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# The contraction types of parallelohedra in $E^5$

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Using the process of zone contraction and its inverse, zone extension, the 179372 contraction types of parallelohedra in  $E^5$  were derived from the 84 combinatorial types of relatively or totally zone-contracted parallelohedra.

## 1. Introduction

The concept of translation lattices to explain the regular shape of crystals has been well established in the field of crystallography since the time of Haüy (1774-1822). The crystallographer Fedorov (1893) initialized a systematic investigation of the topological properties of translation lattices. In 1885, Fedorov (1885) described the five combinatorial types of parallelohedra in Euclidean space  $E^3$ , that is convex polyhedra, congruent copies of which tile space facet-to-facet and in parallel position. Minkowski (1897) proved that, for a convex body to admit a facet-to-facet tiling by translation, it must be a centrosymmetric polytope with centrosymmetric facets. Venkov (1954), and independently McMullen (1980), achieved the complete characterization of parallelohedra in  $E^d$  by proving that each belt has four or six (d-2) faces. A parallelohedron is called *primitive* if, in its lattice tiling, in each vertex, exactly d + 1 adjacent parallelohedra meet. Voronoï (1908a,b) investigated parallelohedra in higher dimensions and he conjectured that each parallelohedron is affinely equivalent to a Dirichlet domain of some translation lattice. He proved the conjecture for the primitive parallelohedra. He also derived the three combinatorial types of primitive parallelohedra in  $E^4$ . Delaunay (1929*a*,*b*) determined 51 combinatorial types of parallelohedra in  $E^4$  and the one he missed was discovered by Štogrin (1973). In recent years, the determination of parallelohedra in  $E^5$  was attacked. Baranovskii & Ryškov (1973) determined 221 combinatorial types of primitive parallelohedra. The complete list of the 222 combinatorial types of primitive parallelohedra was finally reported in 1998 (Engel, 1998), and it was shown that Voronoï's conjecture holds for dimension d = 5.

For dimensions d < 5, the combinatorial types of parallelohedra coincide with the contraction types and it was realized that, beginning with dimension d = 5, the classification into contraction types is a refinement of the classification into combinatorial types (precise definitions of the classification schemes used will be given in §4).

In Engel (1988), the concept of a maximal parallelohedron was introduced that allows the derivation of its complete zonecontraction lattice and the problem of finding all maximal parallelohedra was raised. A partial solution was given by Erdahl & Ryškov (1994) and Erdahl (1998), who determined the maximal zonohedra in  $E^5$ . In this paper, the method of Erdahl & Ryškov is generalized and a combination of zone contraction and zone extension leads to a general solution.

## 2. Zone contraction and zone extension

Let E be a 1-face (edge) of a parallelohedron P in Euclidean space  $E^d$ ,  $d \ge 2$ . A zone Z of P is defined as the set of all 1-faces of P that are parallel to the zone vector  $\mathbf{t}^*$ ,

$$\mathsf{Z} = \{\mathsf{E} \subset \mathsf{P} \mid \mathsf{E} \parallel \mathsf{t}^*\}.$$

A zone Z is called *closed* if every 2-face of P contains either two edges of Z or else none, otherwise it is called *open*. Let  $E_s$ be a shortest edge in a closed zone  $Z_c$ . By a *zone contraction*  $P^{\downarrow}$ , we understand the process of contracting every edge of  $Z_c$ by  $E_s$ . As a result, the zone becomes open or vanishes completely but all properties of a parallelohedron, as given by Venkov (1954) and McMullen (1980), are maintained and, thus, the polytope resulting from a zone contraction is a parallelohedron but of a different combinatorial type compared to the original one. The reverse process  $P^{\uparrow}$  is called a *zone extension*.

A parallelohedron  $P_0$  is called *totally contracted* if all its zones are open. It is called *relatively contracted* if any further contraction leads to a collapse into a parallelohedron of lower dimension. A parallelohedron  $P_m$  is called *maximal* if it does not allow any zone extension. Already in dimension d = 6, in the neighbourhoods of the Gram matrix of the root lattices  $E_6$ and  $E_6^*$ , there exist parallelohedra, even primitive ones, that are at the same time maximal and totally zone contracted.

