)$	1815
$(8, 12, 6)$	$(0, 0, 0)$	1
$(6, 11, 7)$	$(1815/3632, 907/1816, 0)$	1 646 205
$(8, 13, 7)$	$(1817/7264, 1817/7264, 1815/7264)$	3 296 040
$(6, 12, 8)$	$(1/2, 0, 0)$	2
$(8, 16, 10)$	$(1/2, 1815/3632, 0)$	1815
$(14, 24, 12)$	$(1/4, 1/4, 1/4)$	1816
$(16, 27, 13)$	$(15/227, 45/3632, 7/3632)$	996 502 760

Space group type $(3, 7, 1, 2, 1)$**;** IT(196) $= F23$

Normalizer: IT(229) $= Im\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{196} = \operatorname{conv}\big\{(0,0,0), (1/8,1/8,1/8), (1/4,0,0), (1/4,1/4,0)\big\}$$

Upper bound on number of facets: $f_2 \leq 10$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 12 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5, 8, 5)$	$(1817/14528, 1817/14528, 1815/14528)$	2 446 166
$(8, 12, 6)$	$(1/8, 1/8, 1/8)$	1816
$(6, 12, 8)$	$(1/4, 0, 0)$	1817
$(8, 16, 10)$	$(15/454, 45/7264, 7/7264)$	751 819 081
$(14, 24, 12)$	$(0, 0, 0)$	1

Space group type $(3, 7, 1, 3, 1)$**;** IT(197) $= I23$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{197} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 21$ [SS08, Section 5] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 17 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/2, 1/4, 0)$	1
$(5, 9, 6)$	$(3/8, 3/8, 0)$	454
$(8, 12, 6)$	$(1/4, 1/4, 1/4)$	1
$(6, 12, 8)$	$(1/4, 1/4, 0)$	908
$(10, 17, 9)$	$(909/3632, 909/3632, 453/1816)$	453
$(12, 19, 9)$	$(1817/7264, 1817/7264, 1815/7264)$	1 980 209
$(8, 15, 9)$	$(13/32, 13/32, 1/32)$	908
$(10, 18, 10)$	$(1815/3632, 1/4, 0)$	907
$(11, 19, 10)$	$(1815/3632, 1815/3632, 0)$	1 303 152

f-vector	generating grid point	frequency
$(12, 20, 10)$	$(907/3632, 907/3632, 0)$	823 556
$(7, 15, 10)$	$(3/16, 1/8, 0)$	1
$(9, 17, 10)$	$(1361/3632, 1361/3632, 0)$	453
$(13, 22, 11)$	$(121/454, 967/3632, 789/3632)$	545 615
$(14, 23, 11)$	$(1817/7264, 1817/7264, 1813/7264)$	491 821
$(10, 20, 12)$	$(1/2, 0, 0)$	2
$(13, 23, 12)$	$(909/3632, 1/4, 53/227)$	408 105
$(14, 25, 13)$	$(1/2, 1815/3632, 0)$	1814
$(15, 26, 13)$	$(179/3632, 125/3632, 67/3632)$	3420
$(17, 28, 13)$	$(1815/3632, 0, 0)$	1815
$(18, 29, 13)$	$(15/227, 45/3632, 7/3632)$	760 106 234
$(20, 32, 14)$	$(249/7264, 247/7264, 243/7264)$	190 266 816
$(24, 36, 14)$	$(0, 0, 0)$	1
$(20, 33, 15)$	$(3285/7264, 3283/7264, 229/7264)$	20 486 921
$(22, 35, 15)$	$(3285/7264, 3279/7264, 229/7264)$	73 198
$(26, 39, 15)$	$(1815/7264, 1815/7264, 1815/7264)$	1815
$(24, 38, 16)$	$(251/7264, 247/7264, 241/7264)$	15 412 212
$(24, 39, 17)$	$(207/454, 1515/3632, 101/3632)$	3 606 077

Space group type $(3, 7, 1, 1, 2)$**;** $\mathrm{IT}(198) = P2_13$

Normalizer: $\mathrm{IT}(230) = Ia\bar{3}d$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{198} = \mathrm{conv}\big\{(0,0,0), (1/8,1/8,1/8), (-1/8,1/8,1/8), (-1/8,-1/8,1/8), (1/8,-1/8,1/8), (1/8,1/8,1/4), (-1/8,1/8,1/4), (-1/8,-1/8,1/4), (1/8,-1/8,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 69$ [SS11] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 18 facets, see [Koc72, p. 87].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8, 14, 8)$	$(-1/8, -1/8, 1/8)$	2619
$(11, 21, 12)$	$(-51/776, -79/776, 121/776)$	4335
$(12, 22, 12)$	$(-455/6984, -655/6984, 545/3492)$	801 918 314
$(14, 24, 12)$	$(0, 0, 0)$	667
$(19, 31, 14)$	$(65/582, 19/1164, 13/72)$	1041
$(21, 35, 16)$	$(847/6984, 547/6984, 1547/6984)$	260
$(22, 36, 16)$	$(-455/6984, -709/6984, 545/3492)$	159 598 648
$(26, 40, 16)$	$(239/2328, 239/6984, 1403/6984)$	168
$(26, 42, 18)$	$(871/6984, 19/776, 183/776)$	146

f-vector	generating grid point	frequency
$(30, 46, 18)$	$(1/8, 1/24, 5/24)$	843
$(32, 48, 18)$	$(1/8, 1/8, 1/8)$	207
$(29, 47, 20)$	$(10/97, 0, 45/194)$	1
$(30, 48, 20)$	$(851/6984, 15/776, 1627/6984)$	284
$(32, 50, 20)$	$(1/8, 535/6984, 1577/6984)$	24 345 171
$(33, 53, 22)$	$(857/6984, 169/2328, 173/776)$	2
$(34, 54, 22)$	$(871/6984, 1/24, 1567/6984)$	104
$(36, 56, 22)$	$(1/8, 149/2328, 511/2328)$	12 349 276
$(40, 62, 24)$	$(1/8, 419/6984, 1519/6984)$	2 455 911

Space group type $(3, 7, 1, 3, 2)$**;** IT(199) $= I2_13$

Normalizer: IT(230) $= Ia\bar{3}d$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{199} = \text{conv}\big\{(0,0,0), (1/8,1/8,1/8), (-1/8,1/8,1/8), (-1/8,-1/8,1/8), (1/8,-1/8,1/8), (1/8,1/8,1/4), (-1/8,1/8,1/4), (-1/8,-1/8,1/4), (1/8,-1/8,1/4)\big\}$$

Upper bound on number of facets: $f_2 \leq 46$ [SS11] for points with trivial stabilizer and $f_2 \leq 102$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 20 facets, see [Koc72, p. 88].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8, 12, 6)$	$(0, 0, 0)$	1
$(10, 17, 9)$	$(0, 0, 1/2328)$	436
$(13, 22, 11)$	$(-1/8, 5/72, 5/24)$	5646
$(13, 24, 13)$	$(211/6984, 539/6984, 527/2328)$	3088
$(14, 25, 13)$	$(1/24, 1/8, 5/24)$	1
$(15, 26, 13)$	$(121/2328, 613/6984, 179/776)$	256
$(16, 27, 13)$	$(-455/6984, -655/6984, 545/3492)$	319 640 243
$(18, 29, 13)$	$(7/72, 1/24, 1/8)$	1
$(17, 29, 14)$	$(67/6984, 71/6984, 113/6984)$	339 289
$(19, 31, 14)$	$(29/6984, 67/6984, 1675/6984)$	240
$(19, 32, 15)$	$(221/6984, 655/6984, 509/2328)$	680
$(21, 34, 15)$	$(271/2328, 815/6984, 1513/6984)$	392
$(22, 35, 15)$	$(-13/3492, 10/97, 863/6984)$	300 082 779
$(23, 36, 15)$	$(175/2328, 257/2328, 5/24)$	381
$(22, 36, 16)$	$(-1/8, 7/2328, 473/3492)$	118 346 173
$(23, 37, 16)$	$(289/6984, 295/6984, 73/873)$	395
$(24, 38, 16)$	$(31/1746, 109/873, 1369/6984)$	94 655 719
$(25, 39, 16)$	$(145/1164, 145/3492, 727/3492)$	347

f-vector	generating grid point	frequency
$(26, 40, 16)$	$(13/388, 59/1746, 55/1164)$	579
$(23, 38, 17)$	$(577/6984, 1/776, 581/2328)$	12
$(25, 40, 17)$	$(371/6984, 205/2328, 64/291)$	101
$(26, 41, 17)$	$(253/2328, 761/6984, 319/1746)$	8 729 121
$(27, 42, 17)$	$(871/6984, 19/776, 183/776)$	840
$(28, 43, 17)$	$(815/6984, 817/6984, 1385/6984)$	918
$(29, 44, 17)$	$(145/1164, 109/873, 1505/6984)$	25 457 960
$(30, 45, 17)$	$(1/8, 1/8, 1/8)$	115
$(27, 43, 18)$	$(175/6984, 221/6984, 283/6984)$	31
$(28, 44, 18)$	$(1/2328, 41/6984, 71/291)$	3 581 726
$(31, 47, 18)$	$(145/1164, 109/873, 1135/6984)$	51 073 549
$(30, 47, 19)$	$(439/6984, 49/776, 527/2328)$	168
$(33, 50, 19)$	$(145/1164, 109/873, 1435/6984)$	50 529 910
$(32, 50, 20)$	$(149/2328, 259/2328, 157/776)$	4865
$(33, 51, 20)$	$(15/194, 28/291, 455/2328)$	24
$(34, 52, 20)$	$(71/776, 235/2328, 153/776)$	76
$(35, 53, 20)$	$(11/873, 49/3492, 109/6984)$	7 342 771
$(36, 54, 20)$	$(379/3492, 379/3492, 379/3492)$	758
$(34, 53, 21)$	$(145/2328, 1/8, 437/2328)$	37
$(37, 56, 21)$	$(295/6984, 287/2328, 81/388)$	288 840
$(36, 56, 22)$	$(7/97, 41/388, 153/776)$	245
$(37, 57, 22)$	$(1/12, 35/388, 77/388)$	7
$(38, 58, 22)$	$(61/776, 715/6984, 449/2328)$	27
$(39, 59, 22)$	$(721/6984, 241/2328, 147/776)$	1 934 183
$(41, 62, 23)$	$(539/6984, 755/6984, 701/3492)$	858 361
$(43, 65, 24)$	$(139/1746, 355/3492, 1343/6984)$	454 748

Space group type $(3, 7, 2, 1, 1)$**;** IT(200) $= Pm\bar{3}$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{200} = \text{conv}\left\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 10 facets, see [Koc72, p. 81].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5, 8, 5)$	$(1817/7264, 1817/7264, 1815/7264)$	3 297 855
$(5, 9, 6)$	$(1815/3632, 1815/3632, 0)$	1815
$(6, 10, 6)$	$(15/227, 45/3632, 7/3632)$	987 665 556
$(8, 12, 6)$	$(0, 0, 0)$	1817

f-vector	generating grid point	frequency
$(6, 11, 7)$	$(1815/3632, 907/1816, 0)$	1 646 205
$(6, 12, 8)$	$(1/2, 0, 0)$	2
$(8, 16, 10)$	$(1/2, 1815/3632, 0)$	1815

Space group type $(3, 7, 2, 1, 2)$**;** IT(201) $= Pn\bar{3}$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{201} = \text{conv}\left\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 23$ [SS08, Section 5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(6, 12, 8)$	$(1/2, 1815/3632, 0)$	3630
$(12, 19, 9)$	$(435/908, 19/908, 9/1816)$	2 452 464
$(11, 19, 10)$	$(1/4, 907/3632, 849/3632)$	538 173
$(12, 20, 10)$	$(909/3632, 1/4, 907/3632)$	3 292 410
$(7, 15, 10)$	$(3/8, 1/4, 1/16)$	2
$(13, 22, 11)$	$(1/4, 439/1816, 849/3632)$	267 949
$(14, 24, 12)$	$(0, 0, 0)$	3
$(15, 26, 13)$	$(75/1816, 15/454, 6/227)$	8164
$(17, 28, 13)$	$(1/4, 1/4, 0)$	908
$(18, 29, 13)$	$(15/227, 45/3632, 7/3632)$	651 503 995
$(17, 29, 14)$	$(90/227, 18/227, 15/227)$	4
$(20, 32, 14)$	$(111/1816, 13/1816, 25/3632)$	299 205 822
$(24, 36, 14)$	$(1/4, 1/4, 1/4)$	1
$(22, 35, 15)$	$(491/7264, 39/7264, 3/7264)$	750 704
$(24, 38, 16)$	$(239/3632, 43/3632, 1/454)$	24 158 006
$(25, 39, 16)$	$(1817/7264, 1817/7264, 1815/7264)$	5445

Space group type $(3, 7, 2, 2, 1)$**;** IT(202) $= Fm\bar{3}$

Normalizer: IT(221) $= Pm\bar{3}m$ with basis $\frac{1}{2}b'_1, \frac{1}{2}b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{202} = \text{conv}\left\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 12 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(1815/7264, 1815/7264, 907/3632)$	1 646 205
$(5,8,5)$	$(1/4, 1/4, 1815/7264)$	3630
$(5,9,6)$	$(1/4, 1815/7264, 1815/7264)$	105 954
$(8,12,6)$	$(1/4, 1/4, 1/4)$	1
$(6,11,7)$	$(247/7264, 13/1816, 7/3632)$	609 531 852
$(6,12,8)$	$(1/4, 0, 0)$	1817
$(8,16,10)$	$(1/4, 1815/7264, 0)$	444 978
$(14,24,12)$	$(0,0,0)$	1

Space group type $(3,7,2,2,2)$**;** IT(203) $= Fd\bar{3}$

Normalizer: IT(224) $= Pn\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{203} = \operatorname{conv}\big\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/8,1/8,1/8), (1/8,1/8,-1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 14$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: We used 1 000 520 885 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5,8,5)$	$(360/1441, 360/1441, 0)$	1680
$(8,12,6)$	$(0,0,0)$	2
$(10,15,7)$	$(180/1441, 180/1441, 180/1441)$	2880
$(8,13,7)$	$(721/5764, 180/1441, -180/1441)$	4 104 085
$(9,14,7)$	$(721/5764, 721/5764, 719/5764)$	1 035 360
$(8,15,9)$	$(107/5764, 103/5764, -1/1441)$	319 644
$(10,20,12)$	$(1/8, 1/8, -1/8)$	721
$(12,22,12)$	$(1/8, 1/8, 1439/11528)$	720
$(14,24,12)$	$(107/5764, 103/5764, 1/1441)$	729 064 290
$(14,25,13)$	$(107/5764, 103/5764, -5/5764)$	156 709 442
$(18,30,14)$	$(107/5764, 103/5764, 2/131)$	25 031 717
$(16,30,16)$	$(1/8, 1/8, 1/8)$	1

Space group type $(3,7,2,3,1)$**;** IT(204) $= Im\bar{3}$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{204} = \operatorname{conv}\big\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \le 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \le 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 14 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(1/2,1/4,0)$	908
$(5,8,5)$	$(121/454,967/3632,789/3632)$	206 492
$(5,9,6)$	$(3/8,3/8,0)$	454
$(8,12,6)$	$(1/4,1/4,1/4)$	1
$(10,15,7)$	$(1815/7264,1815/7264,1815/7264)$	1815
$(6,11,7)$	$(179/3632,125/3632,67/3632)$	1475
$(7,12,7)$	$(909/3632,1/4,53/227)$	396 005
$(8,13,7)$	$(15/227,45/3632,7/3632)$	683 530 603
$(9,14,7)$	$(1815/7264,1815/7264,1813/7264)$	822 649
$(10,16,8)$	$(249/7264,247/7264,243/7264)$	155 997 990
$(6,12,8)$	$(1/4,1/4,0)$	1
$(10,18,10)$	$(1815/3632,1/4,0)$	907
$(11,19,10)$	$(1815/3632,1815/3632,0)$	1 303 152
$(12,20,10)$	$(907/3632,907/3632,0)$	907
$(7,15,10)$	$(3/16,1/8,0)$	1
$(9,17,10)$	$(1361/3632,1361/3632,0)$	453
$(13,22,11)$	$(907/1816,909/3632,0)$	342 145
$(10,20,12)$	$(1/2,0,0)$	2
$(14,25,13)$	$(1/2,1815/3632,0)$	1814
$(17,28,13)$	$(1815/3632,0,0)$	1815
$(24,36,14)$	$(0,0,0)$	1

Space group type $(3,7,2,1,3)$**;** IT(205) $= Pa\bar{3}$

Normalizer: IT(206) $= Ia\bar{3}$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{205} = \text{conv}\left\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(0,1/2,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \le 86$ [SS11] for points with trivial stabilizer and $f_2 \le 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 13 facets, see [Koc72, p. 84].

