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The complete classification of five-dimensional Dirichlet–Voronoi polyhedra of translational lattices

research paper

Check for

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This paper reports on the full classification of Dirichlet–Voronoi polyhedra and Delaunay subdivisions of five-dimensional translational lattices. A complete list is obtained of 110 244 affine types (*L*-types) of Delaunay subdivisions and it turns out that they are all combinatorially inequivalent, giving the same number of combinatorial types of Dirichlet–Voronoi polyhedra. Using a refinement of corresponding secondary cones, 181 394 contraction types are obtained. The paper gives details of the computer-assisted enumeration, which was verified by three independent implementations and a topological mass formula check.

1. Introduction

The study of translational lattices and their Dirichlet–Voronoi polyhedra are classical subjects in crystallography. Fedorov (1885) (*cf.* Senechal & Galiulin, 1984) determined the five combinatorial types of possible Dirichlet–Voronoi polyhedra in the Euclidean 3-space \mathbb{R}^3 . These are also all the parallelohedra in \mathbb{R}^3 , that is, polyhedra admitting a facet-to-facet tiling of \mathbb{R}^3 by translation. Voronoi (1908, 1909) developed a theory to classify Dirichlet–Voronoi polyhedra for arbitrary *d*-dimensional Euclidean spaces \mathbb{R}^d . His theory allows them to be classified *via* a classification of Delaunay subdivisions up to affine equivalence (so-called *L-types*). In this context Voronoi also came up with his famous and still unsolved conjecture, stating that every parallelohedron in \mathbb{R}^d is affinely equivalent to a Dirichlet–Voronoi polyhedron for some translational lattice.

In this paper we report on the enumeration of the fivedimensional combinatorial types of Dirichlet–Voronoi polyhedra or equivalently Delaunay subdivisions (Theorem 3.5). We find in total 110 244 different combinatorial types and hereby go beyond the partial classification according to subordination schemes previously obtained by Engel (2000). In Table 3 we list the number of Delaunay subdivisions that have been computed so far. By our work, a full classification is known for $d \le 5$ so far. Recent partial results on primitive types in dimension 6 (Baburin & Engel, 2013) seem to indicate that a full classification beyond five dimensions is out of reach at the moment.

Our paper is organized as follows. In 2 we start with some notation and background on Dirichlet–Voronoi and Delaunay polytopes. Voronoi's *L*-type theory is briefly reviewed in 3. In particular we describe how the classification of Dirichlet– Voronoi polyhedra is reduced to the classification of Delaunay subdivisions and how this can practically be done. Algorithms and implementations for our classification result are briefly described in §4 and references to online sources are given. Additional data and tables are presented in §5, where we also relate our work to the theory of contraction types.

2. Dirichlet-Voronoi and Delaunay polytopes

Let Λ denote a *translational lattice* in \mathbb{R}^d . That is, Λ is a full rank-discrete subgroup of \mathbb{R}^d and, equivalently, can be written as

$$\Lambda = \{\lambda_1 b_1 + \ldots + \lambda_d b_d : \lambda_1, \ldots, \lambda_d \in \mathbb{Z}\}$$

with linearly independent vectors $b_1, \ldots, b_d \in \mathbb{R}^d$. Latter vectors, as well as a matrix B with these as columns, are referred to as a *basis* of Λ and we simply write $\Lambda = B\mathbb{Z}^d$. Viewing \mathbb{R}^d as a Euclidean space with norm $|\cdot|$, the *Dirichlet-Voronoi polytope* DV(Λ) of Λ is defined as the set of points in \mathbb{R}^d which are at least as close to the origin than to any other element of Λ :

$$DV(\Lambda) = \{x \in \mathbb{R}^d : |x| \le |x - y| \text{ for all } y \in \Lambda\}.$$

2.1. General facts about polytopes

The term polytope refers to the fact that $DV(\Lambda)$ can be described as a convex hull (a set of all convex combinations) of finitely many points. A point that cannot be omitted in such a description is called a *vertex* of the polytope. Let us briefly review some basics from the theory of polytopes [see Ziegler (1995) and Grünbaum (2003) for details]. A *supporting hyperplane* is an affine hyperplane having the property that the polytope is fully contained in one of the two halfspaces bounded by it. A *k*-dimensional face of a polytope is defined as a *k*-dimensional intersection of the polytope with a supporting hyperplane. The (d - 1)-dimensional faces of a *d*-dimensional faces. Every polytope also has a description by linear inequalities and the non-redundant ones in such a description are in 1-to-1-correspondence to its facets.

Altogether, the faces of a polytope form a poset (partially ordered set, ordered by inclusion), which is called the *face lattice* of the polytope. Two polytopes are called *combinato-rially equivalent* if they possess the same face lattice. For instance, two two-dimensional *n*-gons (which are the two-dimensional polytopes with *n* vertices) are always combinatorially equivalent. However, they might not be *affinely equivalent*, that is, there does not exist an affine map mapping one to the other [see Bremner *et al.* (2014) for details on this and how to compute equivalence].

We note that Engel (2000) uses a so-called *subordination* scheme (sometimes called a *polyhedral scheme*) which is an invariant to classify Dirichlet–Voronoi polytopes. Two combinatorially different polytopes can however have the same subordination scheme. In fact, several combinatorially different Dirichlet–Voronoi polyhedra in \mathbb{R}^5 have the same subordination scheme. Therefore this invariant cannot be used for a full classification of all combinatorial types.

2.2. Affine and combinatorial types of Dirichlet–Voronoi polytopes

In dimension 2 there exist only two combinatorially inequivalent types of Dirichlet–Voronoi polytopes: either centrally symmetric hexagons or rectangles. We note that there are infinitely many affine types of Dirichlet–Voronoi polytopes. Actually, any centrally symmetric hexagon with vertices on a unit circle is a Dirichlet–Voronoi polytope of a lattice. However, they are not all affinely equivalent to each other. For instance, none of them is affinely equivalent to a regular hexagon (except the regular hexagon itself). For more information on affine types of Dirichlet–Voronoi polytopes the interested reader is referred to Dolbilin *et al.* (2011) and Gavrilyuk (2014).

The combinatorial types of Dirichlet–Voronoi polytopes in dimensions 3 and 4 are known as well. There exist five different combinatorial types of Dirichlet–Voronoi polytopes in dimension 3 and 52 different combinatorial types in dimension 4. In this paper we report on the classification in dimension 5 and we show:

Theorem 2.1. There are precisely 110 244 combinatorially inequivalent types of Dirichlet–Voronoi polytopes of five-dimensional translational lattices.

In the following we explain in more detail how to obtain the above classification result, based on Voronoi's second reduction theory for positive definite quadratic forms.

2.3. Delaunay subdivisions

The notion of Delaunay subdivisions was introduced by Delone (1934). Here we give their definition and briefly describe major properties.

Given a translational lattice Λ in \mathbb{R}^d , an empty sphere S(c, r) of centre *c* and radius r > 0 is a sphere such that there is no lattice point in its interior. A *Delaunay cell* is an intersection $\Lambda \cap S(c, r)$. A *Delaunay polytope* is a *d*-dimensional polytope of the form conv $(\Lambda \cap S(c, r))$.

The set of all Delaunay polytopes of Λ form a polytopal subdivision of \mathbb{R}^d , called the *Delaunay subdivision* of Λ . In general, a polytopal subdivision is a non-overlapping union of polytopes that fill all of \mathbb{R}^d and such that the intersection of any two polytopes is either empty or a *k*-dimensional face. DV(Λ) together with all its translates by lattice vectors form another polytopal subdivision of \mathbb{R}^d . Both subdivisions are invariant by lattice translates by *x* of some Delaunay polytope with vertex at $x \in \Lambda$ are translates by *x* of some Delaunay polytope with vertex at 0. Thus to know the full Delaunay subdivision of a lattice Λ , it suffices to know the Delaunay polytopes with vertex 0. The centres of these Delaunay polytopes coincide with the vertices of DV(Λ).