Each maximal parallelohedron defines a *zone-contraction lattice*  $\mathbf{L}(\mathsf{P}_m)$  by contracting all combinations of closed zones (it is partially ordered by zone contraction, least upper and greatest lower bounds are defined by union and intersection, respectively, of closed zones). Each relatively or totally zonecontracted parallelohedron defines a *zone-contraction family*  $\mathbf{F}(\mathsf{P}_0)$  by extending all combinations of extendable zone vectors. In general, a zone-contraction family is the union of several zone-contraction lattices which have the same type of relatively or totally zone-contracted parallelohedron,

$$\mathbf{F}(\mathsf{P}_0) = \bigcup_{\mathbf{L}(\mathsf{P}_m) \cap \mathsf{P}_0 = \mathsf{P}_0} \mathbf{L}(\mathsf{P}_m).$$

A parallelohedron is *zonohedral* if all its zones are closed and if the edges within a zone all have the same length. Then it is the direct sum of straight line segments, *i.e.* a special kind of *zonohedron*. There exists exactly one zone-contraction family, defined by the relatively contracted hypercube, where all the members of it are zonohedral parallelohedra. In general, for non-zonohedral parallelohedra, the number of open zones is much larger than the number of closed zones.

In Engel (1988), the problem of how to find the maximal parallelohedra was raised. We have found a complete answer to that problem: *The successive application of both processes, the zone contraction and the zone extension, allows us, in a most general way, to find all contraction types of parallelohedra starting from the combinatorial types of relatively and totally zone-contracted ones.* 

#### 3. The cone of positive-definite quadratic forms

A translation lattice

 $\Lambda^d = \{\mathbf{t} \mid \mathbf{t} = m_1 \mathbf{a}_1 + \ldots + m_d \mathbf{a}_d, m_i \in \mathbb{Z}\}$ 

in  $E^d$  defines by its basis vectors  $\mathbf{a}_1, \ldots, \mathbf{a}_d$  a Gram matrix  $\mathbf{Q} = (q_{ij})$ , where  $q_{ij} = |\mathbf{a}_i| |\mathbf{a}_j| \cos \alpha_{ij}$ ,  $i \leq j = 1, \ldots, d$ . The Gram matrix  $\mathbf{Q}$  determines the translation lattice in  $E^d$  up to an isometry. It is a point within the *open convex cone*  $C^+$  of *positive-definite quadratic forms* in  $\mathbb{R}^{\binom{d+1}{2}}$ . Its closure is denoted by  $C = \operatorname{clos}(C^+)$  and its boundary by  $C^0 = C \setminus C^+$ . The functional  $\varphi(\mathbf{x}) = \mathbf{x}^t \mathbf{Q} \mathbf{x}$  ( $\mathbf{x}^t$  is the transpose of  $\mathbf{x}$ ) is called a positive-definite *d*-nary quadratic form.

Following Erdahl & Ryškov (1994), a family  $\{D_1, \ldots, D_r\}$  of r sets of equi-spaced parallel hyperplanes is called a *dicing* if it is non-degenerate and vertex transitive. Every dicing corresponds to a zonohedral parallelohedron. Let  $\mathbf{t}_1^*, \ldots, \mathbf{t}_r^*$  be the normal vectors for the r sets of equi-spaced hyperplanes of a dicing. For zonohedral parallelohedra, it was shown by Erdahl & Ryškov that the functional  $\varphi(\mathbf{x})$  is given by

$$\varphi(\mathbf{x}) = \sum_{i=1}^r \lambda_i (\mathbf{t}_i^* \mathbf{x})^2,$$

where  $\lambda_i > 0$ . The normal vectors  $\mathbf{t}_i^*$  are parallel to the edges of the zonohedron  $\mathsf{P}(\mathsf{Q})$ , which is obtained, at the origin of  $E^d$ , by Dirichlet's (1850) famous construction:

$$\mathsf{P}(\mathsf{Q}) = \{ \mathbf{x} \in E^d \mid \varphi(\mathbf{x}) \le \varphi(\mathbf{x} - \mathbf{t}), \forall \mathbf{t} \in \Lambda^d \}.$$