Metrical parameters: We used 1 000 520 885 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8, 12, 6)$	$(1/4, 1/4, 1/4)$	1
$(6, 12, 8)$	$(721/2882, 360/1441, 360/1441)$	10 800
$(7, 13, 8)$	$(360/1441, 721/2882, 0)$	1440
$(10, 18, 10)$	$(720/1441, 1/2882, 0)$	1440
$(11, 21, 12)$	$(1343/2882, 1427/2882, 1/1441)$	741 739
$(12, 22, 12)$	$(456/1441, 481/1441, 433/2882)$	100 165
$(13, 23, 12)$	$(105/2882, 105/2882, 50/1441)$	1 035 360
$(14, 24, 12)$	$(897/2882, 496/1441, 224/1441)$	245 230
$(15, 25, 12)$	$(9/262, 107/2882, 23/2882)$	4692
$(19, 30, 13)$	$(360/1441, 360/1441, 360/1441)$	1440
$(15, 27, 14)$	$(807/2882, 839/2882, 269/1441)$	765
$(16, 28, 14)$	$(2689/5764, 2867/5764, 1/5764)$	96 725 811
$(17, 29, 14)$	$(38/1441, 127/2882, 73/2882)$	298 649
$(18, 30, 14)$	$(103/2882, 107/2882, 51/1441)$	447 854 805
$(19, 31, 14)$	$(353/2882, 99/262, 337/2882)$	371
$(20, 32, 14)$	$(211/5764, 19/524, 199/5764)$	200 379 547
$(21, 33, 14)$	$(747/5764, 2133/5764, 705/5764)$	501
$(20, 34, 16)$	$(1819/5764, 1919/5764, 871/5764)$	31 900 381
$(21, 35, 16)$	$(18/131, 40/131, 14/131)$	1
$(22, 36, 16)$	$(1957/5764, 937/5764, 735/5764)$	74 827 770
$(24, 38, 16)$	$(221/5764, 199/5764, 191/5764)$	98 525 278
$(25, 39, 16)$	$(73/524, 2075/5764, 485/5764)$	505
$(26, 42, 18)$	$(3/22, 1139/2882, 5/131)$	170 301
$(28, 44, 18)$	$(197/5764, 223/5764, 195/5764)$	47 395 035

Space group type $(3, 7, 2, 3, 2)$**;** $\mathrm{IT}(206) = Ia\bar{3}$

Normalizer: $\mathrm{IT}(230) = Ia\bar{3}d$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$\begin{aligned} R_{206} = \operatorname{conv}\big\{&(0,0,0), (1/8,1/8,1/8), (-1/8,1/8,1/8),\\ &(-1/8,-1/8,1/8), (1/8,-1/8,1/8), (1/8,1/8,1/4),\\ &(-1/8,1/8,1/4), (-1/8,-1/8,1/4), (1/8,-1/8,1/4)\big\} \end{aligned}$$

Upper bound on number of facets: $f_2 \leq 57$ [SS11] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 17 facets, see [Koc72, p. 85].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5, 8, 5)$	$(0, 0, 1/2328)$	436
$(8, 12, 6)$	$(0, 0, 0)$	1
$(10, 18, 10)$	$(-1/24, -1/8, 1/6)$	436

f-vector	generating grid point	frequency
$(9, 17, 10)$	$(-1/8, -1/8, 1/4)$	1648
$(10, 19, 11)$	$(-1/8, -1/8, 1/8)$	2619
$(13, 22, 11)$	$(-9/388, -6/97, 33/388)$	1
$(8, 17, 11)$	$(1/8, -1/24, 5/24)$	1
$(13, 23, 12)$	$(-1/6984, -1/8, 1/4)$	328 474
$(14, 24, 12)$	$(-1/6984, -233/2328, 131/873)$	84 229
$(15, 25, 12)$	$(0, 187/1746, 1121/6984)$	526 290
$(16, 26, 12)$	$(-1/8, -167/6984, 130/873)$	105 946
$(14, 25, 13)$	$(-1/8, 145/2328, 1/4)$	63 722
$(16, 27, 13)$	$(1/8, 145/2328, 1/4)$	97 920
$(17, 28, 13)$	$(317/3492, 0, 317/2328)$	29 943
$(18, 29, 13)$	$(1/8, -125/2328, 187/1164)$	41 466 623
$(17, 29, 14)$	$(-869/6984, 341/6984, 11/72)$	137 526
$(18, 30, 14)$	$(-1/8, 55/6984, 116/873)$	25 744 231
$(19, 31, 14)$	$(-805/6984, -535/6984, 1607/6984)$	103 743
$(20, 32, 14)$	$(-13/3492, 10/97, 863/6984)$	344 538 059
$(21, 33, 14)$	$(-283/2328, -1/2328, 377/2328)$	88
$(22, 34, 14)$	$(31/1746, 109/873, 1369/6984)$	145 823 351
$(17, 30, 15)$	$(-1/8, -437/6984, 1745/6984)$	252
$(18, 31, 15)$	$(37/388, 0, 15/97)$	134
$(19, 32, 15)$	$(-1/8, 145/2328, 581/2328)$	11 752
$(20, 33, 15)$	$(-457/6984, -211/2328, 545/3492)$	36 467
$(21, 34, 15)$	$(-59/776, -595/6984, 119/776)$	453
$(22, 35, 15)$	$(-57/776, -577/6984, 545/3492)$	4 479 902
$(19, 33, 16)$	$(-841/6984, 269/6984, 361/2328)$	59
$(21, 35, 16)$	$(-241/2328, -179/2328, 427/2328)$	51 129
$(22, 36, 16)$	$(-457/6984, -475/6984, 545/3492)$	51 774 410
$(23, 37, 16)$	$(-713/6984, 211/6984, 1219/6984)$	12 318
$(24, 38, 16)$	$(-1/8, -1/6984, 319/2328)$	25 827 890
$(25, 39, 16)$	$(-595/6984, -17/6984, 1037/6984)$	55
$(26, 40, 16)$	$(799/6984, 89/776, 49/388)$	9 805 841
$(23, 38, 17)$	$(-1/8, 35/776, 189/776)$	643
$(24, 39, 17)$	$(-455/6984, -655/6984, 545/3492)$	14 629 703
$(25, 40, 17)$	$(1/8, 437/6984, 1745/6984)$	1024
$(26, 41, 17)$	$(-57/776, -193/2328, 545/3492)$	36 088 498
$(28, 43, 17)$	$(211/2328, 1/6984, 475/3492)$	1 849 214
$(30, 45, 17)$	$(1/8, 1/8, 1/8)$	873
$(23, 39, 18)$	$(-865/6984, 173/6984, 1211/6984)$	16
$(25, 41, 18)$	$(-1/8, 1/24, 13/72)$	80
$(26, 42, 18)$	$(-1/8, 55/2328, 437/3492)$	9 494 176
$(27, 43, 18)$	$(-821/6984, 199/6984, 1229/6984)$	80
$(28, 44, 18)$	$(-1/8, 335/6984, 18/97)$	4 091 645
$(29, 45, 18)$	$(-25/1164, -17/1164, 65/1164)$	8
$(30, 46, 18)$	$(785/6984, 787/6984, 425/3492)$	30 035 545
$(25, 42, 19)$	$(-1/8, 85/2328, 461/2328)$	160
$(27, 44, 19)$	$(-1/582, -5/3492, 101/2328)$	72
$(28, 45, 19)$	$(-457/6984, -491/6984, 545/3492)$	3 768 069
$(29, 46, 19)$	$(19/194, 19/291, 211/1164)$	190
$(30, 47, 19)$	$(-461/6984, -473/6984, 545/3492)$	8 842 620

f-vector	generating grid point	frequency
$(32, 49, 19)$	$(1/8, 523/6984, 1571/6984)$	17 287 516
$(29, 47, 20)$	$(-545/6984, 37/2328, 157/776)$	26
$(30, 48, 20)$	$(-1/8, 37/776, 1207/6984)$	1 676 938
$(31, 49, 20)$	$(-857/6984, -463/6984, 1453/6984)$	3
$(32, 50, 20)$	$(-457/6984, -51/776, 545/3492)$	4 326 364
$(34, 52, 20)$	$(691/6984, 463/6984, 317/1746)$	5 767 035
$(32, 51, 21)$	$(-1/8, 209/6984, 323/1746)$	1 601 262
$(33, 52, 21)$	$(11/194, 77/3492, 671/6984)$	767
$(34, 53, 21)$	$(-515/6984, -565/6984, 545/3492)$	144 144
$(36, 55, 21)$	$(1/8, 379/6984, 1499/6984)$	13 657 787
$(34, 54, 22)$	$(-1/8, 35/776, 1253/6984)$	427 874
$(36, 56, 22)$	$(-1/776, -1/6984, 1567/6984)$	16 987
$(38, 58, 22)$	$(80/873, 221/3492, 1181/6984)$	5 013 031
$(37, 58, 23)$	$(27/388, 11/291, 155/1164)$	304
$(40, 61, 23)$	$(1/8, 125/2328, 499/2328)$	22 842 322
$(42, 64, 24)$	$(13/194, 179/3492, 881/6984)$	995 100
$(41, 64, 25)$	$(1/194, 17/3492, 61/6984)$	104
$(44, 67, 25)$	$(1/8, 373/6984, 187/873)$	3 931 406
$(46, 70, 26)$	$(415/6984, 109/2328, 131/1164)$	272 968
$(50, 76, 28)$	$(7/582, 1/97, 9/388)$	90 445

Space group type $(3, 7, 3, 1, 1)$**;** IT(207) $= P432$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{207} = \operatorname{conv}\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 11$ [SS08, Corollary 4.3] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 9 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/2, 1815/3632, 0)$	1 648 020
$(5, 8, 5)$	$(1817/7264, 1817/7264, 1815/7264)$	3 297 855
$(5, 9, 6)$	$(1815/3632, 1815/3632, 0)$	1815
$(8, 12, 6)$	$(0, 0, 0)$	1817
$(6, 12, 8)$	$(1/2, 0, 0)$	2
$(8, 15, 9)$	$(15/227, 45/3632, 7/3632)$	638 181 275

Space group type $(3, 7, 3, 1, 3)$**;** IT(208) $= P4_232$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{208} = \text{conv}\left\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 25$ [SS08, Section 6] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Corollary 6.2 in [SS08] states that every stereohedron with "base point" in general position has at least 11 facets. Furthermore, examples were found of stereohedra with facets any number between 14 and 17.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5,9,6)$	$(3/8,3/8,0)$	454
$(6,11,7)$	$(1817/7264,1817/7264,1815/7264)$	3630
$(6,12,8)$	$(1/4,1/4,0)$	908
$(7,13,8)$	$(907/1816,907/3632,0)$	907
$(11,18,9)$	$(909/3632,909/3632,453/1816)$	453
$(12,19,9)$	$(1/4,907/3632,907/3632)$	1 646 205
$(9,16,9)$	$(1513/3632,1513/3632,151/1816)$	151
$(11,19,10)$	$(909/3632,1/4,53/227)$	1 440 089
$(12,20,10)$	$(907/3632,907/3632,0)$	823 556
$(8,16,10)$	$(1/2,1/4,0)$	454
$(9,17,10)$	$(1347/3632,469/3632,409/3632)$	755
$(13,22,11)$	$(435/908,19/908,9/1816)$	889 541
$(14,23,11)$	$(121/454,967/3632,789/3632)$	1 027 254
$(10,20,12)$	$(1/2,0,0)$	2
$(14,24,12)$	$(1/4,1/4,1/4)$	1 645 299
$(15,25,12)$	$(31/908,123/3632,61/1816)$	822 649
$(16,27,13)$	$(1/4,907/3632,849/3632)$	548 282
$(17,28,13)$	$(185/3632,31/1816,61/3632)$	412 384
$(16,28,14)$	$(1/2,1815/3632,0)$	1814
$(17,29,14)$	$(279/908,189/908,315/1816)$	13
$(20,32,14)$	$(15/227,45/3632,7/3632)$	753 863 053
$(24,36,14)$	$(0,0,0)$	1
$(17,30,15)$	$(427/908,73/227,3/227)$	3
$(20,33,15)$	$(1937/7264,1935/7264,1577/7264)$	111 858 167
$(24,38,16)$	$(251/7264,247/7264,241/7264)$	114 444 764
$(25,39,16)$	$(1815/7264,1815/7264,1815/7264)$	1815
$(24,39,17)$	$(2989/7264,2987/7264,525/7264)$	12 019 663

Space group type $(3,7,3,2,1)$**;** IT(209) $= F432$

Normalizer: IT(221) $= Pm\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{209} = \text{conv}\left\{(0,0,0),(1/4,0,0),(1/4,1/4,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 14$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 12 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/4, 1815/7264, 0)$	3 294 225
$(5, 8, 5)$	$(1/4, 1/4, 1815/7264)$	3630
$(5, 9, 6)$	$(1/4, 1815/7264, 1815/7264)$	1 599 344
$(8, 12, 6)$	$(1/4, 1/4, 1/4)$	1
$(6, 12, 8)$	$(1/4, 0, 0)$	1817
$(8, 15, 9)$	$(247/7264, 13/1816, 7/3632)$	654 164 225
$(14, 24, 12)$	$(0, 0, 0)$	1

Space group type $(3, 7, 3, 2, 2)$**;** IT(210) $= F4_132$

Normalizer: IT(224) $= Pn\bar{3}m$ with basis $\frac{1}{2}b'_1, \frac{1}{2}b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{210} = \text{conv}\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/8,1/8,1/8), (1/8,1/8,-1/8)\}$$

Upper bound on number of facets: $f_2 \leq 17$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 10 facets, see [Koc72, p. 68].

Metrical parameters: We used 1 000 520 885 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5, 8, 5)$	$(1443/11528, 1443/11528, 1437/11528)$	811
$(8, 12, 6)$	$(1/8, 1/8, 1/8)$	1
$(10, 15, 7)$	$(180/1441, 180/1441, 180/1441)$	1440
$(8, 13, 7)$	$(1/8, 1/8, 1439/11528)$	2 694 599
$(9, 14, 7)$	$(180/1441, 719/5764, 719/5764)$	222 045
$(10, 18, 10)$	$(1631/11528, 1439/11528, 1249/11528)$	247 069
$(8, 16, 10)$	$(1443/11528, 1/8, 1439/11528)$	188
$(10, 20, 12)$	$(1/4, 0, 0)$	722
$(12, 22, 12)$	$(180/1441, 0, 0)$	720
$(13, 23, 12)$	$(215/11528, 205/11528, 195/11528)$	494 662
$(14, 24, 12)$	$(1/8, 1/8, -1/8)$	1441
$(15, 26, 13)$	$(3/88, 19/11528, 1/1048)$	390

f-vector	generating grid point	frequency
$(16, 27, 13)$	$(107/5764, 103/5764, 2/131)$	230 824 607
$(16, 28, 14)$	$(769/5764, 673/5764, 61/524)$	116 802 788
$(19, 32, 15)$	$(257/11528, 1/88, 125/11528)$	244
$(20, 33, 15)$	$(219/11528, 201/11528, 185/11528)$	110 275 905
$(16, 30, 16)$	$(0, 0, 0)$	1
$(24, 39, 17)$	$(215/11528, 205/11528, 203/11528)$	7 479 832

Space group type $(3, 7, 3, 3, 1)$**;** IT(211) $= I432$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{211} = \text{conv}\left\{(0, 0, 0), (1/2, 0, 0), (1/2, 1/2, 0), (1/4, 1/4, 1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 22$ [SS08, Corollary 4.3] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 16 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/2, 1/4, 0)$	454
$(5, 8, 5)$	$(1/4, 1/4, 907/3632)$	2267
$(6, 9, 5)$	$(1/2, 1815/3632, 0)$	1814
$(5, 9, 6)$	$(3/8, 3/8, 0)$	1
$(7, 11, 6)$	$(907/1816, 909/3632, 0)$	205 209
$(8, 12, 6)$	$(1/4, 1/4, 1/4)$	1 439 637
$(10, 15, 7)$	$(1815/7264, 1815/7264, 1815/7264)$	1815
$(8, 13, 7)$	$(1817/7264, 1817/7264, 1815/7264)$	2 472 031
$(9, 14, 7)$	$(1815/7264, 1815/7264, 1813/7264)$	822 649
$(6, 12, 8)$	$(1/4, 1/4, 0)$	1
$(10, 17, 9)$	$(121/454, 967/3632, 789/3632)$	179 872
$(8, 15, 9)$	$(909/3632, 1/4, 907/3632)$	907
$(10, 18, 10)$	$(909/3632, 1/4, 53/227)$	366 253
$(11, 19, 10)$	$(1815/3632, 1815/3632, 0)$	453
$(12, 20, 10)$	$(907/3632, 907/3632, 0)$	907
$(9, 17, 10)$	$(1361/3632, 1361/3632, 0)$	453
$(12, 21, 11)$	$(1819/7264, 1817/7264, 1813/7264)$	1 645 298
$(13, 22, 11)$	$(31/908, 123/3632, 61/1816)$	683 840
$(10, 20, 12)$	$(1/2, 0, 0)$	2
$(15, 25, 12)$	$(115/1816, 14/227, 5/1816)$	1041
$(16, 26, 12)$	$(15/227, 45/3632, 7/3632)$	429 155 207
$(16, 27, 13)$	$(1819/7264, 1817/7264, 1695/7264)$	111 811 155
$(17, 28, 13)$	$(1815/3632, 0, 0)$	1815
$(19, 31, 14)$	$(257/7264, 255/7264, 225/7264)$	886

f-vector	generating grid point	frequency
$(20, 32, 14)$	$(489/7264, 487/7264, 3/7264)$	270 726 064
$(24, 36, 14)$	$(0, 0, 0)$	1
$(24, 38, 16)$	$(249/7264, 247/7264, 243/7264)$	42 951 936

Space group type $(3, 7, 3, 1, 2)$**;** IT(212) $= P4_332$**,** IT(213) $= P4_132$

Normalizer: IT(214) $= I4_132$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{212} = \operatorname{conv}\{(1/8, 1/8, 1/8), (1/8, 1/8, 3/8), (1/8, -1/8, 1/8), (-1/8, 1/8, 1/8), (-1/8, -1/8, -1/8), (-3/8, 1/8, 3/8), (-3/8, -1/8, 1/8)\}$$

Upper bound on number of facets: $f_2 \leq 92$ [SS11] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 22 facets, see [Koc72, p. 70].