The Delaunay subdivision is said to be *dual* to the subdivision with Dirichlet-Voronoi polytopes. The Dirichlet-Voronoi polytope of a lattice can be obtained from the Delaunay polytopes with vertex 0 and vice versa: there is a bijection between the k-dimensional faces of these Delaunay polytopes and the (d - k)-dimensional faces of the Dirichlet-Voronoi polytope. In particular, each d-dimensional Delaunay polytope corresponds to a vertex of the Dirichlet-Voronoi polytope. Moreover, the face lattice structure with respect to inclusion is preserved as well: if two faces of Delaunay polytopes with vertex 0 are contained in each other, the corresponding dual faces of the Dirichlet-Voronoi polytope are contained in each other with the inclusion reversed. Therefore, the classification of combinatorial types of Dirichlet-Voronoi polytopes is equivalent to the classification of combinatorial types of Delaunay subdivisions.

The different combinatorial types can be derived from possible affine types. Here, two Delaunay subdivisions, or lattices Λ and Λ' , are *affinely equivalent* (are of the *same affine type*) if there is a matrix (linear map) $A \in GL_d(\mathbb{R})$ with $\Lambda' = A\Lambda$, mapping all Delaunay polytopes of Λ to those of Λ' . Note that two Delaunay subdivisions with different combinatorial types cannot be affinely equivalent. The opposite could be possible though: two different affine types of Delaunay subdivisions could possibly have the same combinatorial type – although we do not know of a single example among Delaunay subdivisions for translational lattices at this point. In particular, up to dimension 5, all affine types of Delaunay subdivisions are not only affinely inequivalent, but also combinatorially inequivalent.

3. Voronoi's second reduction theory

In the following we give a short sketch of Voronoi's second reduction theory (Voronoi, 1908, 1909), as far as it is necessary to describe how our classification of affine types of fivedimensional Delaunay subdivisions is obtained. For a more detailed description and extensions of the theory we refer the reader to Schürmann (2009).

3.1. Working with Gram matrices

The set of real symmetric positive definite matrices is denoted $S_{>0}^d$. When dealing with lattices up to orthogonal transformations, it is often convenient to work with Gram matrices $Q = B^t B \in S_{>0}^d$ instead of using matrices of lattice bases *B*. Up to orthogonal transformations, the basis matrix *B* can be uniquely recovered from *Q* using the Cholesky decomposition. Geometrically this is equivalent to reconstruction of a basis knowing vector lengths and angles between them. Every positive definite symmetric matrix *Q* defines a corresponding positive definite quadratic form $x \mapsto Q[x]$ $= x^t Qx$ on \mathbb{R}^d .

In particular for studying affine types of Delaunay subdivisions it is convenient to use the same coordinates of vertices v_1, \ldots, v_n from a fixed translational lattice $\Lambda \subseteq \mathbb{R}^d$ (often $\Lambda = \mathbb{Z}^d$) for different affine images $B \times \operatorname{conv}\{v_1, \ldots, v_n\}$ of Delaunay polytopes, which we represent by a corresponding matrix $Q \in S_{>0}^d$. A polytope $P = \operatorname{conv}\{v_1, \ldots, v_n\}$ with vertices $v_i \in \Lambda$ is called a *Delaunay polytope* of Q if it is *d*-dimensional and if there exists a centre $c \in \mathbb{R}^d$ and a real number r such that $Q[c - v_i] = r^2$ for $i = 1 \ldots, n$ and $Q[c - v] > r^2$ for all other $v \in \Lambda$. The set $\operatorname{Del}(\Lambda, Q)$ of all Delaunay polytopes of $Q \in S_{>0}^d$ is a polytopal subdivision of \mathbb{R}^d , called the *Delaunay subdivision* of Q with respect to Λ .

We speak of a *Delaunay triangulation* if all the Delaunay polytopes are simplices, that is, if all of them have affinely independent vertices. We say that $Del(\Lambda, Q)$ is a *refinement* of $Del(\Lambda, Q')$ [and $Del(\Lambda, Q')$ is a *coarsening* of $Del(\Lambda, Q)$], if every Delaunay polytope of Q is contained in a Delaunay polytope of Q'. Any Delaunay subdivision can be refined to a Delaunay triangulation by perturbing Q if necessary. Voronoi's theory of secondary cones which we explain below gives us an explicit description of the set of positive definite matrices having the same Delaunay subdivision.

3.2. Secondary cones and L-types

Voronoi's second reduction theory is based on *secondary cones* (also called *L-type domains*):

$$SC(\mathcal{D}) = \{Q \in \mathcal{S}_{>0}^d : Del(\mathbb{Z}^d, Q) = \mathcal{D}\}$$

which can be seen to be non-empty polyhedral cones in $S_{>0}^d$ (which are open within their linear hull), if \mathcal{D} is a Delaunay subdivision for some Q. In order to give an explicit description of SC(\mathcal{D}) we define for an affinely independent set $V \subseteq \mathbb{Z}^d$ of cardinality d + 1 and a point $w \in \mathbb{Z}^d$ the symmetric matrix

$$N_{V,w} = ww^t - \sum_{v \in V} \alpha_v vv^t, \tag{1}$$

where the coefficients α_{ν} are uniquely determined by the affine dependency:

$$w = \sum_{v \in V} \alpha_v v$$
 with $1 = \sum_{v \in V} \alpha_v$.

In the special situation of $V = \{v_1, \ldots, v_{d+1}\}$ being vertices of a Delaunay simplex *L* and *w* being the additional vertex of a Delaunay simplex $L' = \operatorname{conv}\{v_2, \ldots, v_{d+1}, w\}$ adjacent to *L*, we use the notation $N_{L,L'}$ for $N_{V,w}$. In the following we use $\langle A, B \rangle = \operatorname{Trace}(AB)$ to denote the standard inner product defined for two symmetric matrices *A*, *B* on S^d . The following result by Voronoi gives an explicit description of a secondary cone in terms of linear inequalities.

Theorem 3.1 (Voronoi, 1908, 1909). Let Q be a positive definite symmetric matrix whose Delaunay subdivision $\mathcal{D} = \text{Del}(\mathbb{Z}^d, Q)$ is a triangulation. Then

$$SC(\mathcal{D}) = \{ Q' \in \mathcal{S}^d : \langle N_{L,L'}, Q' \rangle > 0 \text{ for adjacent } L, L' \in \mathcal{D} \}.$$
(2)

This theorem of Voronoi shows that the secondary cone SC(D) of a Delaunay triangulation D is a full-dimensional

open polyhedral cone, that is, the intersection of finitely many open halfspaces. If we use weak inequalities ≥ 0 in equation (2) instead of strict inequalities, we obtain a description of the closed polyhedral cone $\overline{SC(D)}$. We will use these closed versions and their facial structure in the sequel. Just as for polytopes (cf. §2.1), faces can be defined for these closed polyhedral cones and the set of all faces forms a combinatorial lattice – the face lattice of the cone. Voronoi discovered that the faces of $\overline{SC(D)}$ correspond to all the possible coarsenings of D.

Two full-dimensional secondary cones touch in a facet if and only if the corresponding Delaunay triangulations can be transformed into each other by *bistellar flips*. That is, we first apply a coarsening of some of the simplices to repartitioning polytopes (*d*-dimensional polytopes with d + 2 vertices) and then apply a refinement procedure. Since these changes of Delaunay triangulations are not important for what follows, we omit a detailed description here and refer the interested reader to Schürmann (2009).

The rational closure $S^d_{\operatorname{rat},\geq 0}$ of $S^d_{>0}$ is the set of positive semidefinite quadratic forms whose kernel is defined by rational equations. At the core of Voronoi's theory is the action of the matrix group $\operatorname{GL}_d(\mathbb{Z})$ on the polyhedral tiling by closures of secondary cones:

Theorem 3.2 (Voronoi's second reduction theory). The topological closures $\overline{\mathrm{SC}(\mathcal{D})}$ give a polyhedral subdivision of $\mathcal{S}^d_{\mathrm{rat},\geq 0}$ on which the group $\mathrm{GL}_d(\mathbb{Z})$ acts by $\overline{\mathrm{SC}(\mathcal{D})} \mapsto U^{\mathrm{I}} \overline{\mathrm{SC}(\mathcal{D})} U$. Under this group action there are only finitely many inequivalent secondary cones.