Conversely, P(Q) uniquely determines the lattice  $\Lambda^d$ . An edge  $E \subset P$  is determined by d-1 facets of P, therefore E is parallel to a dual lattice vector  $\mathbf{t}^* = h_1 \mathbf{a}_1^* + \ldots + h_d \mathbf{a}_d^*$ ,  $h_i \in \mathbb{Z}$ , which is the outer product of the (d-1) facet vectors, with dual basis  $\mathbf{a}_1^*, \ldots, \mathbf{a}_d^*$ , and Gram matrix  $Q^{-1}$ , where  $\mathbf{a}_i \mathbf{a}_j^* = \delta_{ij}$ . One can see that, for  $\mathbf{x} \in E^d$ ,  $\mathbf{x} = x_1 \mathbf{a}_1 + \ldots + x_d \mathbf{a}_d$ , it holds that  $\mathbf{t}^* \mathbf{x} = h_1 x_1 + \ldots + h_d x_d$ , and  $(\mathbf{t}^* \mathbf{x})^2 \ge 0$  can formally be written as  $\mathbf{x}'(\mathbf{t}^* \mathbf{t}^{*t})\mathbf{x}$ , hence, it is a semi-definite quadratic form. Since det $(\mathbf{t}^* \mathbf{t}^{*t}) = 0$ , it follows that  $\mathbf{t}^* \mathbf{t}^{*t}$  is a point in the boundary  $C^0$ .

Let  $\varphi_0(\mathbf{x})$  be the positive-definite quadratic form of a totally zone-contracted parallelohedron  $\mathsf{P}_0$ . For a general parallelohedron  $\mathsf{P}_s$  in  $\mathbf{F}(\mathsf{P}_0)$  with *s* closed zones  $\mathsf{Z}_{c,i}$  and zone vectors  $\mathbf{t}_i^*$ ,  $i = 1, \ldots, s$ , it holds that

$$\varphi(\mathbf{x}) = \varphi_0(\mathbf{x}) + \sum_{i=1}^s \lambda_i (\mathbf{t}_i^* \mathbf{x})^2,$$

where  $\lambda_i > 0$ . Denote by **Q** and **Q**<sub>0</sub> the Gram matrices of  $\varphi(\mathbf{x})$  and  $\varphi_0(\mathbf{x})$ , respectively, then

$$\varphi(\mathbf{x}) = \mathbf{x}^{t} \mathbf{Q} \mathbf{x} = \mathbf{x}^{t} \mathbf{Q}_{0} \mathbf{x} + \mathbf{x}^{t} \Big[ \sum_{i=1}^{s} \lambda_{i} \mathbf{t}_{i}^{*} \mathbf{t}_{i}^{*t} \Big] \mathbf{x}$$

and the Gram matrix for the translation lattice corresponding to  $P_s$  is given by

$$\mathsf{Q} = \mathsf{Q}_0 + \sum_{i=1}^s \lambda_i \mathbf{t}_i^* \mathbf{t}_i^{*t},$$

where  $\lambda_i > 0$ , i = 1, ..., s. An upper bound for *s* is given by  $s \le {\binom{d+1}{2}} - d_0$ , where  $d_0$  is the dimension of the affine hull of the *domain of existence* of  $\mathsf{P}_0$ . The domain of existence of a contraction type of parallelohedron  $\mathsf{P}$  is defined as the open domain of Gram matrices

$$\Phi^+(\mathsf{P}) = \{\mathsf{Q} \in \mathcal{C}^+ \mid \mathsf{P}(\mathsf{Q}) \stackrel{\text{contr}}{\simeq} \mathsf{P}\}.$$

The Gram matrices, as functions of  $\lambda_i > 0$ ,  $Q(\lambda_1, \ldots, \lambda_s)$ , define a *rational open convex polyhedral cone*  $\Phi_s^+ \subset C^+$ . Its extreme quadratic forms are the trivial edge forms  $\mathbf{t}_i^* \mathbf{t}_i^{*t} \subset C^0$ . Let  $\Phi_0^+$  be the domain of existence of the totally zone-contracted parallelohedron  $\mathsf{P}_0$  of the family of  $\mathsf{P}$ . The cone  $\Phi_0^+$  has non-trivial edge forms. The cone of  $\mathsf{P}$  is the direct sum

$$\Phi^+(\mathsf{P}) = \Phi_0^+ \oplus \Phi_s^+.$$

The dimension of the cone  $\Phi^+$  is given by  $k = \dim(\text{aff hull } \Phi^+)$ . Let *s* be the number of closed zones of P, then  $k = d_0 + s$ . A *base polytope* B is obtained by cutting the cone with a hyperplane of dimension k - 1 such that all its edge forms are intersected. The base polytope can be used to classify the cones.