Metrical parameters: We used 1 000 964 383 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8, 14, 8)$	$(-1/8, -1/8, 1/8)$	2
$(10, 17, 9)$	$(-1/4, -353/4248, 89/1062)$	177
$(8, 15, 9)$	$(-95/472, -47/472, 1/472)$	36
$(10, 18, 10)$	$(-5/24, 1/8, 7/24)$	2
$(12, 20, 10)$	$(-1063/4248, -71/1416, 637/4248)$	16
$(9, 17, 10)$	$(-1/8, -133/2124, 133/2124)$	353
$(11, 20, 11)$	$(-89/708, -529/4248, 133/1062)$	281 583
$(12, 21, 11)$	$(-1/4248, -1/8, 1/8)$	1572
$(13, 22, 11)$	$(-11/1416, -167/1416, 131/1416)$	2998
$(14, 23, 11)$	$(-103/1416, -103/1416, 103/1416)$	353
$(12, 22, 12)$	$(-133/1062, -89/1416, 133/2124)$	69 380
$(13, 23, 12)$	$(-9/472, -251/2124, 85/1062)$	49 023
$(14, 24, 12)$	$(-181/1416, -127/1416, -73/1416)$	41
$(13, 24, 13)$	$(0, 0, 1/8)$	1
$(14, 25, 13)$	$(1/12, 1/12, 1/4)$	407
$(15, 26, 13)$	$(-20/59, 227/4248, 569/2124)$	181 534
$(16, 27, 13)$	$(15/472, -265/2124, 22/177)$	177 122 240
$(17, 28, 13)$	$(-89/4248, -503/4248, 341/4248)$	225 284
$(16, 28, 14)$	$(-19/472, 4/531, 100/531)$	119 784 137
$(17, 29, 14)$	$(-305/4248, -115/1062, -32/531)$	723
$(18, 30, 14)$	$(-13/177, -65/1416, 23/236)$	205 167
$(19, 31, 14)$	$(-151/2124, -95/1062, -28/531)$	479 396
$(16, 29, 15)$	$(-229/1062, -229/2124, 83/4248)$	17
$(17, 30, 15)$	$(0, 0, 923/4248)$	948

f-vector	generating grid point	frequency
$(19, 32, 15)$	$(25/4248, -149/4248, 799/4248)$	2411
$(20, 33, 15)$	$(-355/4248, -179/2124, -44/531)$	22 087 236
$(21, 34, 15)$	$(317/4248, -107/4248, 745/4248)$	557 632
$(22, 35, 15)$	$(-151/2124, -127/1416, -28/531)$	251 030 427
$(23, 36, 15)$	$(-1223/4248, -103/1416, 605/4248)$	13
$(16, 30, 16)$	$(0, 0, 0)$	1
$(19, 33, 16)$	$(-833/4248, -437/4248, 79/4248)$	10
$(20, 34, 16)$	$(-535/4248, -269/4248, 263/4248)$	1 257 193
$(21, 35, 16)$	$(131/1416, 19/472, 123/472)$	3205
$(22, 36, 16)$	$(-13/177, -73/2124, 463/4248)$	49 080 272
$(23, 37, 16)$	$(-40/531, -527/4248, -319/4248)$	246 332
$(24, 38, 16)$	$(-151/2124, -119/1416, -31/472)$	32 341 849
$(20, 35, 17)$	$(-43/1416, -11/177, 89/708)$	185
$(21, 36, 17)$	$(-35/354, -14/177, 55/1416)$	1130
$(22, 37, 17)$	$(-47/177, -83/708, 61/1416)$	19
$(23, 38, 17)$	$(-37/177, -77/708, 13/1416)$	1556
$(24, 39, 17)$	$(41/4248, -11/4248, 953/4248)$	41 433 937
$(25, 40, 17)$	$(-151/2124, -179/2124, -41/708)$	112 271
$(26, 41, 17)$	$(-151/2124, -95/1062, -223/4248)$	103 302 207
$(30, 45, 17)$	$(-3/8, -1/8, 1/8)$	179
$(24, 40, 18)$	$(-29/118, -29/236, 27/472)$	3
$(25, 41, 18)$	$(-103/1416, -14/177, -157/4248)$	1088
$(26, 42, 18)$	$(-13/177, -49/1062, 7/72)$	36 076 144
$(27, 43, 18)$	$(-355/4248, -361/4248, -39/472)$	12 539
$(28, 44, 18)$	$(-151/2124, -119/1416, -91/1416)$	21 520 727
$(29, 45, 18)$	$(-1/12, -43/531, -157/2124)$	163
$(30, 46, 18)$	$(-55/708, -239/2124, -329/4248)$	7 322 558
$(32, 48, 18)$	$(1/8, 1/8, 1/8)$	1
$(25, 42, 19)$	$(-12/59, -56/531, 71/4248)$	6
$(27, 44, 19)$	$(-77/1416, -283/4248, 7/72)$	1085
$(28, 45, 19)$	$(-163/2124, -313/4248, 47/708)$	18 007 434
$(29, 46, 19)$	$(145/2124, -53/4248, 193/1062)$	49 730
$(30, 47, 19)$	$(-151/2124, -179/2124, -65/2124)$	52 233 655
$(31, 48, 19)$	$(-5/36, -45/472, -1/59)$	410
$(32, 49, 19)$	$(-607/4248, -58/531, -25/708)$	5 939 349
$(28, 46, 20)$	$(-293/1416, -415/4248, -49/4248)$	41
$(29, 47, 20)$	$(-1/8, -7/72, 1/72)$	47
$(30, 48, 20)$	$(-415/2124, -109/1062, 55/4248)$	63 324
$(31, 49, 20)$	$(-977/4248, -529/4248, 139/4248)$	10 946
$(32, 50, 20)$	$(-151/2124, -179/2124, -199/4248)$	13 855 341
$(33, 51, 20)$	$(-265/1062, -7/59, 1/72)$	141
$(34, 52, 20)$	$(-40/531, -22/177, -319/4248)$	7 330 859
$(29, 48, 21)$	$(-104/531, -221/2124, 67/4248)$	7
$(30, 49, 21)$	$(-455/2124, -19/177, -73/4248)$	7
$(31, 50, 21)$	$(-11/1062, -83/1416, 317/2124)$	1041
$(32, 51, 21)$	$(7/472, -215/4248, 257/1416)$	139 197
$(33, 52, 21)$	$(-289/1416, -51/472, 23/4248)$	3081
$(34, 53, 21)$	$(-161/2124, -13/177, 287/4248)$	16 159 109
$(35, 54, 21)$	$(-191/1416, -191/2124, -7/1062)$	314

f-vector	generating grid point	frequency
$(36, 55, 21)$	$(-401/2124, -265/2124, 1/1416)$	4 176 683
$(32, 52, 22)$	$(-217/1062, -217/2124, -23/4248)$	3
$(33, 53, 22)$	$(131/1062, 439/4248, 313/2124)$	7
$(34, 54, 22)$	$(-104/531, -73/708, 55/4248)$	20 995
$(35, 55, 22)$	$(-67/1416, -281/4248, 451/4248)$	5780
$(36, 56, 22)$	$(-21/236, -37/472, 35/708)$	2 625 931
$(37, 57, 22)$	$(-511/2124, -29/236, 1/72)$	1027
$(38, 58, 22)$	$(-124/531, -265/2124, 73/4248)$	337 899
$(35, 56, 23)$	$(5/177, -115/2124, 275/1416)$	149
$(36, 57, 23)$	$(-104/531, -439/4248, 7/531)$	20 653
$(37, 58, 23)$	$(-95/472, -45/472, -25/1416)$	1528
$(38, 59, 23)$	$(-337/4248, -317/4248, 89/1416)$	8 678 192
$(39, 60, 23)$	$(-481/1416, 73/1416, 383/1416)$	148
$(40, 61, 23)$	$(-217/1062, -115/1062, 23/4248)$	2 574 890
$(39, 61, 24)$	$(119/4248, 323/4248, 1181/4248)$	1122
$(40, 62, 24)$	$(-319/4248, -311/4248, 97/1416)$	608 694
$(41, 63, 24)$	$(-83/236, 25/708, 19/72)$	3
$(42, 64, 24)$	$(-889/4248, -463/4248, 35/4248)$	804 747
$(39, 62, 25)$	$(-815/4248, -455/4248, 107/4248)$	19
$(40, 63, 25)$	$(-34/177, -493/4248, 85/2124)$	170
$(41, 64, 25)$	$(-833/4248, -49/472, 1/72)$	21
$(42, 65, 25)$	$(17/531, -223/4248, 209/1062)$	501 550
$(43, 66, 25)$	$(-121/531, -1/9, -3/472)$	7
$(44, 67, 25)$	$(-299/1416, -233/2124, 17/2124)$	1 446 228
$(43, 67, 26)$	$(-1457/4248, 193/4248, 1183/4248)$	26
$(44, 68, 26)$	$(-97/531, -29/236, 7/1416)$	5763
$(45, 69, 26)$	$(-875/4248, -7/72, -7/472)$	20
$(46, 70, 26)$	$(-889/4248, -463/4248, 11/1416)$	399 754
$(46, 71, 27)$	$(-833/4248, -73/708, 13/1062)$	2528
$(48, 73, 27)$	$(-1441/4248, 227/4248, 1141/4248)$	107 586
$(50, 76, 28)$	$(-733/2124, 103/2124, 127/472)$	49 893
$(52, 79, 29)$	$(-113/531, -49/472, -4/531)$	565

Space group type $(3, 7, 3, 3, 2)$**;** $\mathrm{IT}(214) = I4_132$

Normalizer: $\mathrm{IT}(230) = Ia\bar{3}d$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{214} = \operatorname{conv}\{(0,0,0), (1/8,1/8,1/8), (-1/8,1/8,1/8), (-1/8,-1/8,1/8), (1/8,-1/8,1/8), (1/8,1/8,1/4), (-1/8,1/8,1/4), (-1/8,-1/8,1/4), (1/8,-1/8,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 55$ [SS11] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel found for this group four stereohedra with 38 facets, see [Eng81a; GS80].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(9, 16, 9)$	$(-145/2328, 145/2328, 437/2328)$	654
$(13, 21, 10)$	$(-871/6984, 871/6984, 875/6984)$	218
$(13, 22, 11)$	$(-1/8, -1/8, 1/8)$	5
$(14, 24, 12)$	$(-1/6984, -1/8, 1/8)$	1875
$(16, 26, 12)$	$(145/1164, 109/873, 437/3492)$	478 096
$(17, 27, 12)$	$(1/8, -1/8, 1/4)$	3490
$(14, 25, 13)$	$(1/24, 1/8, 5/24)$	1
$(15, 26, 13)$	$(-1/8, 1/24, 5/24)$	409
$(16, 27, 13)$	$(1/8, 1/24, 5/24)$	1018
$(17, 28, 13)$	$(7/97, 41/388, 153/776)$	93
$(18, 29, 13)$	$(-871/6984, 869/6984, 875/6984)$	349 676
$(19, 30, 13)$	$(1/2328, 233/2328, 155/776)$	17
$(16, 28, 14)$	$(-1/8, 289/6984, 1457/6984)$	95 193
$(17, 29, 14)$	$(293/6984, 289/2328, 1459/6984)$	139
$(18, 30, 14)$	$(281/6984, 289/2328, 1453/6984)$	29
$(19, 31, 14)$	$(-661/6984, -871/6984, 121/776)$	319 860
$(20, 32, 14)$	$(-443/6984, -73/776, 121/776)$	272 521
$(24, 36, 14)$	$(0, 0, 0)$	873
$(19, 32, 15)$	$(289/6984, 1/8, 727/3492)$	217
$(20, 33, 15)$	$(-73/776, -659/6984, 121/776)$	983 215
$(21, 34, 15)$	$(-167/2328, -75/776, 355/2328)$	6660
$(22, 35, 15)$	$(-443/6984, -659/6984, 121/776)$	1 070 500
$(23, 36, 15)$	$(-67/776, -625/6984, 121/776)$	1544
$(24, 37, 15)$	$(-3/776, 719/6984, 133/873)$	72 045 809
$(21, 35, 16)$	$(-53/776, -845/6984, 1087/6984)$	59 276
$(23, 37, 16)$	$(-1/8, 205/6984, 1283/6984)$	58 000
$(24, 38, 16)$	$(-661/6984, -871/6984, 545/3492)$	103 290 708
$(25, 39, 16)$	$(1/72, 817/6984, 151/776)$	241
$(26, 40, 16)$	$(-455/6984, -655/6984, 545/3492)$	226 770 401
$(24, 39, 17)$	$(-1/6984, 697/6984, 1397/6984)$	65 328
$(25, 40, 17)$	$(31/1746, 109/873, 655/3492)$	28 759
$(26, 41, 17)$	$(-455/6984, -673/6984, 545/3492)$	10 781 542
$(27, 42, 17)$	$(703/6984, 235/2328, 1091/6984)$	448
$(28, 43, 17)$	$(-457/6984, -51/776, 545/3492)$	320 083 741
$(30, 45, 17)$	$(1/8, 1/8, 1/8)$	1
$(25, 41, 18)$	$(-55/776, -77/776, 121/776)$	1155
$(26, 42, 18)$	$(-73/776, -659/6984, 545/3492)$	49 928 325
$(27, 43, 18)$	$(-677/6984, -851/6984, 355/2328)$	41 242
$(28, 44, 18)$	$(-455/6984, -841/6984, 545/3492)$	68 451 893
$(29, 45, 18)$	$(109/873, 37/1746, 401/1746)$	110
$(30, 46, 18)$	$(31/1746, 109/873, 1309/6984)$	19 665 278
$(26, 43, 19)$	$(305/6984, 281/2328, 1465/6984)$	29
$(27, 44, 19)$	$(329/6984, 77/776, 173/776)$	81
$(29, 46, 19)$	$(1/24, 289/2328, 1457/6984)$	27 993
$(30, 47, 19)$	$(-455/6984, -73/776, 545/3492)$	48 889 552

f-vector	generating grid point	frequency
$(31, 48, 19)$	$(-281/6984, 293/6984, 5/24)$	256
$(32, 49, 19)$	$(31/1746, 109/873, 223/1164)$	17 734 901
$(31, 49, 20)$	$(325/6984, 91/776, 491/2328)$	4755
$(32, 50, 20)$	$(-463/6984, -73/776, 545/3492)$	12 459 956
$(33, 51, 20)$	$(1/2328, 583/6984, 5/24)$	168
$(34, 52, 20)$	$(31/1746, 109/873, 1369/6984)$	14 570 609
$(30, 49, 21)$	$(7/97, 33/388, 161/776)$	1
$(33, 52, 21)$	$(653/6984, 655/6984, 1249/6984)$	7681
$(34, 53, 21)$	$(-1/8, 331/6984, 64/291)$	12 005 153
$(35, 54, 21)$	$(69/776, 7/72, 421/2328)$	17
$(36, 55, 21)$	$(869/6984, 871/6984, 439/3492)$	3 519 504
$(35, 55, 22)$	$(409/6984, 277/2328, 511/2328)$	4133
$(36, 56, 22)$	$(293/6984, 865/6984, 1459/6984)$	205 405
$(37, 57, 22)$	$(75/776, 7/72, 407/2328)$	101
$(38, 58, 22)$	$(217/1746, 145/1164, 49/388)$	4 966 452
$(34, 55, 23)$	$(19/291, 21/194, 19/97)$	31
$(37, 58, 23)$	$(115/1746, 379/3492, 1367/6984)$	2568
$(38, 59, 23)$	$(-1/2328, 695/6984, 233/1164)$	1 114 000
$(39, 60, 23)$	$(295/6984, 859/6984, 1459/6984)$	171
$(40, 61, 23)$	$(10/97, 361/3492, 1123/6984)$	1 660 625
$(39, 61, 24)$	$(103/6984, 239/6984, 1663/6984)$	1364
$(41, 63, 24)$	$(1/24, 511/6984, 509/2328)$	38
$(42, 64, 24)$	$(865/6984, 289/2328, 295/2328)$	1 919 321
$(41, 64, 25)$	$(349/3492, 39/388, 599/3492)$	302
$(43, 66, 25)$	$(43/388, 1/9, 529/3492)$	106
$(44, 67, 25)$	$(1/24, 869/6984, 182/873)$	1 771 396
$(43, 67, 26)$	$(223/6984, 655/6984, 1525/6984)$	3049
$(45, 69, 26)$	$(455/6984, 5/72, 1571/6984)$	25
$(46, 70, 26)$	$(289/2328, 869/6984, 49/388)$	2 191 033
$(45, 70, 27)$	$(283/6984, 45/776, 1571/6984)$	244
$(47, 72, 27)$	$(1/24, 469/6984, 515/2328)$	41
$(48, 73, 27)$	$(865/6984, 289/2328, 443/3492)$	781 779
$(47, 73, 28)$	$(121/1746, 94/873, 685/3492)$	919
$(49, 75, 28)$	$(65/1164, 1/9, 239/1164)$	11
$(50, 76, 28)$	$(227/2328, 683/6984, 1229/6984)$	686 356
$(49, 76, 29)$	$(85/1164, 121/1164, 227/1164)$	59
$(51, 78, 29)$	$(151/2328, 689/6984, 5/24)$	22
$(52, 79, 29)$	$(71/582, 427/3492, 455/3492)$	252 540
$(51, 79, 30)$	$(5/72, 5/72, 2/9)$	51
$(53, 81, 30)$	$(55/776, 7/72, 159/776)$	34
$(54, 82, 30)$	$(37/388, 167/1746, 209/1164)$	89 693
$(53, 82, 31)$	$(473/6984, 247/2328, 1387/6984)$	32
$(55, 84, 31)$	$(56/873, 41/388, 709/3492)$	4
$(56, 85, 31)$	$(461/6984, 517/6984, 1541/6984)$	137 402
$(55, 85, 32)$	$(653/6984, 343/6984, 797/3492)$	1
$(58, 88, 32)$	$(463/6984, 517/6984, 257/1164)$	66 313
$(57, 88, 33)$	$(215/2328, 119/2328, 529/2328)$	3
$(59, 90, 33)$	$(22/291, 1/12, 247/1164)$	2
$(60, 91, 33)$	$(473/6984, 757/6984, 343/1746)$	11 108

f-vector	generating grid point	frequency
$(61, 93, 34)$	$(15/194, 1/12, 41/194)$	8
$(62, 94, 34)$	$(115/1746, 32/291, 691/3492)$	9984
$(61, 94, 35)$	$(47/776, 87/776, 39/194)$	10
$(63, 96, 35)$	$(52/873, 45/388, 77/388)$	1
$(64, 97, 35)$	$(17/291, 100/873, 39/194)$	1474
$(66, 100, 36)$	$(445/6984, 259/2328, 347/1746)$	10 040
$(68, 103, 37)$	$(443/6984, 259/2328, 1387/6984)$	242
$(70, 106, 38)$	$(427/6984, 761/6984, 1421/6984)$	153

Space group type $(3, 7, 4, 1, 1)$**;** IT(215) $= P\bar{4}3m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{215} = \operatorname{conv}\left\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 12 facets, see [Koc72, p. 61].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/2, 1815/3632, 0)$	1 648 020
$(5, 8, 5)$	$(1815/3632, 0, 0)$	1815
$(6, 9, 5)$	$(15/227, 45/3632, 7/3632)$	996 502 759
$(5, 9, 6)$	$(1815/3632, 1815/3632, 0)$	1815
$(8, 12, 6)$	$(0, 0, 0)$	1
$(8, 13, 7)$	$(1817/7264, 1817/7264, 1815/7264)$	3 296 040
$(6, 12, 8)$	$(1/2, 0, 0)$	2
$(14, 24, 12)$	$(1/4, 1/4, 1/4)$	1816

Space group type $(3, 7, 4, 2, 1)$**;** IT(216) $= F\bar{4}3m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis $\frac{1}{2}b'_1, \frac{1}{2}b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{216} = \operatorname{conv}\left\{(0,0,0), (1/8,1/8,1/8), (1/4,0,0), (1/4,1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 12 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(15/454, 45/7264, 7/7264)$	996 103 483
$(5, 8, 5)$	$(1817/14528, 1817/14528, 1815/14528)$	3 297 855
$(8, 12, 6)$	$(1/8, 1/8, 1/8)$	1816
$(6, 12, 8)$	$(1/4, 0, 0)$	1817
$(14, 24, 12)$	$(0, 0, 0)$	1

Space group type $(3, 7, 4, 3, 1)$**;** IT(217) $= I\bar{4}3m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3

Reduced fundamental domain:

$$R_{217} = \text{conv}\left\{(0, 0, 0), (1/2, 0, 0), (1/2, 1/2, 0), (1/4, 1/4, 1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Engel [Eng81b] found a stereohedron with 15 facets for this group.