Note that one can subdivide the secondary cones into smaller cones and obtain a reduction domain for the action of $\operatorname{GL}_d(\mathbb{Z})$ on $\mathcal{S}_{>0}^d$. This is the reason why Voronoi's theory of Delaunay subdivisions and secondary cones is referred to as *Voronoi's second reduction theory* (for positive definite quadratic forms).

For our classification of affine types, the following observation is crucial:

Theorem 3.3. Let $Q, Q' \in S_{>0}^d$ be two positive definite matrices with Cholesky decompositions Q = B'B and Q' = (B')'(B') and corresponding lattices $\Lambda = B\mathbb{Z}^d$ and $\Lambda' = B'\mathbb{Z}^d$. Then the Delaunay subdivisions of Λ and Λ' are of the same affine type if and only if Q and Q' are in $\operatorname{GL}_d(\mathbb{Z})$ -equivalent secondary cones.

Proof. We are not aware of an explicit reference for this result, so for clarity we give an argument here. First we note that by transforming a set Λ and a Delaunay decomposition $Del(\Lambda, Q)$ by a linear map $A \in GL_d(\mathbb{R})$ we get a new Delaunay decomposition $Del(\Lambda', (A^{-1})^t Q A^{-1})$ with vertex set $\Lambda' = A \Lambda$.

Suppose now that the Delaunay decompositions of Λ and Λ' are of the same affine type. Then $A \operatorname{Del}(\Lambda, \operatorname{Id}_d) = \operatorname{Del}(\Lambda', (A^{-1})^t A^{-1}) = \operatorname{Del}(\Lambda', \operatorname{Id}_d)$. Therefore

$$Del(\mathbb{Z}^d, Q) = B^{-1}Del(\Lambda, Id_d)$$
$$= B^{-1}A^{-1}Del(\Lambda', Id_d)$$
$$= UDel(\mathbb{Z}^d, Q')$$

with $U = B^{-1}A^{-1}B'$. Since $\mathbb{Z}^d = U\mathbb{Z}^d$ we have $U \in GL_d(\mathbb{Z})$ and therefore Q and $(U^{-1})^t Q' U^{-1}$ are in the same secondary cone.

On the other hand, if Q and Q' are in $\operatorname{GL}_d(\mathbb{Z})$ -equivalent secondary cones, then there exists a $U \in \operatorname{GL}_d(\mathbb{Z})$ with $\operatorname{Del}(\mathbb{Z}^d, Q') = U\operatorname{Del}(\mathbb{Z}^d, Q)$. Thus

$$(B')^{-1}$$
Del $(\Lambda', \operatorname{Id}_d) = UB^{-1}$ Del $(\Lambda, \operatorname{Id}_d),$

and hence $A = B'UB^{-1}$ satisfies $A\text{Del}(\Lambda, \text{Id}_d) = \text{Del}(\Lambda', \text{Id}_d)$.

With the knowledge of how to perform bistellar flips, Theorems 3.2 and 3.3 easily lead to an algorithm to enumerate all affine types of Delaunay triangulations in a given dimension [see Algorithm 3 in Schürmann (2009)]. For it, Schürmann and Vallentin developed the program *scc* (*secondary cone cruiser*). The first version from Schürmann & Vallentin (2005) already allowed one to reproduce the known classification of all $GL_d(\mathbb{Z})$ -inequivalent Delaunay triangulations up to dimension d = 5. We will use their result, *i.e.* the output of the program *scc*.

Beginning with dimension 6 the number of inequivalent Delaunay triangulations starts to explode. At the moment, we still do not know how many inequivalent triangulations to expect in dimension 6. Baburin & Engel (2013) report that they found 567 613 632 so far.

3.3. Enumeration of all Delaunay subdivisions

Arbitrary Delaunay subdivisions are limiting cases of Delaunay triangulations. Their secondary cones occur on the boundaries of full-dimensional secondary cones of Delaunay triangulations. The following theorem seems to be folklore. One can find a proof for example in proposition 2.6.1 of Vallentin (2003).

Theorem 3.4. Let \mathcal{D} be a Delaunay triangulation.

(i) A positive definite symmetric matrix Q lies in $\overline{\operatorname{SC}(\mathcal{D})}$ if and only if \mathcal{D} is a refinement of $\operatorname{Del}(Q)$.

(ii) If two positive definite symmetric matrices Q and Q' both lie in $\overline{SC(D)}$, then Del(Q + Q') is a common refinement of Del(Q) and Del(Q').

We note that this theorem can be extended to positive semidefinite symmetric matrices in the rational closure $S^d_{rat,\geq 0}$ of $S^d_{>0}$. For those among them which are not positive definite, one can define a polyhedral Delaunay subdivision with unbounded polyhedra. For details we refer the reader to ch. 4 of Schürmann (2009).

By Theorem 3.4, the classification of all inequivalent Delaunay subdivisions is equivalent to the classification of all inequivalent secondary cones. In order to prove our Theorem 2.1, we show the following equivalent result:

Theorem 3.5. In dimension 5 there are 110 244 affine types of Delaunay subdivisions. Equivalently, there are that many secondary cones of positive definite quadratic matrices in S^5 up to $GL_5(\mathbb{Z})$ -equivalence.

3.4. Related works

At this juncture, we should point out that there is a parallel theory that considers a single Delaunay polytope in a lattice, irrespective of the other Delaunay polytopes in the tessellation. This theory is expounded by Deza & Laurent (2010) and recent developments can be found in Dutour Sikiríc (2016). The possible Delaunay polytopes of dimension 5 were classified by Kononenko (2002) in terms of 138 combinatorial types. The classification in dimension 6 in Dutour (2004) gives 6241 combinatorial types.

In Schürmann (2009, cf. Table 2 on p. 60) it is reported that Engel (2000) found 179 372 inequivalent five-dimensional Delaunay subdivisions. This, however, is unfortunately a misinterpretation of Engel's result who classifies so-called contraction types (of parallelohedra). From these contraction types, he derives 103 769 'combinatorial types'. These types are not the true combinatorial types that are classified here however, but a coarser notion, which classifies parallelohedra in dimension 5, or equivalently Delaunay subdivisions, up to their subordination schemes. The subordination scheme of a d-dimensional polytope P is a list of numbers containing, for every k = 2, ..., d - 1 and for every *n*, the number of (k - 1)faces of P incident to exactly n of the k-faces of P [see §4 of Engel (2000) for details]. Thus, the subordination scheme encodes certain properties of the face lattice of a polytope, but not the whole face lattice. Two combinatorially different polytopes can have the same subordination scheme. They may even be the same for different affine types of Dirichlet-Voronoi polytopes, having even secondary cones of different dimension. In fact, during our work we discovered two such examples for d = 5.

Note that combinatorial types of polytopes can only truly be distinguished by checking whether or not their face lattices are different. It has been shown by Kaibel & Schwartz (2003) that the incidence relations between vertices and facets of two polytopes are sufficient to distinguish their face lattices. Practically such differences can be checked using graph isomorphism software as we describe in the next section. Invariants like the number of faces of a given dimension or the subordination scheme used by Engel may be useful in computations, for instance when limiting the number of equivalence tests. However, such invariants are not sufficient for complete enumerations. Engel's invariant appears to distinguish the known 52 combinatorial types in dimension 4, but it does not distinguish types in any dimension greater than or equal to 5. While it is conceivable that the subordination scheme could be extended to better distinguish between types, it should never be used alone without checking for equivalence since there is always the possibility that non-isomorphic structures have the same invariant.

4. Algorithms and implementations

Before we explain the details of our computations for d = 5, we start with some general observations, which are valid in all dimensions and quite useful for practical purposes.

4.1. Using reduced generators and central forms

Each closure of a secondary cone is given by a finite list of linear inequalities (coming from Voronoi's regulators, cf. Theorem 3.1). From it one can obtain a number of generating rays. In fact, one of these descriptions (by rays or inequalities) can be obtained from the other by a polyhedral representation conversion. Since all of the involved inequalities involve rational numbers only, we may assume that the generators for rays are given by integral vectors (matrices in S^d), with coordinates having a greatest common divisor (gcd) of 1. We refer to these generators as reduced (or normalized) generators. As we are using Theorem 3.4 for the classification of Delaunay subdivisions, we only need to consider closures of secondary cones which are faces of closures of fulldimensional secondary cones. All such faces are themselves generated by a subset of the reduced generators of the fulldimensional cone.