Not all zones of a contracted parallelohedron can be extended. Let  $P_s$  be a parallelohedron with *s* closed zones and Gram matrix Q. For some zone vector  $\mathbf{t}_j^*$ , the Gram matrix  $Q' = Q + \mathbf{t}_i^* \mathbf{t}_j^{*t}$  is an extension of Q by  $\mathbf{t}_i^*$  if

and

$$\mathsf{P}^{\uparrow}_{s} = \mathsf{P}_{(s+1)}$$

 $\mathsf{P}_{(s+1)}^{\downarrow} = \mathsf{P}_{s}.$ 

For a given zone-contraction family  $\mathbf{F}(\mathbf{P}_0)$ , a minimal set  $\mathbf{M}(\mathbf{P}_0)$  of *extendable zone vectors*  $\mathbf{t}^*$  is obtained by considering all zone extensions of  $\mathbf{P}_0$ . A zone can be extended by the zone vector  $\mathbf{t}^* \in \mathbf{M}(\mathbf{P}_0)$  if  $\mathbf{P}_0^{\uparrow} = \mathbf{P}_1$  and  $\mathbf{P}_1^{\downarrow} = \mathbf{P}_0$ . Because the  $\lambda_i > 0$  can be chosen arbitrarily, it is sufficient to consider for  $\mathbf{t}^*$  primitive vectors with integral components only. Let  $\mathbf{H}(\mathbf{P}_0)$  be the upper bound for the magnitude of the components of all  $\mathbf{t}^*$ . Since each  $\mathbf{t}^* \in \mathbf{M}(\mathbf{P}_0)$  is the outer product of d - 1 facets of  $\mathbf{P}$ , their components  $h'_i$  depend on the components  $m'_i$  of the facet vectors  $\mathbf{t}$ . In Engel (1988), the concept of an *optimal basis* was

**Table 1** The structure of the *k*-dimensional cones of the totally contracted parallelohedra in  $E^5$ .

Туре	Gram matrix
k = 1	
$U_{24,24}$	2a0 - a0a/2a - a0a/2a0 - a/00/2a
40.42	2a - a - aa0/2a0 - aa/2a - a0/2a - a/2a
42.96	3a - a - a a a / 3a - a - a a / 3a - a - a / 2a 0 / 2a
48.180	3a - a - a a a / 4a - a - a 2a / 3a - a - a / 3a - a / 4a
50.192	3a - a - a a a / 3a - a - a a / 3a - a - a / 3a - a / 3a
50.282	5a - a - 2aa2a/5a - 2a - a2a/5a - a - 2a/3a - a/5a
54.342	6a - 2a - 2a 2a 2a / 6a - 2a - 2a 2a / 6a - 2a - 2a / 5a - a / 5a
54.366-2	4a - 2a - a 2a a / 6a - a - 2a 3a / 4a - 2a - a / 6a - 2a / 6a