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4, 6, 4)$	$(1/2, 1/4, 0)$	1361
$(5, 8, 5)$	$(909/3632, 1/4, 53/227)$	411 778
$(6, 9, 5)$	$(1/2, 1815/3632, 0)$	1814
$(5, 9, 6)$	$(3/8, 3/8, 0)$	1
$(6, 10, 6)$	$(3337/7264, 2819/7264, 177/7264)$	1392
$(7, 11, 6)$	$(121/454, 967/3632, 789/3632)$	410 418
$(8, 12, 6)$	$(15/227, 45/3632, 7/3632)$	848 891 289
$(10, 15, 7)$	$(1819/7264, 1817/7264, 1695/7264)$	148 432 727
$(6, 12, 8)$	$(1/4, 1/4, 0)$	908
$(10, 17, 9)$	$(909/3632, 909/3632, 453/1816)$	453
$(12, 19, 9)$	$(1817/7264, 1817/7264, 1815/7264)$	1 980 209
$(8, 15, 9)$	$(13/32, 13/32, 1/32)$	1
$(11, 19, 10)$	$(1815/3632, 1815/3632, 0)$	453
$(12, 20, 10)$	$(907/3632, 907/3632, 0)$	823 556
$(9, 17, 10)$	$(1361/3632, 1361/3632, 0)$	453
$(14, 23, 11)$	$(1817/7264, 1817/7264, 1813/7264)$	491 821
$(10, 20, 12)$	$(1/2, 0, 0)$	2
$(17, 28, 13)$	$(1815/3632, 0, 0)$	1815
$(24, 36, 14)$	$(0, 0, 0)$	1
$(26, 39, 15)$	$(1815/7264, 1815/7264, 1815/7264)$	1815

Space group type $(3,7,4,1,2)$**;** IT(218) $= P\bar{4}3n$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{218} = \text{conv}\left\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 23$ [SS08, Section 5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f**-vector**	**generating grid point**	**frequency**
$(5,9,6)$	$(3/8,3/8,0)$	454
$(6,10,6)$	$(909/3632,1/4,907/3632)$	907
$(8,12,6)$	$(1/4,1/4,1/4)$	1
$(6,12,8)$	$(1/4,1/4,0)$	908
$(7,13,8)$	$(907/1816,907/3632,0)$	907
$(10,17,9)$	$(909/3632,909/3632,453/1816)$	453
$(12,19,9)$	$(1817/7264,1817/7264,1815/7264)$	1 980 209
$(8,15,9)$	$(13/32,13/32,1/32)$	1
$(11,19,10)$	$(1815/3632,1815/3632,0)$	1 029 218
$(12,20,10)$	$(907/3632,907/3632,0)$	823 556
$(8,16,10)$	$(1/2,1/4,0)$	454
$(9,17,10)$	$(1361/3632,1361/3632,0)$	453
$(13,22,11)$	$(121/454,967/3632,789/3632)$	820 836
$(14,23,11)$	$(1817/7264,1817/7264,1813/7264)$	491 821
$(10,20,12)$	$(1/2,0,0)$	2
$(14,24,12)$	$(909/3632,1/4,53/227)$	410 871
$(15,26,13)$	$(31/908,123/3632,61/1816)$	824 043
$(16,27,13)$	$(1/4,907/3632,849/3632)$	205 209
$(17,28,13)$	$(1815/3632,0,0)$	1815
$(18,29,13)$	$(15/227,45/3632,7/3632)$	310 229 312
$(19,30,13)$	$(369/7264,205/7264,123/7264)$	2287
$(16,28,14)$	$(1/2,1815/3632,0)$	1814
$(20,32,14)$	$(249/7264,247/7264,243/7264)$	325 683 860
$(24,36,14)$	$(0,0,0)$	1
$(20,33,15)$	$(3285/7264,3283/7264,229/7264)$	23 274 317
$(22,35,15)$	$(249/7264,245/7264,243/7264)$	287 970 712
$(26,39,15)$	$(1815/7264,1815/7264,1815/7264)$	1815
$(24,38,16)$	$(251/7264,247/7264,241/7264)$	46 565 718
$(24,39,17)$	$(3339/7264,2805/7264,175/7264)$	1 006 663
$(26,41,17)$	$(3467/7264,1753/7264,47/7264)$	123 650

Space group type $(3,7,4,2,2)$**;** IT(219) $= F\bar{4}3c$

Normalizer: IT(229) $= Im\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{219} = \operatorname{conv}\left\{(0,0,0),(1/8,1/8,1/8),(1/4,0,0),(1/4,1/4,0)\right\}$$

Upper bound on number of facets: $f_2 \leq 14$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(1/4,1815/7264,0)$	1815
$(5,8,5)$	$(1815/7264,0,0)$	1815
$(5,9,6)$	$(1815/7264,1815/7264,0)$	1815
$(8,12,6)$	$(0,0,0)$	1
$(8,13,7)$	$(1817/14528,1817/14528,1815/14528)$	3 286 478
$(6,12,8)$	$(1/4,0,0)$	2
$(8,15,9)$	$(1815/7264,907/3632,0)$	1 561 509
$(14,24,12)$	$(15/454,45/7264,7/7264)$	928 404 859

Space group type $(3,7,4,3,2)$**;** IT(220) $= I\bar{4}3d$

Normalizer: IT(230) $= Ia\bar{3}d$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{220} = \operatorname{conv}\left\{(0,0,0),(1/8,1/8,1/8),(-1/8,1/8,1/8),\right.$$
$$(-1/8,-1/8,1/8),(1/8,-1/8,1/8),(1/8,1/8,1/4),$$
$$\left.(-1/8,1/8,1/4),(-1/8,-1/8,1/4),(1/8,-1/8,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 76$ [SS11] for points with trivial stabilizer and $f_2 \leq 198$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 17 facets, see [Koc72, p. 64].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8,15,9)$	$(0,0,1/8)$	1
$(12,20,10)$	$(0,0,73/582)$	145
$(10,19,11)$	$(-1/8,-1/8,1/8)$	1164
$(15,24,11)$	$(-1/8,-1/8,1/4)$	2
$(8,17,11)$	$(1/8,-1/24,5/24)$	73
$(9,18,11)$	$(-1/8,-227/6984,355/2328)$	439
$(12,22,12)$	$(143/1746,289/3492,295/3492)$	46
$(13,23,12)$	$(-1/8,-527/6984,1219/6984)$	186 531
$(14,24,12)$	$(1/8,-235/6984,1/8)$	374 107

f-vector	generating grid point	frequency
$(16, 26, 12)$	$(1/8, -1/8, 1/4)$	515
$(17, 27, 12)$	$(-673/6984, -587/6984, 1685/6984)$	985
$(14, 25, 13)$	$(1/9, 0, 1/6)$	217
$(15, 26, 13)$	$(-1/8, 15/776, 155/776)$	15 723
$(16, 27, 13)$	$(-1/8, 29/6984, 157/1164)$	219 449
$(17, 28, 13)$	$(-37/1164, 67/582, 173/1164)$	418
$(18, 29, 13)$	$(1/8, -175/6984, 611/3492)$	56 478 556
$(21, 32, 13)$	$(109/3492, 109/3492, 109/1746)$	732 686
$(16, 28, 14)$	$(-221/2328, 7/2328, 463/2328)$	30
$(17, 29, 14)$	$(-817/6984, -85/6984, 1379/6984)$	12 435
$(18, 30, 14)$	$(-1/8, -197/2328, 1253/6984)$	10 039 845
$(19, 31, 14)$	$(9/776, 277/2328, 833/6984)$	313 969
$(20, 32, 14)$	$(-1/8, -83/776, 1331/6984)$	218 235 938
$(21, 33, 14)$	$(145/2328, 145/2328, 1/8)$	256
$(22, 34, 14)$	$(31/1746, 109/873, 1369/6984)$	60 494 788
$(23, 35, 14)$	$(1/8, 871/6984, 1/8)$	437 810
$(24, 36, 14)$	$(0, 0, 0)$	582
$(18, 31, 15)$	$(1/12, 73/1746, 581/3492)$	181
$(19, 32, 15)$	$(-259/2328, -451/6984, 751/3492)$	3469
$(20, 33, 15)$	$(0, 9/388, 105/776)$	1
$(21, 34, 15)$	$(-503/6984, -791/6984, 11/72)$	82 757
$(22, 35, 15)$	$(-1/8, 55/2328, 437/3492)$	52 090 897
$(24, 37, 15)$	$(-13/3492, 10/97, 863/6984)$	179 647 272
$(25, 38, 15)$	$(109/1746, 109/1746, 109/873)$	173 738
$(19, 33, 16)$	$(-251/2328, -113/2328, 505/2328)$	31
$(23, 37, 16)$	$(289/3492, 145/1746, 293/3492)$	120 217
$(24, 38, 16)$	$(-1/8, 27/776, 1189/6984)$	8 151 923
$(25, 39, 16)$	$(-247/6984, -17/6984, 1627/6984)$	150
$(26, 40, 16)$	$(-3/776, 719/6984, 133/873)$	148 930 926
$(27, 41, 16)$	$(133/1746, 133/1746, 133/873)$	163 682
$(24, 39, 17)$	$(-455/6984, -871/6984, 545/3492)$	2 697 864
$(25, 40, 17)$	$(289/3492, 145/1746, 73/873)$	92 379
$(26, 41, 17)$	$(-455/6984, -7/72, 545/3492)$	25 662 261
$(27, 42, 17)$	$(0, 43/873, 347/2328)$	29 836
$(28, 43, 17)$	$(-455/6984, -655/6984, 545/3492)$	50 738 540
$(29, 44, 17)$	$(25/776, 25/776, 25/388)$	77 647
$(30, 45, 17)$	$(1/8, 1/8, 1/8)$	291
$(26, 42, 18)$	$(-737/6984, -95/2328, 1519/6984)$	1 364 319
$(27, 43, 18)$	$(25/6984, 43/6984, 67/6984)$	18 727
$(28, 44, 18)$	$(-63/776, -7/776, 1489/6984)$	305 143
$(29, 45, 18)$	$(9/97, 3/97, 91/582)$	398
$(30, 46, 18)$	$(88/873, 353/3492, 127/1164)$	96 509 074
$(29, 46, 19)$	$(95/873, 19/291, 19/97)$	15 117
$(32, 49, 19)$	$(-521/6984, -689/6984, 545/3492)$	43 233 216
$(32, 50, 20)$	$(8/97, 40/873, 137/873)$	446
$(34, 52, 20)$	$(83/1164, 251/3492, 511/6984)$	17 388 410
$(33, 52, 21)$	$(235/2328, 47/776, 141/776)$	31 861
$(36, 55, 21)$	$(119/6984, 121/6984, 31/1746)$	8 622 524
$(38, 58, 22)$	$(707/6984, 425/6984, 1273/6984)$	1 526 074

f-vector	generating grid point	frequency
$(37,58,23)$	$(1/8,45/776,159/776)$	2
$(40,61,23)$	$(1/8,365/6984,373/1746)$	12 841 602
$(42,64,24)$	$(647/6984,389/6984,1165/6984)$	78 630
$(44,67,25)$	$(1/8,115/2328,247/1164)$	1 093 237

Space group type $(3,7,5,1,1)$**;** IT(221) $= Pm\bar{3}m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{221} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \le 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \le 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 8 facets, see [Koc72, p. 26].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(15/227,45/3632,7/3632)$	998 150 780
$(5,8,5)$	$(1817/7264,1817/7264,1815/7264)$	3 297 854
$(5,9,6)$	$(1815/3632,1815/3632,0)$	1815
$(8,12,6)$	$(0,0,0)$	1817
$(6,12,8)$	$(1/2,0,0)$	2

Space group type $(3,7,5,1,3)$**;** IT(222) $= Pn\bar{3}n$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{222} = \operatorname{conv}\big\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\big\}$$

Upper bound on number of facets: $f_2 \le 23$ [SS08, Corollary 4.3] for points with trivial stabilizer and $f_2 \le 390$ in general (Theorem 1.2.6).

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5,8,5)$	$(1/2,1815/3632,0)$	3628
$(8,12,6)$	$(1/4,907/3632,849/3632)$	823 077
$(10,15,7)$	$(1817/7264,1817/7264,1815/7264)$	5445
$(8,13,7)$	$(435/908,19/908,9/1816)$	2 469 321
$(9,14,7)$	$(1819/7264,1817/7264,1813/7264)$	3 290 596

f-vector	generating grid point	frequency
$(6, 12, 8)$	$(1/2, 1/4, 0)$	2
$(12, 20, 10)$	$(909/3632, 1/4, 907/3632)$	1814
$(14, 23, 11)$	$(15/227, 45/3632, 7/3632)$	846 570 215
$(17, 28, 13)$	$(1/4, 1/4, 0)$	908
$(18, 29, 13)$	$(111/1816, 13/1816, 25/3632)$	147 289 831
$(24, 36, 14)$	$(1/4, 1/4, 1/4)$	1

Space group type $(3, 7, 5, 1, 2)$**;** IT(223) $= Pm\bar{3}n$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{223} = \text{conv}\left\{(0,0,0), (1/2,0,0), (1/2,1/2,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 14 facets, see [Koc72, p. 38].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(5, 8, 5)$	$(121/454, 967/3632, 789/3632)$	206 569
$(5, 9, 6)$	$(3/8, 3/8, 0)$	454
$(6, 10, 6)$	$(31/908, 123/3632, 61/1816)$	823 556
$(8, 12, 6)$	$(1/4, 1/4, 1/4)$	1
$(10, 15, 7)$	$(1815/7264, 1815/7264, 1815/7264)$	1815
$(7, 12, 7)$	$(1/4, 907/3632, 849/3632)$	205 209
$(8, 13, 7)$	$(15/227, 45/3632, 7/3632)$	625 491 236
$(9, 14, 7)$	$(1815/7264, 1815/7264, 1813/7264)$	822 649
$(10, 16, 8)$	$(249/7264, 247/7264, 243/7264)$	372 249 579
$(6, 12, 8)$	$(1/4, 1/4, 0)$	1
$(7, 13, 8)$	$(907/1816, 907/3632, 0)$	907
$(11, 19, 10)$	$(1815/3632, 1815/3632, 0)$	1 029 218
$(12, 20, 10)$	$(907/3632, 907/3632, 0)$	907
$(8, 16, 10)$	$(1/2, 1/4, 0)$	454
$(9, 17, 10)$	$(1361/3632, 1361/3632, 0)$	453
$(13, 22, 11)$	$(907/1816, 909/3632, 0)$	615 627
$(10, 20, 12)$	$(1/2, 0, 0)$	2
$(17, 28, 13)$	$(1815/3632, 0, 0)$	1815
$(16, 28, 14)$	$(1/2, 1815/3632, 0)$	1814
$(24, 36, 14)$	$(0, 0, 0)$	1

Space group type $(3, 7, 5, 1, 4)$**;** IT(224) $= Pn\bar{3}m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b_1', b_2', b_3'

Reduced fundamental domain:

$$R_{224} = \text{conv}\left\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 16 facets, see [Koc72, p. 40].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8,12,6)$	$(15/227, 45/3632, 7/3632)$	995 679 204
$(6,12,8)$	$(1/2, 1815/3632, 0)$	3630
$(12,19,9)$	$(435/908, 19/908, 9/1816)$	2 470 668
$(12,20,10)$	$(909/3632, 1/4, 907/3632)$	3 292 410
$(14,24,12)$	$(0,0,0)$	3
$(17,28,13)$	$(1/4,1/4,0)$	908
$(24,36,14)$	$(1/4,1/4,1/4)$	1
$(25,39,16)$	$(1817/7264, 1817/7264, 1815/7264)$	5445

Space group type $(3,7,5,2,1)$**;** IT(225) $= Fm\bar{3}m$

Normalizer: IT(221) $= Pm\bar{3}m$ with basis $\frac{1}{2}b'_1, \frac{1}{2}b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{225} = \text{conv}\left\{(0,0,0),(1/4,0,0),(1/4,1/4,0),(1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 12 facets, see [Koc72, p. 27].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(247/7264, 13/1816, 7/3632)$	999 796 985
$(5,8,5)$	$(1/4, 1/4, 1815/7264)$	3630
$(5,9,6)$	$(1/4, 1815/7264, 1815/7264)$	1 649 835
$(8,12,6)$	$(1/4,1/4,1/4)$	1
$(6,12,8)$	$(1/4,0,0)$	1817
$(14,24,12)$	$(0,0,0)$	1

Space group type $(3,7,5,2,2)$**;** IT(226) $= Fm\bar{3}c$

Normalizer: IT(221) $= Pm\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{226} = \text{conv}\left\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/4,1/4,1/4)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 9 facets, see [Koc72, p. 99].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(1/4, 1815/7264, 0)$	1 648 020
$(5,8,5)$	$(1/4, 1/4, 1815/7264)$	3 296 040
$(5,9,6)$	$(1815/7264, 1815/7264, 0)$	3630
$(8,12,6)$	$(0,0,0)$	1817
$(7,12,7)$	$(247/7264, 13/1816, 7/3632)$	994 856 555
$(6,12,8)$	$(1/4,0,0)$	2
$(8,15,9)$	$(1815/7264, 907/3632, 0)$	1 646 205

Space group type $(3,7,5,2,4)$**;** IT(227) $= Fd\bar{3}m$

Normalizer: IT(224) $= Pn\bar{3}m$ with basis $\frac{1}{2}b_1', \frac{1}{2}b_2', \frac{1}{2}b_3'$

Reduced fundamental domain:

$$R_{227} = \text{conv}\left\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/8,1/8,1/8), (1/8,1/8,-1/8)\right\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 16 facets, see [Koc72, p. 28]. Smith [Smi65] even claims to have found a stereohedron with 20 facets.