Having reduced generators R_1, \ldots, R_k of the closure of a secondary cone SC, we define a *central reduced* (or *normalized*) form of the secondary cone as the sum $Q(SC) = \sum_{i=1}^{k} R_i$. It is easy to see that two secondary cones SC and SC' are $GL_d(\mathbb{Z})$ -equivalent if and only if Q(SC) and Q(SC') are $GL_d(\mathbb{Z})$ -equivalent. Hence, for the classification of secondary cones up to $GL_d(\mathbb{Z})$ -equivalence we can equally well classify their central reduced forms up to $GL_d(\mathbb{Z})$ -equivalence.

4.2. Testing equivalence of forms and use of invariants

Testing $GL_d(\mathbb{Z})$ -equivalence of central reduced forms can be done with the Plesken–Souvignier algorithm (Plesken & Souvignier, 1997). Their initial implementation is available (see Plesken & Souvignier, 1995) and is part of computer algebra software such as *MAGMA* (MAGMA, 2006) and *GAP* (The GAP Group, 2015). The algorithm works by building a finite set of vectors that is canonically defined by a given positive definite matrix and spans \mathbb{Z}^d as a lattice. For a given norm bound *n* and a positive definite matrix *Q* let

$$S(Q, n) = \{ v \in \mathbb{Z}^d \mid Q[v] \le n \}.$$

Then we take the smallest *n* such that S(Q, n) spans \mathbb{Z}^d as a lattice and call the vector set Can(Q).

As testing $\operatorname{GL}_d(\mathbb{Z})$ -equivalence of central reduced forms is computationally quite involved, one needs to reduce the

Table 1	
Number of $GL_5(\mathbb{Z})$ -inequivalent secondary cones and contraction	cones
in $S_{>0}^{5}$ by their dimension.	

Table 2 Number of $GL_5(\mathbb{Z})$ -inequivalent secondary cones in $\mathcal{S}_{>0}^5$ by number of

No.	No. secondary cones	No. contraction cones		
1	7	7		
2	37	39		
3	146	161		
4	535	613		
5	1681	2021		
6	4366	5543		
7	9255	12512		
8	15692	22806		
9	21132	33085		
10	22221	37601		
11	18033	32821		
12	10886	21292		
13	4713	9709		
14	1318	2787		
15	222	397		

number of such tests as much as possible since the final number of forms is M = 110244 and so the total number of isomorphism tests is a priori M(M - 1)/2. The basic idea is to use invariants to reduce the number of tests. Some invariants come naturally from the form Q(SC) such as its determinant and size of Can(Q(SC)). Other possible invariants are related to the secondary cone SC under consideration, for example the dimension of SC or its number of generating forms R_1, \ldots, R_k . Further invariants are the rank of R_k and so on. Rather surprisingly, the most efficient invariant tends to be the determinant of Q(SC).

4.3. Putting it all together for five dimensions

Now, finally, let us put the pieces above together, to describe the algorithm behind our classification result for d = 5. To show Theorem 3.5 with computer assistance, we can use Voronoi's theory. We start from the secondary cones of the 222 known Delaunay triangulations. These were classified by Baranovskii & Ryshkov (1973), Ryshkov & Baranovskii (1978) but the classification was incorrect and a final correct classification was obtained by Engel & Grishukhin (2002) which we have independently confirmed (Schürmann & Vallentin, 2006; Dutour Sikirić & Grishukhin, 2009). These open polyhedral cones are full-dimensional in $S_{>0}^5$ and therefore have dimension 15. Their closure is given by a list of non-redundant linear inequalities. From this list, we can obtain the reduced generators of each cone and also a description by generators and by equations/inequalities for each of their facets. These facets are themselves closures of 14-dimensional secondary cones which correspond to Delaunay subdivisions that are a true coarsening of the considered Delaunay triangulation at hand. Some of them may be $GL_d(\mathbb{Z})$ -equivalent, so for our classification we have to obtain a list of $GL_d(\mathbb{Z})$ inequivalent 14-dimensional secondary cones in $S_{>0}^5$ from them, using their central reduced forms. In a next step, we obtain a list of $GL_d(\mathbb{Z})$ -inequivalent 13-dimensional secondary cones from our list of 14-dimensional secondary cones in a similar way. We continue this process until we subsequently

rank-k generating rays.	-		20	
In line <i>i</i> , the rank- <i>k</i> colum	k = 1, 4, 5, contain	ns the number	of se	condary cones

In line *i*, the rank-*k* column, k = 1, 4, 5, contains the number of secondary cones which have *i* generating rays of rank *k*. (There exist no generating rays for k = 2, 3.)

No. generating rays (of particular rank)	Rank-1	Rank-4	Rank-5
0	82	51900	1572
1	410	35316	15421
2	1658	21574	32939
3	5029	1354	26811
4	11301	0	19302
5	18923	100	6841
6	23802	0	3662
7	22411	0	2150
8	15528	0	950
9	7744	0	285
10	2699	0	170
11	548	0	38
12	97	0	76
13	9	0	0
14	2	0	0
15	1	0	9
16	0	0	18

obtain a full list of $\operatorname{GL}_d(\mathbb{Z})$ -inequivalent cones of dimensions 15, ..., 1. See Table 1 for the number of secondary cones obtained in each dimension in this way.

4.4. Practical implementations

The computer code of our first implementation in Haskell of the algorithm described above, together with detailed documentation (in German), are available at http://www.math. uni-rostock.de/~waldmann. In particular, data of the full classification can be obtained at http://www.math.uni-rostock.de/~waldmann/matrizen_dim5, with a matrix of a central reduced form for each secondary cone in $S_{>0}^5$.

Our second implementation used the *GAP* package *polyhedral* (Dutour Sikirić, 2015) with some external calls to *isom* (Plesken & Souvignier, 1995) for equivalence tests and *lrs* (Avis, 2015) for polyhedral representation conversions. In our third implementation, we adapted the program *scc*. In its latest version (Garber *et al.*, 2015) we included the program *isom* to produce all secondary cones of a given dimension.

In order to avoid the dependency on *isom* in all three implementations, we also performed equivalence computations with *nauty* (McKay, 2014), applied to test equivalence of the sets Can(Q(SC)) of vectors, by using the method explained in §3.4 of Bremner *et al.* (2014). Overall, the full computation, its resulting data and in particular the numbers in Table 1 were all sufficiently well cross-checked. All calculations yield the same results and due to the different nature of our three programs we can be certain of the obtained classification, although the computations are large and quite involved.

We can use the obtained results for a computational proof of our main Theorem 2.1, by showing that all Dirichlet– Voronoi polytopes are combinatorially inequivalent. This implies that all Delaunay subdivisions are combinatorially

Table 3 Number of primitive and all combinatorial types of Delaunay subdivisions and the corresponding $GL_u(\mathbb{Z})$ -inequivalent secondary cones.

n	Primitive types	All combinatorial types
2	1	2
3	1 (Fedorov, 1885)	5 (Fedorov, 1885)
4	3 (Voronoi, 1908, 1909)	52 (Delone, 1929 <i>a</i> , <i>b</i> ; Stogrin, 1975)
5	222 (Baranovskii & Ryshkov, 1973; Ryshkov & Baranovskii, 1978; Engel & Grishukhin, 2002)	110244
6	≥ 567 613 632 (Baburin & Engel, 2013)	

inequivalent. This is shown by checking whether their face lattices are non-isomorphic. Since the face lattice of a polytope is determined by the incidence graph of vertices and facets, we can check whether these graphs are non-isomorphic. These isomorphism checks can be performed using, for instance, graph isomorphism software such as *nauty* (McKay, 2014). We computed 'canonical forms' for each of the graphs with *nauty* and then used *md5sum* (a special hash function) for each of them in order to decide computationally (in a reasonable amount of time) that they are all different.