Туре	(k-1) subordinations
k = 2	
40 122	Unior 40.42
42.132-1	$U_{24,24}$ , 10.12 $U_{24,24}$ , 42.96
42 132-2	$\mathbf{U}_{24,24}, \mathbf{U}_{24,35}$
48 188	40 42 48 180
48 202	40.42, 42.96
48 246	U 48 180
50.232	40.42, 50.192
50.280	48 180 50 192
50.298	40.42, 50.282
50.304	48.180, 50.282
50.312-1	$U_{24,24}, 50.282$
50.330	50.192, 50.282
52.308	42.96, 48.180
54.364	50.192, 54.342
54.366-1	40.42, 54.342
54.374	48.180, 54.366-2
54.376-1	42.96, 54.342
54.376-2	42.96, 50.282
54.386	48.180, 54.342
54.388-2	50.282, 54.342
54.402-1	$\mathbf{U}_{24,24}^{I}$ , 54.366–2
k = 3	
42.168	42.132–1, 42.132–1 <sup>I</sup> , 42.132–2
48.242–1	40.122, 40.122 <sup>I</sup> , 42.132–2
48.242–2	40.122, 42.132–1, 48.202
48.254	40.122, 48.188, 48.246
50.288	48.188, 50.232, 50.280
50.312-2	48.188, 50.298, 50.304
50.328	40.122, 50.298, 50.312-1
50.334	48.246, 50.304, 50.312-1
50.346	50.232, 50.298, 50.330
50.352	50.280, 50.304, 50.330
52.316	48.188, 48.202, 52.308
52.344	$42.132-2, 48.246, 48.246^{1}$
52.346	42.132–1, 48.246, 52.308
54.382	48.188, 48.188 <sup>1</sup> , 54.374, 54.374 <sup>1</sup>
54.388-1	50.232, 54.364, 54.366-1
54.392	48.202, 50.298, 54.376–2
54.394	48.188, 54.366–1, 54.386
54.398	50.304, 52.308, 54.376-2
54.400	48.202, 54.366-1, 54.376-1
54.402-2	42.132–1, 50.312–1, 54.376–2
54.404	50.298, 54.366-1, 54.388-2
54.408	50.280, 54.364, 54.386
54.410-1	48.246, 54.374, 54.402–1
54.410-2	50.304, 54.386, 54.388-2
54.410-3	50.330, 54.364, 54.388-2
34.420 54.422	54.500, 54.570-1, 54.580 54.276, 1, 54.276, 2, 54.289, 2
54.422	54.570-1, 54.570-2, 54.588-2
50.402 k = 4	42.132-2, 34.402-1, 34.402-1
n = 4	42 168 42 168 <sup>I</sup> 42 169 <sup>V</sup>
42.204	$42.100, 42.100, \dots, 42.100$ A2 168 A8 242 1 A8 242 2 A8 242 2 <sup>I</sup>
40.202 50.342	42.100, 40.242-1, 40.242-2, 40.242-2 48 254 50 212 2 50 228 50 224
50.342	40.234, JU.312-2, JU.326, JU.334 50.288 50.312 7, 50.346, 50.357
50.300	10.200, 50.512-2, 50.540, 50.552
54.554	40.242-1, 40.234, 40.234, 32.344

Table 1 (continued)

Туре	(k-1) subordinations
52.354	48.242-2, 48.254, 52.316, 52.346
52.384	42.168, 52.344, 52.346, 52.346 <sup>I</sup>
54.406	50.312-2, 52.316, 54.392, 54.398
54.416	50.288, 54.388-1, 54.394, 54.408
54.418–1	48.254, 48.254 <sup>I</sup> , 54.410–1, 54.410–1 <sup>I</sup> , 54.382
54.418–2	48.242-2, 50.328, 54.392, 54.402-2
54.418–3	50.312-2, 54.394, 54.404, 54.410-2
54.424	50.334, 52.346, 54.398, 54.402-2
54.426	50.346, 54.388-1, 54.404, 54.410-3
54.428	52.316, 54.398, 54.400, 54.420
54.432–2	50.352, 54.408, 54.410-2, 54.410-3
54.438	54.392, 54.400, 54.404, 54.422
54.444	54.398, 54.410-2, 54.420, 54.422
56.470	52.344, 54.410–1, 54.410–1 <sup>I</sup> , 56.462
k = 5	
42.240	$42.204, 42.204^{I}, \ldots, 42.204^{IX}$
48.322	$42.204, 48.282, 48.282^{I}, \ldots, 48.282^{V}$
52.392	48.282, 52.352, 52.354, 52.354 <sup>I</sup> , 52.382
54.432–1	50.342, 52.354, 54.406, 54.418-2, 54.424
54.440	50.360, 54.416, 54.418-3, 54.426, 54.432-2
54.452	54.406, 54.418-3, 54.428, 54.438, 54.444
56.478	52.352, 52.352 <sup>I</sup> , 54.418–1, 54.418–1 <sup>I</sup> , 56.470, 56.470 <sup>I</sup>

introduced that minimizes the components of the facet vectors. It simultaneously reduces the Gram matrices Q and  $Q^{-1}$  such that  $\Delta_{opt} = tr(Q_{opt} - \rho^2 Q_{opt}^{-1})^2$  is minimal, where  $\rho = [det(Q)]^{1/d}$ ,

$$\Delta_{\text{opt}} = \min_{\mathsf{A} \in GL_d(\mathbb{Z})} \operatorname{tr}(\mathsf{A}\mathsf{Q}\mathsf{A}^t - \rho^2 \mathsf{A}^\circ \mathsf{Q}^{-1} \mathsf{A}^{-1})^2.$$

With respect to an optimal basis, the magnitude of the components of the zone vectors  $\mathbf{t}^*$  are also minimal and are small integers for low dimensions. For zonohedra, it holds that H = 1, which follows from the dicing conditions. For dimension d = 5, in all cases, with respect to an optimal basis, H = 1 was found to be sufficient.