Metrical parameters: We used 1 000 520 885 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(107/5764, 103/5764, -1/1441)$	345 600
$(5,8,5)$	$(360/1441, 360/1441, 0)$	1680
$(6,9,5)$	$(107/5764, 103/5764, 2/131)$	994 981 920
$(8,12,6)$	$(0,0,0)$	2

f-vector	generating grid point	frequency
$(10, 15, 7)$	$(180/1441, 180/1441, 180/1441)$	2880
$(8, 13, 7)$	$(721/5764, 180/1441, -180/1441)$	4 150 560
$(9, 14, 7)$	$(721/5764, 721/5764, 719/5764)$	1 035 360
$(10, 20, 12)$	$(1/8, 1/8, -1/8)$	721
$(12, 22, 12)$	$(1/8, 1/8, 1439/11528)$	720
$(14, 24, 12)$	$(1/4, 0, 0)$	1441
$(16, 30, 16)$	$(1/8, 1/8, 1/8)$	1

Space group type $(3, 7, 5, 2, 3)$**;** IT(228) $= Fd\bar{3}c$

Normalizer: IT(224) $= Pn\bar{3}m$ with basis $\frac{1}{2}b'_1, \frac{1}{2}b'_2, \frac{1}{2}b'_3$

Reduced fundamental domain:

$$R_{228} = \operatorname{conv}\big\{(0,0,0), (1/4,0,0), (1/4,1/4,0), (1/8,1/8,1/8), (1/8,1/8,-1/8)\big\}$$

Upper bound on number of facets: $f_2 \leq 25$ [SS08, Corollary 3.5] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 12 facets, see [Koc72, p. 47].

Metrical parameters: We used 1 000 520 885 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(6, 11, 7)$	$(721/5764, 180/1441, -180/1441)$	4320
$(6, 12, 8)$	$(1/4, 360/1441, 0)$	2880
$(12, 19, 9)$	$(721/5764, 721/5764, 719/5764)$	3 108 240
$(12, 20, 10)$	$(1443/11528, 1/8, 1439/11528)$	2 072 160
$(10, 20, 12)$	$(1/8, 1/8, -1/8)$	1
$(14, 24, 12)$	$(0, 0, 0)$	3
$(15, 25, 12)$	$(1101/5764, 503/2882, -163/2882)$	799 102
$(15, 26, 13)$	$(247/11528, 169/11528, 65/11528)$	6630
$(17, 28, 13)$	$(2141/11528, 1951/11528, -469/11528)$	236 188
$(18, 29, 13)$	$(215/11528, 205/11528, 203/11528)$	604 933 404
$(17, 29, 14)$	$(519/2882, 865/5764, -45/2882)$	2
$(20, 32, 14)$	$(107/5764, 103/5764, 2/131)$	214 368 477
$(24, 36, 14)$	$(1/8, 1/8, 1/8)$	1
$(22, 35, 15)$	$(215/11528, 205/11528, 199/11528)$	162 095 446
$(24, 38, 16)$	$(2089/11528, 1899/11528, -417/11528)$	10 432 173
$(25, 39, 16)$	$(180/1441, 180/1441, 180/1441)$	4320

Space group type $(3, 7, 5, 3, 1)$**;** IT(229) $= Im\bar{3}m$

Normalizer: IT(229) $= Im\bar{3}m$ with basis b'_1, b'_2, b'_3; so the normalizer is identical with the group itself.

Reduced fundamental domain:

$$R_{229} = \text{conv}\,\{(0,0,0),(1/2,0,0),(1/2,1/2,0),(1/4,1/4,1/4)\}$$

Upper bound on number of facets: $f_2 \leq 8$ [BS01, Theorem 2.4] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 14 facets, see [Koc72, p. 29].

Metrical parameters: We used 1 001 452 269 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(4,6,4)$	$(909/3632, 1/4, 53/227)$	617 441
$(5,8,5)$	$(1/4, 1/4, 907/3632)$	2267
$(6,9,5)$	$(15/227, 45/3632, 7/3632)$	995 887 587
$(5,9,6)$	$(3/8, 3/8, 0)$	1
$(7,11,6)$	$(907/1816, 909/3632, 0)$	205 209
$(8,12,6)$	$(1/4, 1/4, 1/4)$	1 439 637
$(10,15,7)$	$(1815/7264, 1815/7264, 1815/7264)$	1815
$(8,13,7)$	$(1817/7264, 1817/7264, 1815/7264)$	2 472 031
$(9,14,7)$	$(1815/7264, 1815/7264, 1813/7264)$	822 649
$(6,12,8)$	$(1/4, 1/4, 0)$	1
$(11,19,10)$	$(1815/3632, 1815/3632, 0)$	453
$(12,20,10)$	$(907/3632, 907/3632, 0)$	907
$(9,17,10)$	$(1361/3632, 1361/3632, 0)$	453
$(10,20,12)$	$(1/2, 0, 0)$	2
$(17,28,13)$	$(1815/3632, 0, 0)$	1815
$(24,36,14)$	$(0,0,0)$	1

Space group type $(3,7,5,3,2)$**;** IT(230) $= Ia\bar{3}d$

Normalizer: IT(230) $= Ia\bar{3}d$ with basis b_1', b_2', b_3'; so the normalizer is identical with the group itself.

Reduced fundamental domain:

$$\begin{aligned} R_{230} = \text{conv}\,\{&(0,0,0),(1/8,1/8,1/8),(-1/8,1/8,1/8),\\ &(-1/8,-1/8,1/8),(1/8,-1/8,1/8),(1/8,1/8,1/4),\\ &(-1/8,1/8,1/4),(-1/8,-1/8,1/4),(1/8,-1/8,1/4)\} \end{aligned}$$

Upper bound on number of facets: $f_2 \leq 68$ [SS11] for points with trivial stabilizer and $f_2 \leq 390$ in general (Theorem 1.2.6).

Remarks concerning lower bounds: Koch found for this group a stereohedron with 23 facets, see [Koc72, p. 57].

Metrical parameters: We used 1 000 677 997 grid points in the approximating grid.

f-vector	generating grid point	frequency
$(8, 13, 7)$	$(-1/8, -1/8, 1/4)$	2
$(8, 14, 8)$	$(-1/8, 1/24, 5/24)$	2
$(10, 17, 9)$	$(-1/6984, -1/6984, 1745/6984)$	70
$(12, 20, 10)$	$(1/8, -1/8, 1/4)$	3513
$(10, 19, 11)$	$(-1/8, -1/8, 1/8)$	3
$(11, 20, 11)$	$(289/2328, -293/6984, 1453/6984)$	68
$(12, 21, 11)$	$(-275/2328, 55/2328, 385/2328)$	1945
$(14, 23, 11)$	$(281/6984, 289/2328, 1453/6984)$	118
$(12, 22, 12)$	$(289/2328, -295/6984, 1457/6984)$	35
$(13, 23, 12)$	$(-1/8, -527/6984, 1219/6984)$	682
$(14, 24, 12)$	$(-1/8, -167/6984, 130/873)$	837
$(15, 25, 12)$	$(-1/8, 289/6984, 1451/6984)$	3942
$(16, 26, 12)$	$(1/12, -1/12, 1/6)$	74 941
$(17, 27, 12)$	$(575/6984, 193/2328, 583/6984)$	17 737
$(19, 29, 12)$	$(0, -25/1746, 25/1746)$	639
$(15, 26, 13)$	$(1/8, 871/6984, 877/6984)$	453
$(17, 28, 13)$	$(-69/776, -3/776, 151/776)$	82 800
$(18, 29, 13)$	$(-545/6984, -61/2328, 521/2328)$	88 823
$(19, 30, 13)$	$(19/1164, 12/97, 295/2328)$	83 305
$(15, 27, 14)$	$(1/12, 1/12, 1/12)$	1
$(16, 28, 14)$	$(-155/2328, -775/6984, 1085/6984)$	150
$(17, 29, 14)$	$(-1/8, 173/6984, 1223/6984)$	17 458
$(18, 30, 14)$	$(-1/8, -169/6984, 347/2328)$	177 516
$(19, 31, 14)$	$(347/6984, 91/776, 1507/6984)$	17 968
$(20, 32, 14)$	$(-73/776, -659/6984, 121/776)$	263 654
$(21, 33, 14)$	$(197/2328, 197/6984, 985/6984)$	35 874
$(22, 34, 14)$	$(575/6984, 193/2328, 49/582)$	24 840 979
$(23, 35, 14)$	$(92/873, 185/1746, 127/776)$	48 764
$(24, 36, 14)$	$(0, 0, 0)$	1
$(16, 29, 15)$	$(-217/2328, -661/6984, 1307/6984)$	11
$(19, 32, 15)$	$(-21/388, -59/582, 173/1164)$	8
$(20, 33, 15)$	$(-53/1164, -43/582, 119/1164)$	11
$(21, 34, 15)$	$(-469/6984, -779/6984, 121/776)$	193 621
$(22, 35, 15)$	$(-1/8, -767/6984, 149/776)$	28 444 598
$(23, 36, 15)$	$(-673/6984, -587/6984, 1685/6984)$	103 745
$(24, 37, 15)$	$(-457/6984, -51/776, 545/3492)$	119 145 287
$(21, 35, 16)$	$(-749/6984, -257/6984, 749/3492)$	11 622
$(22, 36, 16)$	$(-1/8, -1/6984, 319/2328)$	78 857
$(23, 37, 16)$	$(-469/6984, -773/6984, 545/3492)$	180 601
$(24, 38, 16)$	$(-1/8, 55/2328, 437/3492)$	5 243 826
$(25, 39, 16)$	$(-67/776, -625/6984, 121/776)$	13 491
$(26, 40, 16)$	$(-199/2328, -205/2328, 545/3492)$	32 078 653
$(20, 35, 17)$	$(-173/2328, -865/6984, 1211/6984)$	3
$(23, 38, 17)$	$(-697/6984, -39/776, 1571/6984)$	17 207
$(24, 39, 17)$	$(-749/6984, -251/6984, 1495/6984)$	3486
$(25, 40, 17)$	$(-455/6984, -815/6984, 545/3492)$	20 236
$(26, 41, 17)$	$(-73/776, -659/6984, 545/3492)$	10 941 120
$(27, 42, 17)$	$(-59/776, -595/6984, 119/776)$	21 632
$(28, 43, 17)$	$(-457/6984, -517/6984, 545/3492)$	71 934 443

f-vector	generating grid point	frequency
$(30, 45, 17)$	$(1/8, 1/8, 1/8)$	582
$(25, 41, 18)$	$(-733/6984, -113/2328, 1547/6984)$	5005
$(26, 42, 18)$	$(-83/776, -253/6984, 499/2328)$	276 888
$(27, 43, 18)$	$(-871/6984, -293/6984, 5/24)$	3947
$(28, 44, 18)$	$(-1/8, 77/6984, 51/388)$	11 978 279
$(29, 45, 18)$	$(-859/6984, -287/2328, 1025/6984)$	14 566
$(30, 46, 18)$	$(-455/6984, -73/776, 545/3492)$	53 229 871
$(25, 42, 19)$	$(-653/6984, -73/776, 109/582)$	1259
$(27, 44, 19)$	$(-653/6984, -659/6984, 1307/6984)$	1230
$(28, 45, 19)$	$(-869/6984, -175/2328, 1573/6984)$	476 221
$(29, 46, 19)$	$(-269/2328, -283/2328, 361/2328)$	3521
$(30, 47, 19)$	$(-659/6984, -869/6984, 545/3492)$	5 218 967
$(31, 48, 19)$	$(-833/6984, -623/6984, 1513/6984)$	5
$(32, 49, 19)$	$(-455/6984, -773/6984, 545/3492)$	8 920 763
$(29, 47, 20)$	$(-653/6984, -655/6984, 653/3492)$	987
$(30, 48, 20)$	$(-245/2328, -287/6984, 190/873)$	178 743
$(31, 49, 20)$	$(-805/6984, -425/6984, 527/2328)$	497
$(32, 50, 20)$	$(-281/2328, -283/6984, 61/291)$	2 735 367
$(33, 51, 20)$	$(-767/6984, -869/6984, 1027/6984)$	12
$(34, 52, 20)$	$(-455/6984, -655/6984, 545/3492)$	6 769 464
$(36, 54, 20)$	$(109/873, 109/873, 109/873)$	290
$(32, 51, 21)$	$(-433/6984, -445/6984, 871/3492)$	114 082
$(33, 52, 21)$	$(-265/2328, -169/2328, 265/1164)$	34
$(34, 53, 21)$	$(-187/2328, -51/776, 847/3492)$	355 297
$(36, 55, 21)$	$(-661/6984, -869/6984, 545/3492)$	870 762
$(34, 54, 22)$	$(-439/6984, -871/6984, 109/582)$	17 779
$(35, 55, 22)$	$(77/2328, 7/2328, 287/1164)$	88
$(36, 56, 22)$	$(-5/97, -355/3492, 355/2328)$	60 060
$(37, 57, 22)$	$(499/6984, 83/6984, 821/3492)$	1
$(38, 58, 22)$	$(-583/6984, -65/776, 545/3492)$	419 837
$(35, 56, 23)$	$(-655/6984, -761/6984, 1327/6984)$	3
$(36, 57, 23)$	$(-653/6984, -73/776, 1307/6984)$	40 225
$(38, 59, 23)$	$(-809/6984, -59/776, 179/776)$	4317
$(39, 60, 23)$	$(-865/6984, -173/2328, 527/2328)$	1
$(40, 61, 23)$	$(-263/2328, -149/2328, 787/3492)$	132 168
$(38, 60, 24)$	$(-457/6984, -847/6984, 1297/6984)$	379
$(40, 62, 24)$	$(-689/6984, -709/6984, 77/388)$	1223
$(42, 64, 24)$	$(-673/6984, -869/6984, 545/3492)$	31 120
$(42, 65, 25)$	$(-77/776, -707/6984, 1387/6984)$	1431
$(44, 67, 25)$	$(-817/6984, -505/6984, 1589/6984)$	28 571
$(42, 66, 26)$	$(-151/2328, -857/6984, 649/3492)$	84
$(44, 68, 26)$	$(-691/6984, -707/6984, 347/1746)$	53
$(46, 70, 26)$	$(103/2328, 1/776, 217/873)$	2658
$(48, 73, 27)$	$(-863/6984, -173/2328, 175/776)$	1

2.3 Discussion of the results

In Section 2.2 we presented f-vectors of stereohedra of the tetragonal, trigonal, hexagonal, and cubic groups. We investigated a total of 145 space groups and found 3315 combinatorial types of stereohedra, most of them new. These stereohedra yield 238 different f-vectors. Due to the complexity of our investigations we omitted the triclinic, monoclinic, and orthorhombic space groups, since these are either already understood or would not have been able to produce stereohedra with more than 38 facets – the number of facets of Engel's stereohedron.

We found stereohedra with all numbers of vertices from 4 to 70 and with all numbers of facets from 4 to 38. The maximal numbers are both realized by Engel's stereohedron, which is produced by the group IT(214) = $I4_132$. Engel found four different combinatorial types of stereohedra with f-vector $f = (70, 106, 38)$ and we were able to confirm this – and found no further combinatorial types. Since our main focus is on the number of facets of the stereohedra, we created the histogram of Figure 2.1 that shows how many distinct f-vectors realize facet numbers.

In the following we comment on specific groups. For all groups left out there was no previous work done on them and our results are the first. All numbers correspond to numbers given in the International Tables [Hah05].

76 We confirmed the findings of Koch & Fischer [KF72]. However, they made mistakes in calculating the coordinates they present in their paper. These mistakes occurred since they did not compute in exact arithmetic as we were told by Koch.

84 Matching lower bounds for Bochiş & Santos [BS01] are provided.

91 We improved the lower bound of Bochiş & Santos [BS06] from 17 to 26 facets (both DV-stereohedra are generated by points with trivial stabilizer).

98 We improved the lower bound of Bochiş & Santos [BS06] from 29 to 35 facets (both DV-stereohedra are generated by points with trivial stabilizer). This group seems to generate stereohedra with the second most facets after IT(214) = $I4_132$.

141 Matching lower bounds for Bochiş & Santos [BS01] are provided.

150 Matching lower bounds for Bochiş & Santos [BS06] are provided.

152 We improved the lower bound of Bochiş & Santos [BS06] from 13 to 25 facets (both DV-stereohedra are generated by points with trivial stabilizer).

159 Matching lower bounds for Bochiş & Santos [BS06] are provided.

166 We improved the lower bound of Dress et al. [DHM93] from 6 to 22 facets.

178 We improved the lower bound of Bochiş & Santos [BS06] from 32 to 34 facets (both DV-stereohedra are generated by points with trivial stabilizer). This group seems to generate stereohedra with the third most facets after IT(214) = $I4_132$.