5. Tables and data

We provide the following tables, containing additional information: Table 1 gives the number of inequivalent secondary cones by their dimension. Table 2 gives the number of secondary cones by their number of rank-1, -4 or -5 extreme rays. Table 3 gives the known numbers of inequivalent secondary cones (all combinatorial types) and fulldimensional secondary cones (primitive types), together with a reference where these results can be found. Table 4 gives the number of secondary cones according to their dimension and their number of extreme rays. Table 5 gives the number of secondary cones that cannot be extended to a higherdimensional cone by a pyramid construction with a rank-1 extreme ray. Table 6 gives the frequencies of occurrence of Bravais groups according to the nomenclature of *CARAT* (2008). Table 7 and Table 8 relate our classification to notions in the theory of *contraction types* as developed by Engel (2000). In the following we provide some background information (see also Dutour Sikirić *et al.*, 2014).

5.1. Fundamental faces and irreducible cones

For a given secondary cone SC with generating rays R_1, \ldots, R_k we define the *fundamental face* F(SC) to be the smallest face of SC that contains all the generators R_i of rank greater than 1. The face F(SC) may be reduced to zero in which case SC is generated by rank-1 matrices only. From Erdahl & Ryshkov (1994) we know that the number of generators is equal to the dimension of the secondary cone in this case and that this case is equivalent to the Dirichlet–Voronoi polytope being a zonotope and to the Delaunay subdivision being the connected region of a hyperplane arrangement. Up to $GL_5(\mathbb{Z})$ -equivalence, we found 81 secondary cones of this kind, corresponding to different zonotopes in dimension 5.

If F(SC) is non-trivial (non-zero) then the structure of the secondary cone is more complex. For a secondary cone SC we have a decomposition of the form

Table 4

Number of secondary cones according to dimension (at most 15) and number of generators (at most 26).

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	7														
2		37													
3			144												
4			2	517											
5				17	1595										
6					81	4041									
7					1	301	8266								
8				1		12	887	13354							
9					3		62	2007	16862						
10					1	11	2	222	3461	16358					
11						1	36	13	557	4443	11989				
12							2	89	50	944	4259	6395			
13								7	182	122	1103	2945	2346		
14									19	305	181	857	1449	526	
15										43	403	173	430	456	62
16									1		80	390	102	120	84
17										5		92	274	35	13
18											15		72	122	5
19												30		29	33
20													34		13
21										1				23	
22											3				6
23												4			
24													6		
25														7	
26															6

Table 5

Number of $GL_5(\mathbb{Z})$ -inequivalent secondary cones in $\mathcal{S}_{>0}^5$ which are not extendable to a higher-dimensional secondary cone by adding a rank-1 generating ray.

Dimension	10	11	12	13	14	15
No. secondary cones	1	12	40	142	266	222

$$SC = F(SC) + \sum_{i=1}^{h} \mathbb{R}_{+} p(v_i)$$

with $p(v_i) = v_i v_i^t$ the rank-1 matrix (form) associated to a vector v_i . Our computations show that we have dim SC = dim F(SC) + h which means that SC is obtained by a sequence of h pyramid constructions over F(SC). By a pyramid construction we mean an extension to a higher-dimensional secondary cone by adding a rank-1 generating ray.

If F(SC) does not contain any positive definite matrices (and hence lies in the boundary of $S_{>0}^5$), then in dimension 5 there is only one possibility: F(SC) has only one extreme ray that corresponds to the D₄ root lattice, which we denote by F_{D_4} . Up to $GL_5(\mathbb{Z})$ -equivalence, we found 424 different combinatorial types of secondary cones of the form $F_{D_4} + \sum_{i=1}^h \mathbb{R}_+ p(v_i)$. Note that F_{D_4} itself is not a secondary cone, since it does not contain any positive definite forms. By our computation, all such cones have their dimension equal to their number of generators.

The fundamental cones F(SC) may themselves contain rank-1 forms. For example, there exist two secondary cones of dimension 3 with four generators each, three of rank 4 and one of rank 1 (see §5 of Dutour Sikirić *et al.*, 2015). If F(SC)contains only forms of rank higher than 1 then, according to the terminology of Engel (2000), it is *totally zone contracted*. If a secondary cone satisfies SC = F(SC) then it is called *irreducible*. Tables 7 and 8 give key information on irreducible secondary cones we found.

5.2. Contraction types

In Engel (2000) the notion of a contraction type is introduced. This notion is distinct from secondary cones and gives a further refinement of them. That is, if we have a secondary cone SC that is irreducible but not totally zone contracted and has rank-1 forms p_1, \ldots, p_m , then we can decompose it into a number of *contraction cones* (also called *contraction domains*) $SC_i + \sum_{j=1}^m \mathbb{R}_+ p_j$ with SC_i a totally zone-contracted secondary cone. For example, the three-dimensional cone SC with symbol $L_1^2 L_3 p_1$ in Table 8 is a cone over a square (combinatorially) with vertices corresponding to p_1, L_1, L_3 and L_1 . We can decompose it into two isomorphic three-dimensional cones (over triangles) of the form $L_1 L_3 + \mathbb{R}_+ p_1$ and one twodimensional cone of the form $L_3 + \mathbb{R}_+ p_1$.

For other cones the decomposition can be more complicated. Given an irreducible secondary cone SC, let R_1 be the cone of its extreme rays of rank 1. We define S to be the set of all totally zone-contracted irreducible cones whose rays are also rays of SC (of rank greater than 1). Then our computation Table 6

Frequency of occurrence of Bravais groups.

'Name' is the standard name from the *GAP* package (CARAT, 2008). 'Order' is the size of the point group of corresponding lattices. 'Frequency' is the number of secondary cones that are symmetric with respect to the group.

Name	Order	Frequency
1,1,1,1,1: 1	2	105301
1,1,1,1;1: 2	4	4155
1,1,1;1;1: 6	8	159
2-2;1,1,1: 2	12	137
1,1,1;1,1: 2	4	112
1,1,1;1;1: 4	8	90
1,1,1;1;1: 5	8	39
1,1,1,1;1: 1	4	34
2-1;1,1,1: 2	16	31
2-2;1,1;1: 6	24	31
1,1;1;1;1: 15	16	20
1,1;1,1;1: 3	8	14
1,1;1;1;1: 13	16	12
3;1,1: 3	48	10
1,1;1;1;1:6	16	8
3;1;1: 8	96	7
1,1,1;1;1:2	8	6
2-1;1,1;1: 4	32	6
1,1;1,1;1:6	8	6
1,1;1;1;1:17	16	5
3;1,1:2	96	4
3;1,1:5	96	4
2-1;1,1;1: 6	32	4
1;1;1;1;1:8	32	4
1,1,1;1,1:1	4	3
1,1,1;1;1;1:1	8	3
2-2;2-2;1: 3	12	3
1,1;1;1;1:10	10	3
4-3;1: 5	240	2
2-2;1,1;1:4	24	2
1,1,1,1,1,1	52 24	2
2-2,1,1,1, 5	102	2
1.1.1.1.1.1.13	32	2
1 1.1 1.1 1	8	1
1 1.1.1.1.1 1	16	1
1.1.1.1.1.1.1	32	1
3.1.1.7	192	1
4-1.1.2	768	1
4-1:1: 3	2304	1
5-1:3	3840	1
5-2:3	1440	1
3.1.1.4	192	- 1
4-1:1: 4	768	1
2-2:2-2:1: 5	72	1
2-1:1:1:1:6	64	1
2-1;1;1;1: 7	64	1
2-2;1;1;1: 7	48	1
3;1;1: 7	192	1
2-1;1;1;1: 8	64	1
2-1;1;1;1: 11	64	1
1;1;1;1;1: 12	32	1
2-1;1;1;1: 12	64	1
1;1;1;1;1: 15	32	1
1;1;1;1;1: 16	32	1

shows that SC can be decomposed into contraction cones $S + R_1$ with $S \in S$.

The decomposition of an irreducible secondary cone SC into contraction cones induces a decomposition of any secondary cone obtained by adding rank-1 forms. Overall, we thus obtain a decomposition into contraction cones that is finer than the decomposition by secondary cones. For

54,418

54,426

54,444

54,432

42,240

48.322

52,392

56,478

54.432

54,452

54,440

No. SC

4100

1256

786

800

928

628

628

100

689

1815

1088

1392

800

800

Table 7

Information about the 82 totally zone-contracted secondary cones.