In what follows, the cone C is described. The Gram matrix **Q** is represented as a point q with components  $q_{ij}$  in  $\mathbb{R}^{d \times d}$ . A basis of  $\mathbb{R}^{d \times d}$  is given by the  $e_{ij}$  with  $e_{ij}e_{kl} = \delta_{ijkl}$ , i, j, k, l = 1, ..., d. Since **Q** is symmetric,  $\mathbf{Q} = \mathbf{Q}^{t}$ , it follows that the cone C lies in the subspace defined by  $e_{ij} = e_{ji}$ ,  $i \leq j = 1, ..., d$ . Each zone vector  $\mathbf{t}^*$  has a representation in  $\mathbb{R}^{d \times d}$  by  $\mathbf{t}^* \mathbf{t}^{*t} = \mathbf{t}^* \times \mathbf{t}^*$  (× denotes the tensor product). For any  $\mathbf{A} \in GL_d(\mathbb{Z})$ ,  $\mathbf{Q}' = \mathbf{AQA}^t$  is arithmetically equivalent to **Q**. Thus,  $q' = \mathbf{A}^t \times \mathbf{A}^t q$  is arithmetically equivalent to q. If  $\mathbf{S} \in GL_d(\mathbb{Z})$  fixes **Q**, then  $\mathbf{S}^t \times \mathbf{S}^t$  fixes q. For any vector  $\mathbf{v}^*$ ,  $\mathbf{I} = \mathbf{v}^* \times \mathbf{v}^*$  is in  $C^0$  since  $\det(\mathbf{v}^* \times \mathbf{v}^*) = 0$ . Let c be the representation of the identity matrix **I** in  $\mathbb{R}^{d \times d}$ . Then  $\lambda \mathbf{c}$  is the axis of the cone C because for any ray vector **I** we have that the cone angle  $\omega$  becomes

$$\cos \omega = \frac{\mathbf{c} \cdot \mathbf{l}}{|\mathbf{c}||\mathbf{l}|} = \frac{v_1^2 + v_2^2 + \ldots + v_d^2}{d^{1/2}(v_1^4 + 2v_1^2v_2^2 + \ldots + v_d^4)^{1/2}} = \frac{1}{d^{1/2}}.$$

Thus, C is a cone of rotation with rotation axis  $\lambda c$ . It is intersected by subspaces of dimensions  $\binom{k+1}{2}$ , k < d. For large dimensions d, the cone angle  $\omega$  is close to 90°.

# research papers

# Table 2

The numbers of contraction types of parallelohedra in  $E^5$ .