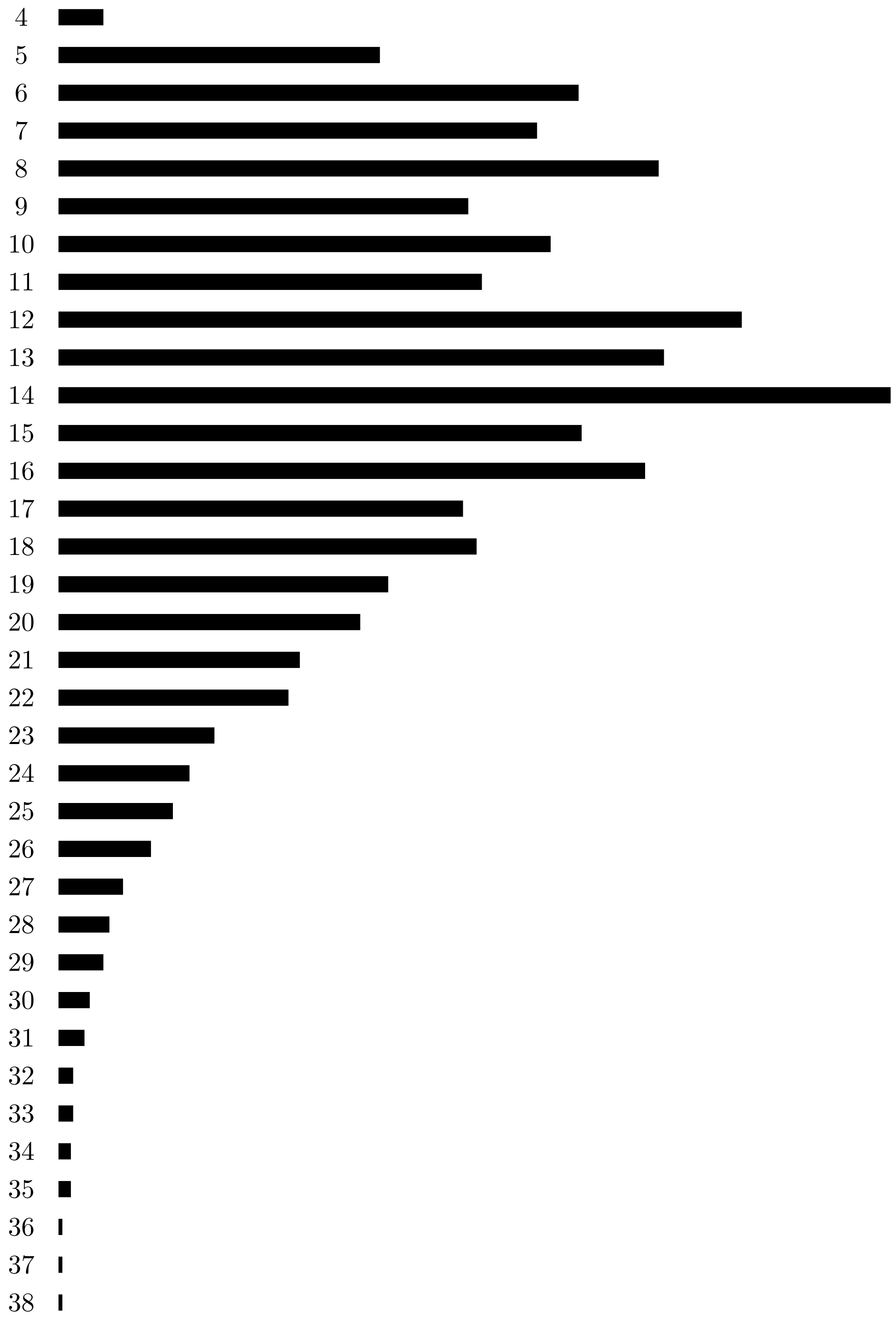


Figure 2.1: Histogram of f-vectors by number of facets.

195 Engel's results [Eng81b] were almost confirmed: We found a second point, namely $(1/2, 1/2, 0)$, that generates the f-vector $(6, 12, 8)$.

196 Matching lower bounds for Sabariego & Santos [SS08] are provided.

197 We were able to Confirmed Engel's results [Eng81b].

198 We improved Koch's result [Koc72] from 18 to 24 facets and found many further f-vectors.

199 We improved Koch's result [Koc72] from 20 to 24 facets and found many further f-vectors.

200 Confirmed Engel's and Koch's results ([Eng81b] and [Koc72], resp.)

202 Found another f-vector not listed by Engel [Eng81b], namely $(8, 16, 10)$.

203 Matching lower bounds for Sabariego & Santos [SS08] are provided.

204 Almost confirmed Engel's results [Eng81b]. We found a second point, namely $(1/2, 1/2, 0)$, that generates the f-vector $(10, 20, 12)$. Matching lower bounds for Bochiş & Santos [BS01] are provided.

205 We improved Koch's result [Koc72] from 13 to 18 facets and found many further f-vectors.

206 We improved Koch's result [Koc72] from 17 to 28 facets and found many further f-vectors.

207 Almost confirmed Engel's results [Eng81b]. We found a second point, namely $(1/2, 0, 0)$, that generates the f-vector $(6, 12, 8)$.

208 Found further stereohedra with less facets than what was already found by Sabariego & Santos [SS08].

209 We were able to confirm Engel's results [Eng81b].

210 We improved Koch's result [Koc72] from 10 to 17 facets and found many further f-vectors. Matching lower bounds for Sabariego & Santos [SS08] are provided.

211 We were able to confirm Engel's results [Eng81b].

212 We improved Koch's result [Koc72] from 22 to 29 facets and found many further f-vectors.

214 Engel's results [Eng81a] were confirmed by our computations and we found many further f-vectors. We also reconstructed the diagram [Abb. 3, p. 207, Ibid]. It shows a slice of the fundamental domain and how it dissects into regions of points that produce stereohedra with the same combinatorial type. Our (coarse) reconstruction of the diagram in Figure 2.3 is a dissection of the same slice into regions of points that produced stereohedra with same f-vector, and it shows that Engel's diagram (shown in Figure 2.2) contains a few mistakes.

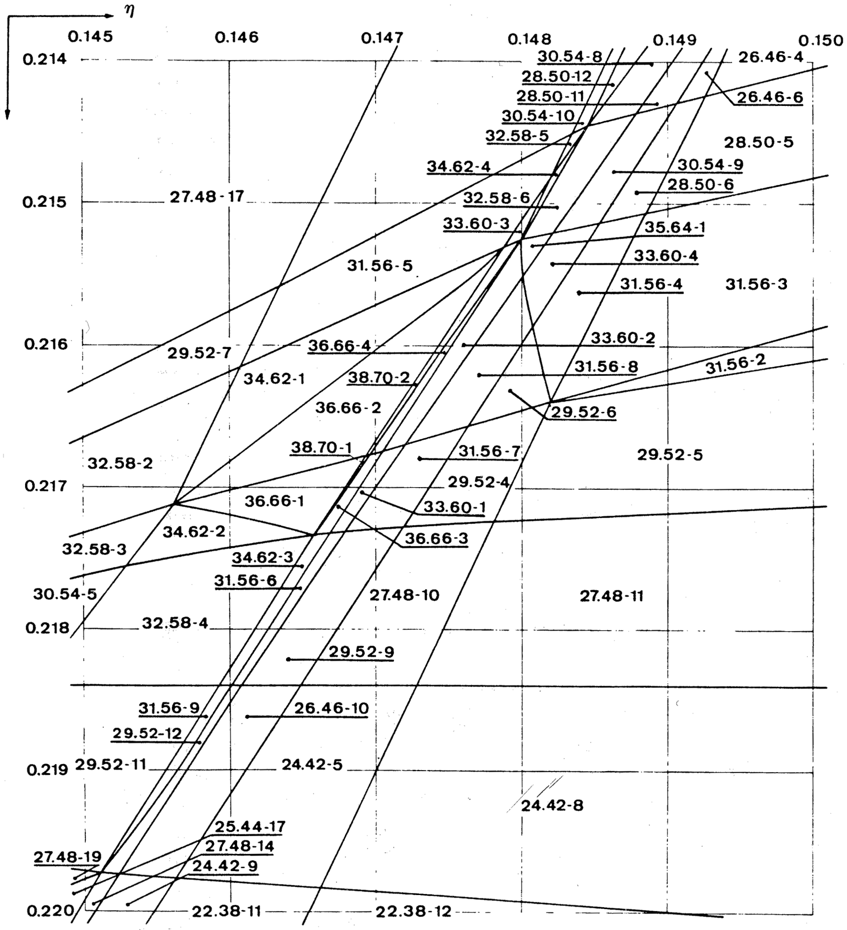


Figure 2.2: Engel's original diagram [Eng81a, Abb. 3, p. 207].

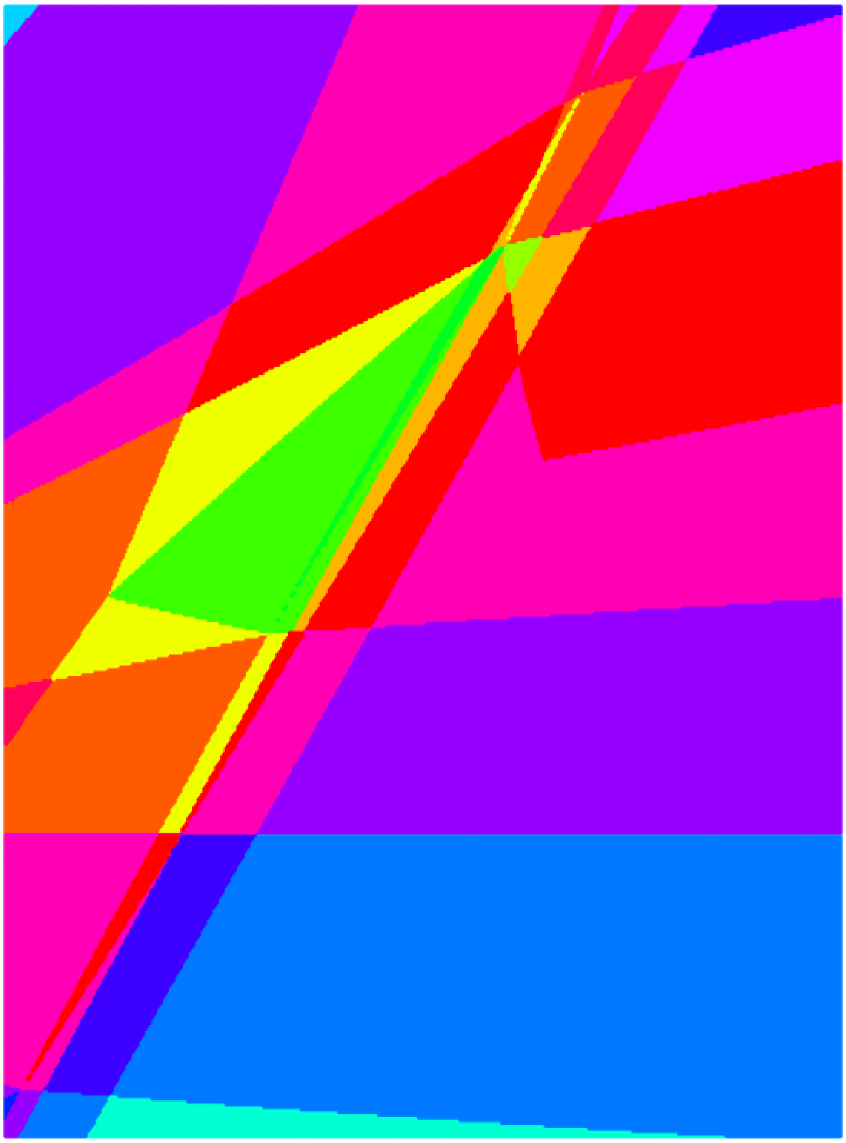


Figure 2.3: Our coarser but corrected reconstruction of Engel's original diagram.

215 Almost confirmed Engel's results [Eng81b]. We found a second point, namely $(1/2, 1/2, 0)$, that generates the f-vector $(6, 12, 8)$.

216 We were able to confirm Engel's results [Eng81b].

217 We were able to confirm Engel's results [Eng81b].

220 We improved Koch's result [Koc72] from 17 to 25 facets and found many further f-vectors.

221 Almost confirmed Engel's results [Eng81b]. We found a second point, namely $(1/2, 1/2, 0)$, that generates the f-vector $(6, 12, 8)$.

223 We were able to confirm Koch's results [Koc72] and found many further f-vectors.

224 We were able to confirm Koch's results [Koc72] and found a few further f-vectors.

225 We were able to confirm Koch's results [Koc72].

226 We were able to confirm Koch's results [Koc72].

227 We were able to confirm Koch's results [Koc72]. The claimed results by Smith [Smi65] we could not reproduce. Since our extremal stereohedra for this group only have 16 facets, we are also skeptical about his rather vague claims.

228 We improved Koch's result [Koc72] from 12 to 16 facets and found many further f-vectors.

229 We were able to confirm Koch's results [Koc72] and almost confirmed Engel's results [Eng81b]. We found a second point, namely $(1/2, 1/2, 0)$, that generates the f-vector $(10, 20, 12)$.

230 We improved Koch's result [Koc72] from 23 to 27 facets and found many further f-vectors.

Chapter 3

On the Number of Space Groups

This chapter is about the number of space group types. We begin in Section 3.1 with a quick summary of what was already known, then derive a new upper bound on the number of types in Section 3.2, and finally discuss the closely related number of $\mathbb{Z}$-classes in Section 3.3. Also in this chapter we have to assume many known (and scattered) results, but always tried to provide exact references.

3.1 Known results

Bieberbach's third theorem states that there are only finitely many isomorphism classes of space groups in each dimension, but little is known about actual numbers or general bounds. The exact numbers are only known up to dimension 6. In Table 3.1 we list these with references provided. For the following discussion let us agree on the abbreviation

$$\mathrm{s}(n) = \text{number of space group types of } \mathbb{R}^n.$$

dim	# types	comment
0	1	
1	2	
2	17	A list of all groups for $n = 2, 3$ with detailed descriptions can be found in [Hah05].
3	219	Ibid.
4	4783	Brown et al. [Bro+78] classified the four-dimensional space groups.
5	222 018	Plesken & Schulz [PS00] counted the space group types in dimensions $n = 5, 6$.
6	28 927 922	Ibid.

Table 3.1: Number of space group types in low dimensions.

The first systematic approach to study the number of space groups in higher dimensions was undertaken by Schwarzenberger [Sch80; Sch82]. He proved a lower bound for $\mathrm{s}(n)$ by only considering so-called orthogonal space groups. An n-dimensional space group is called ***orthogonal*** if its lattice is spanned by n mutually orthogonal vectors and its reflection group is of a particular type.

Schwarzenberger found a way to associate to each n-dimensional orthogonal space group a graph on n vertices. This way he established a bijective correspondence between space group types and equivalence classes of graphs. Using this he proved

$$\mathrm{s}(n) = 2^{\Omega(n^2)}.$$

Based on simple calculations and intuition from low dimensions, he went on to suggest that the asymptotic behaviors of $\mathrm{s}(n)$ and the number of orthogonal space groups are actually similar. While Hiller [Hil86, p. 776] claims that Schwarzenberger explicitly conjectures that $\mathrm{s}(n)$ grows asymptotically like 2^{n^2}, we could only find his more modest suggestions that "$\log_2 \mathrm{s}(n)$ should have an asymptotic approximation involving n^2, $n \log n$, n, $\log n$, etc." [Sch82, p. 244].

Regarding *upper bounds* the only general result was proven by Buser [Bus85]. He showed that $\mathrm{s}(n) \leq \exp\exp 4n^2$, which amounts to

$$\mathrm{s}(n) = 2^{2^{O(n^2)}},$$

which is a fair bit away from Schwarzenberger's lower bound. We will extend his techniques and prove in Theorem 3.2.4 that

$$\mathrm{s}(n) = 2^{2^{O(n \log n)}}.$$

This is a simple consequence of the explicit upper bound we provide there.

3.2 A new upper bound

In this section we derive a new upper bound for the number of isomorphism classes of n-dimensional space groups. Our approach follows Buser [Bus85] and Ratcliffe [Rat06].

Definition 3.2.1. A lattice L is ***scaled*** if all nonzero vectors have norm at least 1. A space group Γ is ***normalized*** if its lattice is scaled and contains n linearly independent translations of length 1.

Of course every lattice can be turned into a scaled one by a homothetic transformation. What is less clear is that every space group is isomorphic to a normalized group.

Proposition 3.2.2 ([Bus85, Prop. 5.3])**.** *Every space group is isomorphic to a normalized space group.*

We also need the following lemma, whose short proof we present.

Lemma 3.2.3. (i) *Let L be a scaled lattice in $\mathbb{R}^n$ and let $\mathrm{N}(r)$ be the number of lattice points of L inside the closed ball of radius r around the origin. Then* $\mathrm{N}(r) \leq (2r+1)^n$.

(ii) *Let* $v_1, \ldots, v_n$ *be a basis of* $\mathbb{R}^n$*. For every* $x \in \mathbb{R}^n$ *there are integers* $\lambda_i \in \mathbb{Z}$ *such that*

$$\Big\| x - \sum \lambda_i v_i \Big\| \leq \frac{1}{2}(\|v_1\| + \ldots + \|v_n\|).$$

(iii) *Consider a scaled lattice* L *in* $\mathbb{R}^n$ *and a vector subspace* U *spanned by* $m < n$ *linearly independent unit vectors from* L*. We then have*

$$\inf \big\{ \mathrm{d}(w, U) : w \in L - U \big\} > (m+3)^{-n}.$$

Proof. (i) Any two lattice points have distance ≥ 1. Putting a ball of radius $1/2$ around each point, we get a sphere packing. The ball $\mathrm{B}(0, r + 1/2)$ encloses all balls that contain all the lattice points of distance at most r from the origin. If we denote by V_n the volume of the unit ball in $\mathbb{R}^n$, we have

$$(1/2)^n\, V_n\, \mathrm{N}(r) \leq (r + 1/2)^n\, V_n$$

from which the desired inequality follows.

(ii) Consider the lattice generated by $v_1, \ldots, v_n$. Centering a fundamental parallelepiped around the origin yields the result, since for every $x \in \mathbb{R}^n$ we can find a representative in this region.

(iii) It is known that the infimum is attained, i.e., among all lattice points not in U there exists $w \in L$ closest to U (see Barvinok [Bar02, Lemma VII.1.3] for details). For the sake of contradiction assume $\|w\| \leq (m+3)^{-n}$. The vectors

$$0w,\ 1w,\ 2w,\ \ldots,\ (m+3)^n w \tag{3.1}$$

are all distance ≤ 1 away from U. By (ii) we get that their U-projections are distance $\leq m/2$ away from the next lattice point contained in U. This yields that (translations of) all vectors in (3.1) are distinct lattice vectors of norm $\leq r := m/2 + 1$. So on the one hand we have $(m+3)^n + 1 \leq \mathrm{N}(r)$, but using (i) we get $\mathrm{N}(r) \leq (m+3)^n$. This is a contradiction and thus $\|w\| > (m+3)^n$ must hold. □

Before we can get to the main theorem of this section, we need to discuss the maximal order of finite subgroups of $\mathrm{GL}(n, \mathbb{Z})$. In Feit [Fei96, Theorem A] it is proven that apart from a few low-dimensional exceptions, the maximal order of a finite subgroup of $\mathrm{GL}(n, \mathbb{Q})$ is $2^n n!$ which is attained by the hyperoctahedral group. Since every finite subgroup of $\mathrm{GL}(n, \mathbb{Q})$ is conjugate to a subgroup of $\mathrm{GL}(n, \mathbb{Z})$, we have an exact upper bound. For a weaker result (the same bound but only proven for $n \gg 0$) with a much easier proof, which does not rely on the classification of finite simple groups, see Friedland [Fri97].