'Dimension' is the dimension of the secondary cone SC, 'generator' gives the type of extreme rays, 'symbol' gives the number of facets and vertices of the corresponding Dirichlet–Voronoi polytopes and 'No. SC' gives the number of secondary cones having SC as their fundamental face.

Dimension	Generator	Symbol	No. SC
1	L_1	40,42	450
1	L_2	42,96	777
1	L_3	48,180	670
1	L_4	50,192	112
1	L_5	50,282	352
1	L_6	54,342	324
1	L_7	54,366	220
2	D_4^2	42,132	1067
2	$L_1 D_4$	40,122	1814
2	$L_2 D_4$	42.132	1825
2	$L_2 D_4$	48.246	1428
2	$L_{5}D_{4}$	50.312	352
2	$L_7 D_4$	54,402	484
2	L_1L_2	48,202	2385
2		48,188	1058
2		50 232	333
2	L_1L_5	50.298	650
2		54.366	758
2		52, 308	1638
2		54 376	650
2		54 376	324
2	L_2L_4	50,280	318
2	 L	50 304	553
2		54 386	582
2		54 374	490
2		50 330	348
2		54 364	318
2		54 388	553
3	$L_1 D_4^2$	48 242	2738
3	$L_1 D_4$ $L_2 D_4^2$	42.168	2047
3	$L_2 D_4^2$	52 344	1344
3	$L_3 D_4$ $L_2 D_2^2$	56 462	484
3		48 242	5029
3	$L_1 L_2 D_4$ $L_2 L_2 D_4$	48 254	2436
3	$L_1 L_3 D_4$ $L_2 L_3 D_4$	50 328	650
3		50,526 52,346	2344
3	$L_2 L_3 D_4$	54 402	650
3	$L_2 L_5 D_4$	50 334	553
3		54 410	1160
3	$L_3L_7U_4$	52 316	2773
3	$L_1 L_2 L_3$	54,302	1256
3	$L_1 L_2 L_5$	54,392	758
3	$L_1 L_2 L_6$ $L_1 L^2 L_6$	54 382	456
3	$L_1L_3L_7$	50 288	516
3	$L_1L_3L_4$	50,200	696
3	$L_1L_3L_5$	54 304	856
2	$L_1L_3L_6$	50.346	630
3	$L_1L_4L_5$	54 388	734
2	$L_1L_4L_6$	54,588	028
2	$L_1 L_5 L_6$	54,404	1002
2	$L_{2}L_{3}L_{5}$	54,590	1092
3	$L_{2}L_{3}L_{6}$	54,420	552
2	$L_2L_5L_6$	50 252	553
3	$L_3L_4L_5$	51 100	535
3	$L_3L_4L_6$	54,400	501
3 2	$L_3L_5L_6$	54,410	028
3 4	$L_4 L_5 L_6$ $L^2 D^3$	34,410	333
	$L_2 U_4$	42,204	2000
4	$L_1 L_2 U_4$	40,282	3988 2272
4	$L_1 L_3 U_4$	52,55Z	1074
4	$L_2 L_3 U_4$	56,384	10/4
4	$L_3L_7U_4$	50,470	1160

Table 7 (conti	nued)	
Dimension	Generator	Symbol
4	$L_1L_2L_3D_4$	52,354
4	$L_1L_2L_5D_4$	54,418
4	$L_1 L_3^2 L_7 D_4$	54,418
4	$L_1L_3L_5D_4$	50,342
4	$L_2L_3L_5D_4$	54,424
4	$L_1 L_2 L_3 L_5$	54,406
4	$L_1 L_2 L_3 L_6$	54,428
4	$L_1 L_2 L_5 L_6$	54,438
4	$L_{1}L_{3}L_{4}L_{5}$	50,360
4	$L_1 L_3 L_4 L_6$	54,416

 $L_1 L_3 L_5 L_6$

 $L_1 L_4 L_5 L_6$

 $L_2 L_3 L_5 L_6 \\ L_3 L_4 L_5 L_6$

 $L_{2}^{5}D_{4}^{5}$

 $L_1L_2^2\mathsf{D}_4^3$

 $L_1 L_2 L_3 D_4^2$

 $L_1 L_3^2 L_7 D_4^2$

 $L_1 L_2 L_3 L_5 D_4$

 $L_1 L_2 L_3 L_5 L_6$

 $L_1 L_3 L_4 L_5 L_6$

4

4

4

5

5

5

5

5

5

5

secondary cones SC whose fundamental face F(SC) is totally zone contracted there is no difference. But for other irreducible secondary cones the contraction types form a strictly finer decomposition. The total number of contraction types that we obtain is 181 394. The number of contraction cones by their dimension is given in Table 1. In Table 8 we give for each irreducible secondary cone D the number of types of contraction cones contained in $D + \sum_k \mathbb{R}_+ p(v_k)$. We note that in Engel (2000) the number of contraction cones is reported to be 179 372. This discrepancy is most likely due to the different notion of equivalence *via* 'subordination schemes' used there.

5.3. Euler Poincaré characteristic check

Another key check of the correctness of our enumeration is to use the Euler Poincaré characteristic. We have the formula

$$\sum_{F} (-1)^{\dim(F)} \frac{1}{|\operatorname{Stab}(F)|} = 0$$

where the sum is over the representatives of cones with respect to the action of $\operatorname{GL}_n(\mathbb{Z})$. This kind of formula comes from the Euler Poincaré characteristic of discrete groups, *i.e.* $\chi(\operatorname{GL}_n(\mathbb{Z})) = 0$ for $n \ge 3$. See Brown (1994) and Dutour Sikirić *et al.* (2016) for more details.

Both our enumeration of secondary cones and our enumeration of contraction cones satisfy this condition, which is yet another strong indication of the correctness of our enumeration. For example, for the secondary cones, if we regroup the cones by their dimension, this gives us the following non-trivial identity:

Table 8

Information about the 125 inequivalent irreducible secondary cones, which are not totally zone contracted.

Table 8 (continued)

Generator

 $L_1 L_3^2 L_5 L_6 p_1^4$

 $L_2 L_3^2 L_6 p_1^4$

Dimension

Same labelling convention as in Table 7; in addition p_1 denotes an extreme ray of rank 1 and 'No. contraction cones' is the number of contraction cones corresponding to this irreducible component.