Family	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Total
10.32	_	_	_	_	_	1	4	8	13	16	17 (1)	11	7 (2)	2	1	1(1)	81 (4)
26.48	_	1	2	6	14	27	50	74	87	78	55 (1)	22 (1)	7 (2)	1(1)			424 (5)
40.42	1	2	4	8	17	33	60	82	91	75	47 (2)	17	5 (5)				442 (7)
40.122	1	4	13	34	81	169	291	376	369	255	123 (3)	33 (3)	6 (6)				1755 (12)
42.96	1	2	6	16	35	66	110	144	154	121	78 (3)	30	11 (4)	2	1(1)		777 (8)
42.132-1	1	4	13	39	90	178	294	379	375	268	136 (4)	39 (4)	8 (3)	1(1)			1825 (12)
42.132-2	1	3	9	25	55	104	169	215	215	154	84 (4)	25 (2)	7 (3)	1 (1)			1067 (10)
42.168	1	5	18	51	117	229	364	447	415	261	112 (10)	23 (5)	4 (4)				2047 (19)
42.204	1	3	9	23	47	84	126	144	125	70	29 (8)	4 (4)					665 (12)
42.240	1	1	2	5	9	13	19	19	16	8	7 (7)						100 (7)
48.180	1	4	12	33	77	145	216	255	230	155	76 (4)	25 (1)	6 (3)	1 (1)			1236 (9)
48.188	1	5	17	51	127	247	375	438	383	243	105 (7)	27	4 (4)				2023 (11)
48.202	1	4	15	4/	122	259	421	516	469	309	143(7)	40	/ (/)				2353 (14)
48.242-1	1	3 7	21	104	276	504 504	052	1126	057	560	$\frac{117}{(12)}$	$\frac{22}{12}$	4 (4)				2724 (21) 4865 (20)
40.242-2	1	6	24	104 76	180	364	533	502	483	277	103(7)	42(13) 10(11)	4(4) 1(1)				2668(10)
48 254	1	8	37	128	336	662	978	1073	849	458	105(7) 149(13)	20(20)	1 (1)				4609 (33)
48.282	1	7	32	106	277	574	858	925	705	355	103(26)	10(10)					3953 (36)
48.322	1	3	9	22	51	97	143	148	108	49	15(15)	10 (10)					646 (15)
50.192	1	1	2	5	9	14	20	22	20	15	9 (1)	3 (2)	1(1)				122 (4)
50.232	1	2	5	13	28	48	68	76	63	38	16 (2)	3 (3)					361 (5)
50.280	1	3	9	24	54	94	130	139	111	63	25 (4)	6 (4)	1 (1)				660 (9)
50.282	1	3	9	26	56	95	129	133	100	55	20 (6)	3 (3)					630 (9)
50.288	1	4	13	38	90	162	226	237	181	94	30 (7)	4 (4)					1080 (11)
50.298	1	5	18	54	127	230	317	323	232	111	31 (15)	3 (3)					1452 (18)
50.304	1	5	19	57	133	235	312	308	216	101	27 (17)	2(2)					1416 (19)
50.312-1	1	3 7	20	20	20	95 425	129	155	100	55 159	20(6)	3 (3)					0.50(9)
50.328	1	5	18	50 54	127	230	317	323	232	111	32(32) 31(15)	3 (3)					1473(32) 1452(18)
50.330	1	3	9	26	56	95	129	133	100	55	20 (6)	3(3)					630 (9)
50.334	1	5	19	57	133	235	312	308	216	101	27 (17)	2(2)					1416 (19)
50.342	1	7	30	98	237	425	568	551	370	158	33 (33)						2478 (33)
50.346	1	5	18	54	127	230	317	323	232	111	31 (15)	3 (3)					1452 (18)
50.352	1	5	19	57	133	235	312	308	216	101	27 (17)	2 (2)					1416 (19)
50.360	1	7	30	98 70	237	425	568	550	369	158	32 (32)	(2)	0 (5)	4 (4)			2475 (32)
52.308	1	6	25	120	198	392	583	655 1191	546	334	146(13)	43 (2)	9 (5)	1(1)			3018(21)
52.510 52.344	1	0 6	39 26	138	202	376	526	553	934 423	225	210(23) 77(14)	33 13 (8)	0 (0) 1 (1)				2512(31) 2512(23)
52.344	1	8	39	136	349	665	940	985	745	388	127(20)	20(12)	1(1)				4404(33)
52.352	1	8	40	140	357	677	950	984	718	352	98 (24)	10(10)	1 (1)				4335 (34)
52.354	1	11	63	239	639	1238	1755	1812	1323	643	183 (40)	20 (20)					7927 (60)
52.384	1	6	24	73	174	326	442	438	306	143	40 (26)	4 (4)					1977 (30)
52.392	1	8	37	122	308	588	799	773	514	214	44 (44)						3408 (44)
54.342	1	2	7	18	40	67	94	102	84	52	24 (3)	6 (4)	1 (1)				498 (8)
54.364	1	2	17	18	40	67	94	102	84	52	24 (3)	6 (4)	1(1)				498 (8)
54.300-1 54.366_2	1	4	15	45 21	110	203	289	307 76	235	120	43 (7)	2 (7)	1 (1)				1385 (14) 304 (8)
54.300-2	1	5	17	46	96	156	192	180	123	29 57	13(7) 17(10)	$\frac{2}{2}(2)$	1 (1)				892 (12)
54.376-1	1	2	7	18	40	67	94	102	84	52	24(3)	$\frac{2}{6}(4)$	1(1)				498 (8)
54.376-2	1	4	15	46	106	185	250	254	186	97	32 (10)	4 (4)					1180 (14)
54.382	1	5	17	46	97	156	192	176	118	51	15 (15)						874 (15)
54.386	1	5	21	62	152	282	394	404	300	156	52 (13)	10 (7)	1 (1)				1840 (21)
54.388–1	1	4	15	45	110	203	289	307	235	126	43 (7)	7 (7)					1385 (14)
54.388-2	1	4	15	46	106	185	250	254	186	97	32 (10)	4 (4)					1180 (14)
54.392	1	/	31	102	252	465	638 717	038	446 510	204	52(27)	4 (4)					2840 (31)
54.394	1	7	33	100	278	320 477	632	613	J10 /10	180	47(21)	$\frac{7}{3}(3)$					2706(23)
54 400	1	4	15	45	110	203	289	307	235	126	47(30) 43(7)	$\frac{3}{7}(3)$					1385(14)
54.402-1	1	4	14	41	88	145	187	179	129	64	24(13)	3	1(1)				880 (14)
54.402-2	1	4	15	46	106	185	250	254	186	97	32 (10)	4 (4)					1180 (14)
54.404	1	7	31	102	252	465	637	638	446	204	52 (27)	4 (4)					2839 (31)
54.406	1	10	54	193	486	881	1169	1115	729	299	56 (56)						4993 (56)
54.408	1	5	21	62	152	282	394	404	300	156	52 (13)	10 (7)	1 (1)				1840 (21)
54.410-1	1	7	31	97 100	221	378	481	454	307	139	37 (23)	3(3)					2156 (26)
54.410-2 54.410-2	1	/	35 15	109	203 106	4/3	027	010	410 194	189	47 (30) 32 (10)	5 (5) 4 (4)					2/80 (33)
54.416	1	7	33	40 110	278	520	230 717	204 718	509	242	64(21)						3206 (28)
54.418-1	1	7	31	97	222	377	477	441	292	124	31 (31)	1 (1)					2100 (31)
54.418-2	1	7	31	102	250	464	638	638	446	204	52 (27)	4 (4)					2837 (31)
54.418-3	1	10	54	192	483	869	1160	1104	722	291	50 (50)						4936 (50)
54.420	1	5	21	62	152	282	394	404	300	156	52 (13)	10 (7)	1 (1)				1840 (21)