We now come to the main result of this section.

Theorem 3.2.4. *The number* $\mathrm{s}(n)$ *of isomorphism classes of* n*-dimensional space groups is bounded by*

$$\mathrm{s}(n) \leq (2^n n!(n+1)^n + n)[(3n(n+2)^n + 1)^n 2^n n!(n+1)^n]^{(2^n n!(n+1)^n + n)^2}$$

for $n > 10$*. In particular,* $\mathrm{s}(n) = 2^{2^{O(n \log n)}}$.

Proof. By Proposition 3.2.2 it is sufficient to bound the number of isomorphism classes of normalized space groups of $\mathbb{R}^n$. Let Γ be such a group with lattice L. Then L contains n translations

$$\tau_1 = (I, t_1), \ldots, \tau_n = (I, t_n)$$

with $t_1, \ldots, t_n$ being linearly independent unit vectors. Consider the sublattice

$$L' = \langle \tau_1, \ldots, \tau_n \rangle,$$

which is a subgroup of L. Since both lattices are of rank n, we must have $[L : L'] < \infty$. Theorem 1.1.5 then implies that $[\Gamma : L'] = [\Gamma : L][L : L'] < \infty$. Let $\tau_{n+1}, \ldots, \tau_m$ be a transversal of L' in Γ, i.e., $m - n = [\Gamma : L']$. By Lemma 3.2.3 (ii) we can assume that the length of the translational parts $t_{n+1}, \ldots, t_m$ is bounded by $n/2$, a requirement we will need later repeatedly.

Every isometry

$$\alpha \in \Gamma = \bigsqcup_{p=n+1}^{m} L'\tau_p$$

has a unique *normal form*

$$\alpha = (I, a_1 t_1 + \ldots + a_n t_n)\tau_p, \tag{3.2}$$

with $a_1, \ldots, a_n \in \mathbb{Z}$ and $n + 1 \leq p \leq m$. In particular, for $1 \leq i, j \leq m$ every product $\tau_i \tau_j$ has a unique normal form

$$\tau_i \tau_j = (I, c_{ij1} t_1 + \ldots + c_{ijn} t_n)\tau_{f(i,j)}, \tag{3.3}$$

with $c_{ijk}, f(i,j) \in \mathbb{Z}$ and $n + 1 \leq f(i,j) \leq m$.

Claim: The integers m, c_{ijk}, and $f(i,j)$ determine the group Γ up to isomorphism. Indeed, suppose Λ is another normalized n-dimensional space group with the same integer parameters. Let $\nu_1, \ldots, \nu_n$ be the unit translations of its lattice and let $\nu_{n+1}, \ldots, \nu_m$ be the transversal of the sublattice in Λ. We then define a mapping

$$\Psi : \Gamma \to \Lambda, \quad (I, a_1 t_1 + \ldots + a_n t_n)\tau_p \mapsto (I, a_1 v_1 + \ldots + a_n v_n)\nu_p.$$

This turns out to be an isomorphism: Bijectivity is clear, so we just show that it is a homomorphism. To this end we will first explain how multiplication in Γ looks like in terms of the normal form (3.2).

Given $\alpha, \beta \in \Gamma$ such that

$$\alpha = (I, a_1 t_1 + \ldots + a_n t_n)\tau_p,$$
$$\beta = (I, b_1 t_1 + \ldots + b_n t_n)\tau_q,$$

the product is

$$\alpha\beta = (I, a_1 t_1 + \ldots + a_n t_n)\tau_p \tau_1^{b_1} \ldots \tau_n^{b_n} \tau_q.$$

Note that $\tau_i^{b_i} = (I, b_i t_i)$. If $b_1 > 0$, we can replace $\tau_p \tau_1$ by its normal form using the integer parameters defined in (3.3). On the other hand, if $b_1 < 0$, we have

$$\begin{aligned} & \tau_p \tau_1^{-1} = (I, d_1 t_1 + \ldots + d_n t_n)\tau_r \\ \Leftrightarrow \quad & \tau_r \tau_1 = (I, -d_1 t_1 - \ldots - d_n t_n)\tau_p \end{aligned}$$

for some $1 \leq r \leq m$. Given the uniqueness of the normal form, we actually must have $-d_k = c_{r1k}$. So again we can replace a product, namely $\tau_p \tau_1^{-1}$, by its normal form with parameters defined in (3.3) – however, this time with an additional sign introduced. By repeating these steps we can reach the normal form of $\alpha\beta$.

The mapping Ψ is defined in such a way that exactly the same procedure explained for Γ will produce analogous results in Λ. Since we assumed that Λ has the same set of integer parameters as Γ, we must have $\Psi(\alpha\beta) = \Psi(\alpha)\Psi(\beta)$. This finishes the proof of the claim.

To derive the claimed upper bounds we will now bound $|c_{ijk}|$ and m. Let us begin with $|c_{ijk}|$. When we chose the transversal, we required the length of the translational parts of τ_i, τ_j, and $\tau_{f(i,j)}$ to be at most $n/2$. Therefore, the length of the translational part of

$$(I, c_{ij1}t_1 + \ldots + c_{ijn}t_n) = \tau_i \tau_j \tau_{f(i,j)}^{-1} \tag{3.4}$$

is bounded by $3n/2$. Set u_k to be the part of t_k that lies in the orthogonal complement of the vector subspace $\langle t_1, \ldots, t_{k-1}, t_{k+1}, \ldots, t_n \rangle \subset \mathbb{R}^n$. Using the bound just derived, we get

$$|c_{ijk} u_k| \leq 3n/2.$$

Lemma 3.2.3 (iii) gives $|u_k| > (n+2)^{-n}$. Altogether this results in

$$|c_{ijk}| \leq \frac{3n}{2}(n+2)^n =: c_{\max}.$$

Let us next derive a bound for m. We have

$$m - n = [\Gamma : L'] = [\Gamma : L][L : L'].$$

Since the translational parts of $\tau_{n+1}, \ldots, \tau_m$ are bounded by $n/2$, Lemma 3.2.3 (i) implies that $[L : L'] \leq (n+1)^n$. Observe that $[\Gamma : L]$ equals the order of the point group of Γ. Since this finite group can be embedded in $\mathrm{GL}(n, \mathbb{Z})$, we know from Feit's result cited above, that

$$[\Gamma : L] \leq 2^n n!$$

for $n > 10$. This yields the bound

$$m \leq 2^n n!(n+1)^n + n =: m_{\max}.$$

We can now derive an upper bound on $\mathrm{s}(n)$ as follows: It is at most the number of triples

$$\big(m, \{c_{ijk}\}, \{f(i,j)\}\big).$$

We have $1 \leq m \leq m_{\max}$. Every c_{ijk} can assume at most $2c_{\max} + 1 \leq 3n(n+2)^n + 1$ values, and $1 \leq i, j \leq m_{\max}$, $1 \leq k \leq n$. Hence,

$$|\{c_{ijk}\}| \leq (2c_{\max} + 1)^{nm_{\max}^2} = (3n(n+2)^n + 1)^{nm_{\max}^2}.$$

Furthermore, $n + 1 \leq f(i,j) \leq m_{\max}$ and therefore

$$|\{f(i,j)\}| \leq (m_{\max} - n)^{m_{\max}^2}.$$

In total we get

$$\begin{aligned} \mathrm{s}(n) &\leq m_{\max}(3n(n+2)^n+1)^{nm_{\max}^2}(m_{\max}-n)^{m_{\max}^2} \\ &\leq (2^n n!(n+1)^n+n)[(3n(n+2)^n+1)^n 2^n n!(n+1)^n]^{(2^n n!(n+1)^n+n)^2} \end{aligned}$$

for $n > 10$. □

In the next section we will apply the bound from Theorem 3.2.4 to the number of $\mathbb{Z}$-classes.

3.3 On the number of $\mathbb{Z}$-classes

Currently there are two ways to show the finiteness of the number of $\mathbb{Z}$-classes. The first is to apply a highly nontrivial theorem of Jordan–Zassenhaus [CR88, Sect. XI.79; Gas06], while the second uses a much more accessible theorem by Eisenstein–Hermite [SO13, Chap. 9; MH73, Chap. II]. Neither approach seems to allow for computing an upper bound. However, our bound for the number of space group types in Theorem 3.2.4 is trivially an upper bound for the number of $\mathbb{Z}$-classes as well. In the remaining part of this section we will derive a lower bound.

Consider the automorphism group $\mathrm{Aut}(L)$ of a lattice $L \subseteq \mathbb{R}^n$. As mentioned in Chapter 1, the group $\mathrm{Aut}(L)$ can be understood as a finite subgroup of $\mathrm{GL}(n, \mathbb{Z})$. To evaluate the bound we will employ the Smith–Minkowski–Siegel *mass formula*. This formula gives an explicit constant C such that

$$\sum \frac{1}{|\operatorname{Aut}(L)|} = C,$$

where the sum is over all inequivalent lattices of the same genus. Two lattices $L, L' \subseteq \mathbb{R}^n$ are ***equivalent*** if there exists an isomorphism $f : L \to L'$ with

$$q'(f(x)) = q(x),$$

where q, q' are the quadratic forms belonging to L, L', respectively. Otherwise, L and L' are called ***inequivalent***. It is not hard to show that two lattices are equivalent if and only if their automorphism groups are conjugate in $\mathrm{GL}(n, \mathbb{Z})$. The ***genus*** is a classification of all lattices in $\mathbb{R}^n$, and two lattices are in the same genus if they are equivalent as $\mathbb{Z}_p$-modules for all $p \in \mathbb{P} \cup \{\infty\}$, where $\mathbb{Z}_p$ denotes the p-adic integers and $\mathbb{Z}_\infty = \mathbb{R}$.

To get a lower bound for the number of $\mathbb{Z}$-classes, we can use the inequality

$$\sum \frac{1}{|\operatorname{Aut}(L)|} \ \leq \ \#\mathbb{Z}\text{-classes}$$

for an arbitrary but fixed genus. We have the following special case of the mass formula for the genus that consists of all odd unimodular lattices.

Theorem (Smith–Minkowski–Siegel; see [CS99, Sect. 16.2])**.** *Let Ω be the set of all inequivalent odd unimodular lattices of dimension n. Then*

$$\sum_{L \in \Omega} \frac{1}{|\operatorname{Aut}(L)|} = \frac{1}{2^{n+1}(\frac{n}{2}-1)!} \cdot |E_{\frac{n}{2}-1}| \cdot |B_2| \cdot |B_4| \cdots |B_{n-2}|$$

for even $n > 1$ and $n \equiv \pm 2 \mod 8$, where $E_{\frac{n}{2}-1}$ is an Euler number and B_{2k} denotes Bernoulli numbers.

In Olver et al. [Olv+10] not only the definitions of the Bernoulli and Euler numbers can be found, but also the following asymptotic approximations. For n large enough we have

$$|B_{2n}| \sim \frac{2(2n)!}{(2\pi)^{2n}} \quad \text{and} \quad |E_{2n}| \sim \frac{2^{2n+2}(2n)!}{\pi^{2n+1}}.$$

Plugging all in, we get the following asymptotic lower bound for the number of $\mathbb{Z}$-classes:

$$\#\big(\mathbb{Z}\text{-classes}\big) = 2^{\Omega(n \log n)}.$$

It is hard to estimate just how accurate this asymptotic lower bound actually is. To calculate it we only used one fixed genus. However, it seems that other genera do not give substantially better results, and furthermore are there only finitely many genera in each dimension. On the other hand, since most finite groups of $\mathrm{GL}(n, \mathbb{Z})$ do not arise as the automorphism group of a lattice, there are many more $\mathbb{Z}$-classes, which might lead to a better asymptotic lower bound.

Appendices

Appendix A

Cohomology of Groups

We recall a few facts from group cohomology that are used in this thesis. In our presentation we closely follow Rotman [Rot95; Rot09; Rot10].

If K and Q are groups, then a group G is called an ***extension*** of K by Q if G contains a normal subgroup $K' \cong K$ with $G/K' \cong Q$. This induces a short exact sequence of groups

$$K \xrightarrow{\ i\ } G \xrightarrow{\ \pi\ } Q,$$

and often the term *extension* is used for such a sequence as well. K is called the ***kernel*** of the extension, while Q is the ***quotient***. The theory of group extensions becomes much easier if the kernel is abelian. Since this case is sufficient for our purposes, we will make this assumption for the rest of this appendix. Furthermore, even though an extension G of K by Q is not abelian in general, we will use additive notation for the operation in G. Otherwise multiplication in G and the scalar multiplication defined by equation (A.1) could easily be confused.

Every extension of K by Q induces a homomorphism

$$\Theta : Q \to \operatorname{Aut}(K),$$

via a so-called lifting as follows. A particular ***lifting*** is a function $\ell : Q \to G$ with $\pi\ell = \mathrm{id}_Q$ and $\ell(1) = 1$. Such a lifting can be used to define for each $x \in Q$ the automorphism

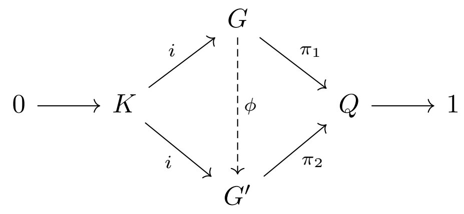
$$\Theta_x : K \to K, \quad a \mapsto \ell(x) + i(a) - \ell(x).$$

Now the homomorphism $\Theta : Q \to \operatorname{Aut}(K)$ is defined by setting $\Theta : x \mapsto \Theta_x$. It is independent of the lifting ℓ and allows us to turn K into a $\mathbb{Z}Q$-module by defining scalar multiplication as $xa = \Theta_x(a)$ for $x \in Q, a \in K$, and then extending linearly. In this context it is common to abbreviate the term "$\mathbb{Z}Q$-module" to "Q-module."

Let K be a Q-module. An extension G of K by Q ***realizes the operators*** if

$$xa = \ell(x) + i(a) - \ell(x) \tag{A.1}$$

for all $x \in Q$ and $a \in K$ (so the given scalar multiplication coincides with the scalar multiplication induced by conjugation). Let G, G' be two extensions realizing the operators, we say that G and G' are ***equivalent*** if there exists a homomorphism $\phi : G \to G'$ making the following diagram commute



The set of all equivalence classes can be given a group structure isomorphic to the ***second cohomology group*** $H^2(Q, K)$.

To introduce the first cohomology group $H^1(Q, K)$ we need to consider the set of all ***derivations*** $\mathrm{Der}(Q, K)$, which are functions of the kind

$$d : Q \to K, \quad d(xy) = xd(y) + d(x).$$

$\mathrm{Der}(Q, K)$ becomes an abelian group under pointwise addition. For a fixed $a \in K$, a derivation of the type $u(x) = xa - a$ is called a ***principal derivation***. The set of all principal derivations forms a subgroup $\mathrm{PDer}(Q, K)$ of $\mathrm{Der}(Q, K)$. We define the ***first cohomology group*** as

$$H^1(Q, K) = \mathrm{Der}(Q, K)/\,\mathrm{PDer}(Q, K).$$

In general the nth cohomology group of Q with coefficients in a Q-module K is defined as follows: Let

$$\cdots \longrightarrow F_2 \longrightarrow F_1 \longrightarrow F_0 \longrightarrow \mathbb{Z}$$

be an arbitrary but fixed $\mathbb{Z}Q$-projective resolution of $\mathbb{Z}$. Applying the contravariant functor $\mathrm{Hom}_Q(-, K)$ yields the cochain complex

$$\cdots \longleftarrow \mathrm{Hom}_Q(F_2, K) \longleftarrow \mathrm{Hom}_Q(F_1, K) \longleftarrow \mathrm{Hom}_Q(F_0, K) \longleftarrow 0.$$

The ***nth cohomology group*** is defined as the cohomology of this complex

$$H^n(Q, K) = H^n(\mathrm{Hom}(F, K)).$$

Given a short exact sequence

$$0 \longrightarrow G' \longrightarrow G \longrightarrow G'' \longrightarrow 0$$

of Q-modules, we can use the projective resolution F to build an exact sequence of chain complexes: Since every F_i is projective, the sequence

$$0 \longrightarrow \mathrm{Hom}_Q(F_i, G') \longrightarrow \mathrm{Hom}_Q(F_i, G) \longrightarrow \mathrm{Hom}_Q(F_i, G'') \longrightarrow 0$$

is exact as well. This induces the diagram

$$\begin{array}{ccccc}
\vdots & & \vdots & & \vdots \\
\downarrow & & \downarrow & & \downarrow \\
\mathrm{Hom}_Q(F_2, G') & \rightarrowtail & \mathrm{Hom}_Q(F_2, G) & \twoheadrightarrow & \mathrm{Hom}_Q(F_2, G'') \\
\downarrow & & \downarrow & & \downarrow \\
\mathrm{Hom}_Q(F_1, G') & \rightarrowtail & \mathrm{Hom}_Q(F_1, G) & \twoheadrightarrow & \mathrm{Hom}_Q(F_1, G'') \\
\downarrow & & \downarrow & & \downarrow \\
\mathrm{Hom}_Q(F_0, G') & \rightarrowtail & \mathrm{Hom}_Q(F_0, G) & \twoheadrightarrow & \mathrm{Hom}_Q(F_0, G'') \\
\downarrow & & \downarrow & & \downarrow \\
0 & & 0 & & 0
\end{array}$$

with exact rows. The snake lemma applied to this short exact sequence of complexes

$$\mathrm{Hom}(F, G') \rightarrowtail \mathrm{Hom}(F, G) \twoheadrightarrow \mathrm{Hom}(F, G'')$$

gives the following ***long exact cohomology sequence***.

$$\begin{array}{l}
0 \longrightarrow H^0(Q, G') \longrightarrow H^0(Q, G) \longrightarrow H^0(Q, G'') \longrightarrow \\
\quad \longrightarrow H^1(Q, G') \longrightarrow H^1(Q, G) \longrightarrow H^1(Q, G'') \longrightarrow \\
\quad \longrightarrow H^2(Q, G') \longrightarrow H^2(Q, G) \longrightarrow H^2(Q, G'') \dashrightarrow \\
\quad \dashrightarrow H^n(Q, G') \longrightarrow H^n(Q, G) \longrightarrow H^n(Q, G'') \longrightarrow \cdots
\end{array} \tag{A.2}$$

We end our summary of group cohomology with the following useful lemma.