				N	7	$L_3^2 L_4 L_6 p_1^4$	54,452	2
Dimension	Generator	Symbol	No. SC	No. contraction cones	7	$L_3 L_4 L_6^2 p_1^4$	58,536	2
					7	$L_1^3 L_3^3 L_5 D_4 p_1^3$	50,378	12
	$L_{1}^{2}L_{3}p_{1}$	48,196	566	2047	/	$L_1^3 L_2 L_3^3 L_5 p_1^3$	54,442	13
	$L_1 L_3 L_5 p_1^2$	50,320	205	3988	7	$L_1^2 L_3^2 L_4 L_5 p_1^2$	50,390	2
	$L_{1}^{2}L_{3}D_{4}p_{1}$	48,262	1240	1074	7	$L_1 L_3 L_5 L_6 p_1$ $L^2 L L L L n^3$	54,454 54,474	3 16
	$L_1^3 L_3^3 L_7 p_1$	54,390	174	665	7	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L^2 L^2 L_n^3$	54,474	70
	$L_1^2 L_2 L_3 p_1$	52,324	1423	1092	7	$L_1 L_3 L_5 L_6 p_1$ $L^2 L^2 L^2 L_p^3$	54,404	1/
ļ.	$L_{1}^{2}L_{3}L_{4}p_{1}$	50,296	274	1256	7	$L_1 L_3 L_5 L_6 p_1$ $L^2 L L L L n^3$	54,404	1-
	$L_1^2 L_3 L_5 p_1$	50,320	205	615	7	$L_1 L_3 L_4 L_5 L_6 p_1$	54,402	10
1	$L_1^2 L_3 L_6 p_1$	54,402	358	4100	7	$L_1 L_2 L_3 L_5 L_6 p_1$ $L_1^3 L^3 L_n^3$	54,480	12
1	$L_1 L_3^2 L_5 p_1$	50,326	182	3503	7	$L_1 L_3 L_5 L_6 p_1$ $L L L^2 L n^3$	54 472	12
1	$L_3 L_5^2 L_6 p_1$	54,434	203	3999	7	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L_1 L^2 L_1 D_1 p^2$	54 454	60
5	$L_1 L_5 L_6 p_1^3$	54,412	97	615	7	$L_1 L_2 L_3 L_5 D_4 p_1$ $L^2 L_1 L^2 L_1 L_p^2$	54,454	20
5	$L_1 L_3 L_5 D_4 p_1^2$	50,350	205	1188	7	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L L L^2 L n^2$	54,474	20
5	$L_1^2 L_3^2 L_5 p_1^2$	50,334	298	5895	7	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L^2 L L L p^2$	54,462	20
5	$L_1 L_2 L_3 L_5 p_1^2$	54,414	396	492	7	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L L^2 L p^2$	54,402	20
5	$L_1 L_3 L_4 L_5 p_1^2$	50,368	197	492	7	$L_1 L_3 L_4 L_5 L_6 p_1$	54,472	14
5	$L_1 L_3 L_5 L_6 p_1^2$	54,426	164	689	7	$L_1 L_2 L_3 L_5 L_6 p_1$ $L_1^2 L_1^2 L_2^2 L_p^2$	54,490	14
5	$L_1 L_3 L_5 L_6 p_1^2$	54,432	164	1815	8	$L_1 L_3 L_4 L_5 L_6 p_1^{-1}$ $I^2 I^2 I^2 I^{-2} I^{-5}$	54,478	14
5	$L_1^2 L_3 D_4^2 p_1$	52,360	1168	3279	8	$L_1 L_3 L_5 L_6 p_1$ $I^3 I^3 I^2 I p^4$	54,478	2
5	$L_1^3 L_3^3 L_7 D_4 p_1$	54,426	396	100	8	$L_1 L_3 L_5 L_6 p_1$ $L^2 L^3 L^3 L_9^4$	54,478	4
5	$L_{1}^{2}L_{2}L_{3}D_{4}p_{1}$	52,362	2060	1392	8	$L_1 L_3 L_5 L_6 p_1$ $L^2 L^3 L^2 L_9^4$	54,400	3
5	$L_{1}^{2}L_{3}L_{5}D_{4}p_{1}$	50,350	205	553	8	$L_1 L_3 L_5 L_6 p_1$ $L L L^2 L L n^4$	54,478	4
5	$L_1 L_3^2 L_5 D_4 p_1$	50,356	182	1092	8	$L_1 L_2 L_3 L_5 L_6 p_1$ $L_1^2 L_1 L_1 p^4$	54,488	5
5	$L_1^2 L_2 L_3 L_5 p_1$	54,414	396	958	8	$L_1 L_3 L_4 L_5 L_6 p_1$	58 544	2
5	$L_1^2 L_2 L_3 L_6 p_1$	54,436	358	480	8	$L_1 L_3 L_4 L_6 p_1$ $L^3 L_4 L^3 L_5 D_{10} D_{10}^3$	54 469	12
5	$L_1^2 L_3 L_4 L_5 p_1$	50,368	205	1490	8	$L_1 L_2 L_3 L_5 U_4 p_1$ $L^3 L_1 J^3 L_1 p^3$	54,408	13
5	$L_1^2 L_3 L_4 L_6 p_1$	54,424	327	990	8	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^3 L^3 L L L p^3$	54,488	3
5	$L_1^2 L_3 L_5 L_6 p_1$	54,426	228	291	8	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L_1^2 L^2 L_n^3$	54,470	7
5	$L_1 L_2 L_3^2 L_5 p_1$	54,420	352	546	8	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L_1 L^2 L^2 L_n^3$	54 498	14
5	$L_1 L_3^2 L_4 L_5 p_1$	50,374	182	800	8	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L^2 L_1 L^2 L_1 p^3$	54 486	17
	$L_1 L_3^2 L_5 L_6 p_1$	54,432	128	628	8	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L^2 L L^2 L n^3$	54,480	14
	$L_1 L_3 L_5^2 L_6 p_1$	54,442	178	328	8	$L_1 L_3 L_4 L_5 L_6 p_1$ $L_1 L_3 L_3 L_3 L_n^3$	54 514	2
)	$L_2 L_3 L_5^2 L_6 p_1$	54,468	203	474	8	$L_1 L_2 L_3 L_5 L_6 p_1$ $L_1 J^3 L_1 J^3 L_n p^3$	54 502	2
	$L_3 L_4 L_5^2 L_6 p_1$	54,456	203	591	9	$L_1 L_3 L_4 L_5 L_6 p_1$	54 502	- 1
) -	$L_{3}^{2}L_{6}p_{1}^{4}$	54,430	34	92	9	$L_1 L_4 L_5 L_6 p_1$ $L^3 L^4 L^3 L_0 p^5$	54 502	1
5	$L_1^3 L_3^3 L_5 p_1^3$	50,348	73	1188	9	$L_1 L_3 L_5 L_6 p_1$ $L^2 L_1 L^2 L^2 L_1 p^5$	54 512	3
5	$L_1^2 L_3 L_5 L_6 p_1^3$	54,440	164	492	9	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L^2 L_1 L^2 L_1 p^5$	54 500	3
5	$L_1 L_2 L_5 L_6 p_1^5$	54,446	97	492	0	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L L L^2 n^5$	58 552	1
5	$L_1 L_3 L_5^2 L_6 p_1^3$	54,450	121	2619	9	$L_1 L_3 L_4 L_6 p_1$ $L^3 L_4 L^3 L^2 L_5 p_4^4$	54 512	1
6	$L_1 L_4 L_5 L_6 p_1^3$	54,434	93	1092	9	$L_1 L_2 L_3 L_5 L_6 p_1$ $I^3 I^3 I I^2 I n^4$	54,512	
5	$L_1^2 L_3^2 L_5 D_4 p_1^2$	50,364	298	958	9	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L_1 J^3 L^3 L_n p^4$	54 522	1
5	$L_1 L_2 L_3 L_5 D_4 p_1^2$	54,440	396	1490	9	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L_1 J^3 L^2 L_n^4$	54 512	1
6	$L_1^2 L_2 L_3^2 L_5 p_1^2$	54,428	606	3030	9	$L_1 L_2 L_3 L_5 L_6 p_1$ $L^2 L^3 L_1 L^3 L_n^4$	54 510	2
5	$L_1^2 L_3^2 L_4 L_5 p_1^2$	50,382	298	639	9	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L^3 L_4 L^2 L_6 p_4$	54 500	4
5	$L_1^2 L_3^2 L_5 L_6 p_1^2$	54,440	200	291	10	$L_1 L_3 L_4 L_5 L_6 p_1$	54 452	
5	$L_1^2 L_3 L_5^2 L_6 p_1^2$	54,450	34	820	10	$L_{3}L_{4}L_{6}p_{1}$ $I^{4}I^{6}I^{4}I^{6}p_{1}^{6}$	54 526	
5	$L_1 L_2 L_3 L_5 L_6 p_1^2$	54,460	164	605	10	$L_1 L_3 L_5 L_6 p_1$	58 582	1
5	$L_1 L_2 L_3 L_5 L_6 p_1^2$	54,466	164	628	10	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^3 L_4 L^3 L_p^5$	54 536	1
6	$L_1 L_3^2 L_5^2 L_6 p_1^2$	54,456	148	328	10	$L_1 L_2 L_3 L_5 L_6 p_1$ $I^3 I^4 I I^3 I n^5$	54,550	3
5	$L_1 L_3 L_4 L_5 L_6 p_1^2$	54,448	164	1000	10	$L_1 L_3 L_4 L_5 L_6 p_1$ $L_1 L^2 p^9$	50.468	
5	$L_1 L_3 L_4 L_5 L_6 p_1^2$	54,454	150	474	11	$L_4 L_5 p_1$	54 524	
6	$L_1^3 L_3^3 L_7 D_4^2 p_1$	56,486	396	740	11	$L_1 L_3 L_4 L_5 L_6 p_1$ $L^2 L_1 L^2 n^8$	58 580	
6	$L_{1}^{2}L_{2}L_{3}D_{4}^{2}p_{1}$	52,400	933	207	11	$L_{3}L_{4}L_{6}p_{1}$ $L_{2}^{2}I_{1}I_{1}I_{2}p^{7}$	58 500	1
6	$L_1^2 L_2 L_3 L_5 D_4 p_1$	54,440	396	492	11	$L_1 L_3 L_4 L_5 L_6 p_1$ $I^4 I_4 I^6 I^4 I_5^6$	54 560	1
6	$L_1 L_2 L_3^2 L_5 D_4 p_1$	54,446	352	450	11	$L_1 L_2 L_3 L_5 L_6 p_1$ $I^4 I^6 I I^4 I r^6$	54 548	
5	$L_1^2 L_2 L_3 L_5 L_6 p_1$	54,460	228	2420	11	$L_1 L_3 L_4 L_5 L_6 \rho_1$ $L L L^2 L p^9$	54 548	
5	$L_1^2 L_3 L_4 L_5 L_6 p_1$	54,448	228	279	12	$L_1 L_4 L_5 L_6 p_1$ $I I^2 I I I^2 r^8$	58 604	
,	$L_1 L_2 L_3^2 L_5 L_6 p_1$	54,466	128	1490	12	$L_1 L_3 L_4 L_5 L_6 \rho_1^2$ $I^2 I^2 I I^2 I^2 r^9$	58 628	
1	$L_1 L_2 L_3 L_5^2 L_6 p_1$	54,476	178	628	13	$L_1 L_3 L_4 L_5 L_6 p_1'$ $L^2 L L L^2 L^2 n^9$	58.620	
)	$L_1 L_3^2 L_4 L_5 L_6 p_1$	54,454	128	328	15	$L_1 L_3 L_4 L_5 L_6 \rho_1$ $I^3 I I^3 n^{12}$	50,020 62 700	
	T T T T 7 T	51 161	170	474	15	$L_2 L_4 L_6 p_1$	02.700	

No. contraction

cones

No. SC

Symbol

54,454

54,464

293 74	63 939	56927 5	5146751	8329297
$-\overline{5760}+\overline{57}$	$\frac{1}{60} - \frac{1}{64} + \frac{1}{64}$	576	11520	5760
3341911	1630783	10308319	13879	9537
960	256	1152	-+	40
1414553	1356727	565595	48907	8923
180	288	288 +	96	$-\frac{1}{144} \equiv 0.$

This kind of mass formula provides a highly non-trivial check of the correctness of an enumeration as any error on a single entry or on a single stabilizer would make the formula wrong.

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References

- Avis, D. (2015). *The lrs program*. http://cgm.cs.mcgill.ca/~avis/C/lrslib/ USERGUIDE.html.
- Baburin, I. A. & Engel, P. (2013). Acta Cryst. A69, 510-516.
- Baranovskii, E. & Ryshkov, S. (1973). Sov. Math. Dokl. 14, 1391– 1395.
- Bremner, D., Dutour Sikirić, M., Pasechnik, D. V., Rehn, T. & Schürmann, A. (2014). LMS J. Comput. Math. 17, 565–581.
- Brown, K. S. (1994). Cohomology of Groups, Vol. 87 of Graduate Texts in Mathematics. New York: Springer-Verlag.
- CARAT (2008). CARAT. Version 2.0. https://wwwb.math.rwth-aachen.de/carat/.
- Delone, B. (1929a). Izv. Akad. Nauk. SSSR Otd. Fiz.-Mater. Nauk, pp. 79–110.
- Delone, B. (1929b). Izv. Akad. Nauk. SSSR Otd. Fiz.-Mater. Nauk, pp. 145–164.
- Delone, B. (1934). Bull. Acad. Sci. USSR, pp. 793-800.
- Deza, M. & Laurent, M. (2010). *Geometry of Cuts and Metrics*, Vol. 15 of *Algorithms and Combinatorics*. Heidelberg: Springer.
- Dolbilin, N., Itoh, J. & Nara, C. (2011). Computational Geometry, Graphs and Applications, Vol. 7033 of Lecture Notes in Computer Science, pp. 55–60. Heidelberg: Springer.
- Dutour, M. (2004). Eur. J. Combin. 25, 535-548.
- Dutour Sikiríc, M. (2015). Polyhedral, a GAP package. http://mathieudutour.altervista.org/Polyhedral/index.html.

- Dutour Sikiríc, M. (2016). Can. J. Math. https://cms.math.ca/10.4153/ CJM-2016-013-7.
- Dutour Sikirić, M., Gangl, H., Gunnells, P., Hanke, J., Schürmann, A. & Yasaki, D. (2016). J. Pure Appl. Algebra, **220**, 2564–2589.
- Dutour Sikirić, M. & Grishukhin, V. (2009). Eur. J. Combin. 30, 853–865.
- Dutour Sikirić, M., Grishukhin, V. & Magazinov, A. (2014). Eur. J. Combin. 42, 49–73.
- Dutour Sikiríc, M., Hulek, K. & Schürmann, A. (2015). *Alg. Geom.* **2**, 642–653.
- Engel, P. (2000). Acta Cryst. A56, 491-496.
- Engel, P. & Grishukhin, V. (2002). Eur. J. Combin. 23, 275-279.
- Erdahl, R. M. & Ryshkov, S. S. (1994). Eur. J. Combin. 15, 459-481.
- Fedorov, E. (1885). Verh. Russ. Kais. Mineral. Ges. St Petersburg, 21, 1–279.
- The GAP Group (2015). *GAP groups, algorithms, programming.* Version 4.7.9. http://www.gap-system.org/.
- Garber, A., Schürmann, A. & Vallentin, F. (2015). scc (secondary cone cruiser). Version 2.0. http://www.geometrie.uni-rostock.de/ software/.
- Gavrilyuk, A. (2014). Math. Notes, 95, 625-633.
- Grünbaum, B. (2003). Convex Polytopes, Vol. 221 of Graduate Texts in Mathematics, 2nd ed. New York: Springer- Verlag.
- Kaibel, V. & Schwartz, A. (2003). Graphs Comb. 19, 215-230.
- Kononenko, P. (2002). Math. Notes, 71, 374-391.
- MAGMA (2006). MAGMA high performance software for algebra, number theory, and geometry. Version 2.13. http://magma.maths. usyd.edu.au/.
- McKay, B. (2014). nauty. Version 2.5. http://cs.anu.edu.au/people/ bdm/nauty/.
- Plesken, W. & Souvignier, B. (1995). ISOM and autom. Published under GPL licence at http://www.math.uni-rostock.de/~waldmann/ ISOM_and_AUTO.zip.
- Plesken, W. & Souvignier, B. (1997). J. Symbolic Comput. 24, 327-334.
- Ryshkov, S. & Baranovskii, E. (1978). Proc. Steklov Inst. Math. 140 pp.
- Schürmann, A. (2009). Computational Geometry of Positive Definite Quadratic Forms, Vol. 48 of University Lecture Series. Providence, RI: American Mathematical Society.
- Schürmann, A. & Vallentin, F. (2005). scc (secondary cone cruiser). Version 1.0. http://www.math.uni-magdeburg.de/lattice_geometry/.
- Schürmann, A. & Vallentin, F. (2006). Discrete Comput. Geom. 35, 73–116.
- Senechal, M. & Galiulin, R. (1984). Structural Topology, 10, 5–22.
- Stogrin, M. (1975). Proc. Steklov Inst. Math. 123, 1-116.
- Vallentin, F. (2003). PhD thesis, Center for Mathematical Sciences, Munich University of Technology. http://mediatum.ub.tum.de/doc/ 602017/602017.pdf.
- Voronoi, G. (1908). J. Reine Angew. Math. 134, 198-287.
- Voronoi, G. (1909). J. Reine Angew. Math. 136, 67-182.
- Ziegler, G. (1995). Lectures on Polytopes. New York: Springer.