Lemma A.1 ([Rob96, Cor. 11.3.8]). *Let Q be a finite group of order m. Suppose that K is a Q-module such that for every element $a \in K$ there exists a unique $b \in K$ with $mb = a$. Then $H^n(Q, K) = 0$ for all $n > 0$.*

Appendix B

Background on Computations

In this appendix we will explain how we calculated the data presented in Chapter 2. Since all our calculations were done in $\mathbb{R}^3$, we will confine ourselves to $n = 3$ here as well. However, most of what we state is true for general dimensions n. The only exception is the existence of a classification of all space groups; these were so far only obtained for dimensions $n \leq 4$ and any further classification would be a *major* undertaking.

The following lemma is crucial for our computations. It was first described by Koch [Koc72] in her thesis and later (re)proved by Bochiş & Santos [BS06, Lemma 1.1].

Definition B.1. Let $a \in \mathbb{R}^3$ be a point and let $\tau = (I, t) \in \Gamma$ be a nontrivial translation of the space group $\Gamma \leq \mathrm{Isom}(\mathbb{R}^3)$. We call

$$S_a(\tau) = \big\{x \in \mathbb{R}^3 : \langle a - t, t\rangle < \langle x, t\rangle < \langle a + t, t\rangle\big\}$$

the ***open slab*** induced by a and τ.

The lemma now states:

Lemma B.2. *For a space group $\Gamma \leq \mathrm{Isom}(\mathbb{R}^3)$, let L be its lattice with basis $\tau_i = (I, t_i)$, $i = 1, 2, 3$. Given a point $a \in \mathbb{R}^3$, the orbit points*

$$\mathcal{O} = \big(\Gamma(a) \cap \bigcap_{i=1}^{3} S_a(\tau_i)\big) \cup \big\{\pm\tau_1(a), \pm\tau_2(a), \pm\tau_3(a)\big\}$$

*suffice for computing $\mathrm{DV}(a)$. We call $\mathcal{O}$ the set of **relevant points** of a.*

Proof. Consider an open slab $S_a(\tau_i)$, an orbit point $b \in \Gamma(a) - S_a(\tau_i)$ for some $i \in \{1, 2, 3\}$ with $b \neq \pm\tau_i(a)$, and assume $\langle b, t_i\rangle \geq \langle a + t_i, t_i\rangle$. We then have the planar parallelogram $\mathrm{conv}(a, \tau_i(a), b, -\tau_i(b))$. The orbit point b is relevant for $\mathrm{DV}(a)$ if and only if there exists a sphere that contains only a, b on the boundary and no other orbit points in the interior. However, this cannot be the case for a, b since we have

$$\angle\big(a, \tau_i(a), b\big) = \angle\big(b, -\tau_i(b), a\big) \geq \pi/2,$$

which is a contradiction. □

We apply this lemma to space groups with an orthogonal sublattice in the following way: Let $\Gamma \leq \text{Isom}(\mathbb{R}^3)$ be a space group with lattice L, such that L contains a sublattice L' that is spanned by an orthogonal basis. Denote by F the (cuboidal) half-open fundamental parallelepiped of L'. It is enough to compute $S = \Gamma(a) \cap F$ to construct the set of relevant points of $a \in \mathbb{R}^3$, because according to Lemma B.2 we only need to translate S to all other orthants of the basis of L'. (Strictly speaking we then might get a superset of all relevant points of a due to boundary effects.) Of course this raises the question of how to determine S. Since we have

$$\Gamma = \bigcup_{i=1}^{k} L\alpha_i \qquad L = \bigcup_{j=1}^{\ell} L'\tau_j$$

for $\alpha_i = (A_i, a_i) \in \Gamma$ and $\tau_j = (I, t_j) \in L$, this yields

$$\Gamma = \bigcup_{i=1}^{k} \bigcup_{j=1}^{\ell} L'\tau_j\alpha_i$$

with $\tau_j\alpha_i = (A_i, a_i + t_j)$. So for each $i = 1, \ldots, k$ and every $j = 1, \ldots, \ell$ we need to find a representative of $L'\tau_j\alpha_i(a)$ in F. We use

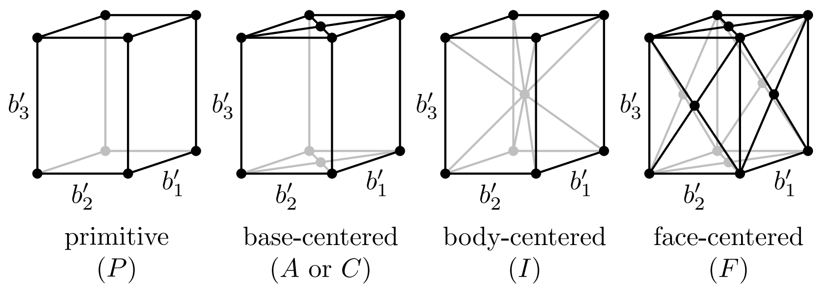
$$\tau_j\alpha_i(a) - \lfloor \tau_j\alpha_i(a) - a \rfloor,$$

where the floor function is applied componentwise. To finalize the computation of S we add translates of a by every basis vector of L'. The above procedure is summarized in Algorithm 1.

We use this algorithm for computations with orthorhombic, tetragonal, trigonal, hexagonal, and cubic groups. A classification of these groups can be found in the International Tables for Crystallography (IT) [Hah05]. The algorithm depends on the set R of representatives of L in Γ and on the set T of representatives of L' in L. R can be extracted from the GAP package Cryst [GAP15]; these representatives are exactly the same as the ones from the IT. The representatives T of L' in L can be read off from the crystal system of Γ. In the following we will show how to do this for the space groups of interest. We denote the basis vectors of the sublattice L' by b'_1, b'_2, b'_3.

Orthorhombic groups

For orthorhombic space groups, the following types of fundamental parallelepipeds of the sublattice L' occur:



Algorithm 1: Compute relevant points of a.

Data: $a \in \mathbb{R}^3$; representatives $R = \{\alpha_1, \dots, \alpha_k\}$ of L in Γ; matrix $B' = \left[b'_1, b'_2, b'_3\right] \in \mathbb{R}^{3\times 3}$ of basis vectors of L'; representatives $T = \{\tau_1, \dots, \tau_\ell\}$ of L' in L.
Result: Superset P of relevant points of a.

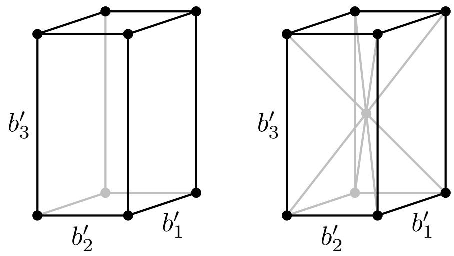
```
begin
    P ⟵ ∅
    S ⟵ ∅
    for j ∈ {1, ..., ℓ} do
        for i ∈ {1, ..., k} do
            p ⟵ τ_j α_i(a)
            p ⟵ p − ⌊p − a⌋
            append p to S
        end
    end
    for v ∈ {0, −1}^3 do
        for s ∈ S do
            P ⟵ B'v + s
        end
    end
    append a + b'_1, a + b'_2, a + b'_3 to P
    return P
end
```

The lengths of b'_1, b'_2, b'_3 can be freely chosen, but the angles between all pairs of vectors always have to be $\pi/2$. The representatives T of L' in L are

- primitive case: $T = \{(0,0,0)\}$
- base-centered case (type A): $T = \{(0,0,0), (0, 1/2, 1/2)\}$
- base-centered case (type C): $T = \{(0,0,0), (1/2, 1/2, 0)\}$
- body-centered case: $T = \{(0,0,0), (1/2, 1/2, 1/2)\}$
- face-centered case: $T = \{(0,0,0), (1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2)\}$

Tetragonal groups

For tetragonal space groups, the following types of fundamental parallelepipeds of the sublattice L' occur:



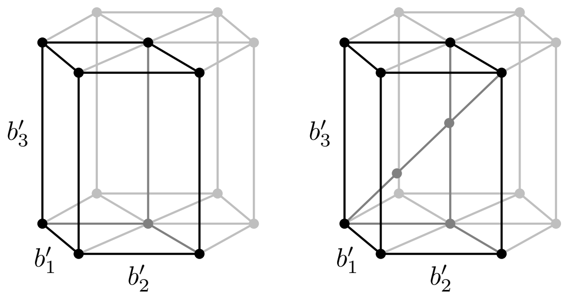
primitive (P) body-centered (I)

The lengths of b'_1 and b'_2 have to be equal, the length of b'_3 can be freely chosen. The angles between all pairs of vectors always have to be $\pi/2$. The representatives T of L' in L are

- primitive case: $T = \{(0,0,0)\}$
- body-centered case: $T = \{(0,0,0), (1/2, 1/2, 1/2)\}$

Trigonal and hexagonal groups

In the case of the trigonal and hexagonal crystal systems we need to apply a change of basis to get cuboidal fundamental parallelepipeds for the sublattice L'. The space groups of these systems are given in the IT with respect to sublattice parallelepipeds of the following types:



primitive (P) rhombohedral (R)

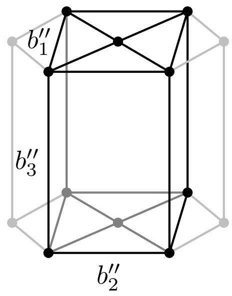
The lengths of b'_1 and b'_2 have to be equal, the length of b'_3 can be freely chosen. The angle between b'_1 and b'_2 must be $\angle(b'_1, b'_2) = 2\pi/3$, the angles between b'_1 and b'_3 and between b'_2 and b'_3 have to be $\angle(b'_1, b'_3) = \angle(b'_2, b'_3) = \pi/2$. The inner points in the rhombohedral case have the coordinates $(2/3, 1/3, 1/3)$ and $(1/3, 2/3, 2/3)$. To obtain orthogonal fundamental cells, we need to apply a coordinate transformation between

$$\mathcal{B}' = (b'_1, b'_2, b'_3) \quad \text{and} \quad \mathcal{B}'' = (b''_1, b''_2, b''_3) = (2b'_1 + b'_2, b'_2, b'_3).$$

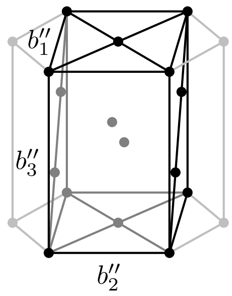
We get the new sublattice $L'' = \langle b''_1, b''_2, b''_3 \rangle$. Of course we have to apply this transformation to the trigonal and hexagonal groups of the IT accordingly. The basis exchange matrix $X = X_{\mathcal{B}'' \to \mathcal{B}'}$ is

$$X = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \text{and} \qquad X^{-1} = \begin{bmatrix} 1/2 & 0 & 0 \\ -1/2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and thus, if Γ is a trigonal or hexagonal group from the IT and $(A, a) \in \Gamma$ is an isometry, we have to work with the isometry $(X^{-1}AX, X^{-1}a)$ instead. After the coordinate transformation we have the following two orthogonal fundamental parallelepiped types for sublattices:



transformed
primitive



transformed
rhombohedral

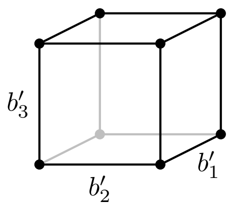
Here we need to have $\|b_1''\| = \sqrt{3}\|b_2''\|$, the length of b_3'' can be freely chosen, and the angles between all pairs of vectors have to be $\pi/2$. The representatives T of L'' in L are

- transformed primitive case: $T = \{(0,0,0), (1/2, 1/2, 0)\}$
- transformed rhombohedral case:

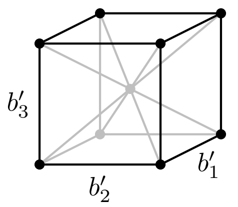
$$T = \{(0,0,0), (1/2, 1/2, 0), (1/3, 0, 1/3), (2/3, 0, 2/3), (1/6, 1/2, 2/3), (5/6, 1/2, 1/3)\}$$

Cubic groups

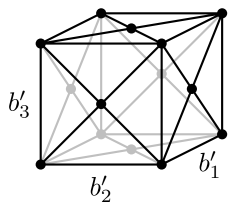
For cubic space groups, the following types of fundamental parallelepipeds of the sublattice L' occur:



primitive
(P)



body-centered
(I)



face-centered
(F)

The lengths of b_1', b_2', and b_3' have to be the same and the angles between all pairs of vectors have to be $\pi/2$. The representatives T of L' in L are

- primitive case: $T = \{(0,0,0)\}$
- body-centered case: $T = \{(0,0,0), (1/2, 1/2, 1/2)\}$
- face-centered case: $T = \{(0,0,0), (1/2, 1/2, 0), (1/2, 0, 1/2), (0, 1/2, 1/2)\}$

Details on implementation and used resources

The above algorithm was implemented in C++ using the Callable Library from Polymake [GJ00]. The resulting software package is called `plesiohedron`, see [Sch]. Exact arithmetic was realized by using the GMP library [Gt15]. Many precomputations were done by using Sage [Ste+15], GAP [GAP15], and Python. In total we produced roughly 14 TB of output data, which we analyzed using Python, the Unix tools sed, awk, and many more command line tools. Visualizations were done with POV-Ray [Vis].

To carry out the computations, we proceeded for each space group Γ as follows:

1. We first applied the normalizer $\mathrm{N}(\Gamma)$ to reduce the part of the fundamental domain, that we needed to examine. This reduced fundamental domain is always denoted by R_k in Chapter 2, where k is the number of Γ from the IT. Each R_k is again a convex three-dimensional polytope.

2. Next we generated a very fine grid inside R_k using a Sage program we developed. This program first triangulates R_k, and for each simplex in the triangulation, it calculates weighted barycenters. As weights we used all rational numbers with denominator $D \in \mathbb{N}$, where D is chosen large enough to get a fine enough grid.

3. For each point of the grid we applied `plesiohedron`.

4. The output was examined using the tools described above.

For the computations we used two clusters at Freie Universität Berlin and around twenty-five stand-alone Linux computers. In total we used

$$3\,073\,014 \text{ hours} \approx 351 \text{ years}$$

of CPU time.

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Deutsche Zusammenfassung

Thematisch gliedert sich diese Dissertation in drei Teile:

(i) Übersichtsartikel über die Theorie der n-dimensionalen Raumgruppen,

(ii) Untersuchung der 3-dimensionalen Raumgruppen in Hinblick auf die möglichen f-Vektoren von Dirichlet–Voronoi-Stereoedern,

(iii) Abschätzung der Anzahl der Isomorphieklassen von Raumgruppen des $\mathbb{R}^n$.

Jeder Teil dieser Arbeit entspricht einem der drei Kapitel, die wir nachfolgend kurz beschreiben werden.

Im ersten Kapitel geben wir eine Einführung in die Theorie der Raumgruppen und fassen übersichtsartig die wichtigsten Resultate aus diesem Gebiet zusammen. Beweise werden nur geführt, falls wir keine oder keine adäquaten in der Literatur finden konnten. Wir halten eine solche Zusammenfassung für dringend notwendig, da andere Einführungen sich entweder auf Raumgruppen der Dimensionen $n \leq 3$ beschränken, sich stark auf kristallographische Aspekte konzentrieren oder veraltet sind. Entsprechend haben wir versucht, die wichtigsten Referenzen zu Raumgruppen zu sichten und im Literaturverzeichnis aufzulisten.

Kapitel 2 widmet sich einer ausführlichen Untersuchung von Dirichlet–Voronoi-Stereoedern. Ein Stereoeder ist ein konvexes Polytop, das den $\mathbb{R}^n$ mittels der Wirkung einer Raumgruppe lückenlos überdeckt. Falls das Stereoeder eine Dirichlet–Voronoi-Zelle eines Voronoi-Diagramms eines Orbits einer Raumgruppe ist, spricht man von einem Dirichlet–Voronoi-Stereoeder. Solche Stereoeder sind spezielle Beispiele sogenannter konvexer monohedraler Pflastersteine, deren Form und Kombinatorik nur rudimentär verstanden sind. Insbesondere ist es ein offenes Problem, ob die Anzahl der Facetten eines konvexen monohedralen Pflastersteins durch eine Funktion beschränkt ist, die nur von der Dimension n abhängt. Durch unsere Untersuchungen wollen wir die Arbeiten von Santos et al. komplementieren und einen realistischen Eindruck der Anzahl der Facetten in Dimension 3 gewinnen. Für die Untersuchungen und Berechnungen wurde von uns das umfangreiche Programmpaket `plesiohedron` entwickelt.

Schließlich präsentieren wir im letzen Kapitel eine neue Abschätzung der Anzahl der Isomorphieklassen $\mathrm{s}(n)$ von Raumgruppen des $\mathbb{R}^n$. Nach einem Satz von Bieberbach ist diese Anzahl in jeder Dimension endlich. Schwarzenberger hat gezeigt, dass

$$\mathrm{s}(n) = 2^{\Omega(n^2)}$$

gilt und Buser konnte eine obere Schranke der Form

$$\mathrm{s}(n) = 2^{2^{O(n^2)}}$$

beweisen. Wir verbessern Busers Resultat und zeigen, dass

$$\mathrm{s}(n) = 2^{2^{O(n \log n)}}$$

gilt. Anschließend schätzen wir mit Hilfe dieses Resultats erstmalig die Anzahl der Konjugationsklassen endlicher Untergruppen von $\mathrm{GL}(n, \mathbb{Z})$ ab und beurteilen die Güte dieser Abschätzung mit Hilfe der Minkowski–Siegelschen Massenformel.

Erklärung

Gemäß §7 (4), der Promotionsordnung des Fachbereichs Mathematik und Informatik der Freien Universität Berlin vom 8. Januar 2007 versichere ich hiermit, dass ich alle Hilfsmittel und Hilfen angegeben und auf dieser Grundlage die vorliegende Arbeit selbstständig verfasst habe. Des Weiteren versichere ich, dass ich diese Arbeit nicht bereits zu einem früheren Promotionsverfahren eingereicht habe.

Berlin, den

Moritz W. Schmitt