Table 2 (																	
Family	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Total
54.422	1	4	15	46	106	185	250	254	186	97	32 (10)	4 (4)					1180 (14)
54.424	1	7	33	109	266	477	632	613	419	189	47 (30)	3 (3)					2796 (33)
54.426	1	7	31	102	252	465	637	638	446	204	52 (27)	4 (4)					2839 (31)
54.428	1	7	33	111	280	523	720	723	513	246	68 (23)	8 (8)					3233 (31)
54.432-1	1	10	54	194	486	885	1175	1115	730	300	60 (60)						5010 (60)
54.432-2	1	7	33	109	265	473	627	610	416	189	47 (30)	3 (3)					2780 (33)
54.438	1	7	31	102	252	465	637	638	446	204	52 (27)	4 (4)					2839 (31)
54.440	1	10	54	192	483	869	1160	1104	722	291	50 (50)						4936 (50)
54.444	1	7	33	109	265	473	627	610	416	189	47 (30)	3 (3)					2780 (33)
54.452	1	10	54	192	483	869	1160	1104	722	293	55 (55)						4943 (55)
56.462	1	4	14	41	88	145	187	179	129	64	24 (13)	3	1 (1)				880 (14)
56.470	1	7	31	96	218	372	470	443	296	135	34 (20)	3 (3)					2106 (23)
56.478	1	7	31	96	218	369	463	432	278	118	27 (27)						2040 (27)

### 4. The classification into contraction types

Table 2 (continued)

The hierarchical structure of the k-faces of P is used to classify the parallelohedra. The k-faces,  $0 \le k \le d$ , together with the empty set, determine a *face lattice*  $\mathcal{L}(\mathsf{P})$  by inclusion. Two polytopes P and P' are called *combinatorially equivalent*,  $\mathsf{P}' \stackrel{\text{comb}}{\simeq} \mathsf{P}$  if there exists an isomorphism  $\tau : \mathcal{L}(\mathsf{P}) \to \mathcal{L}(\mathsf{P}')$ . In order to verify the combinatorial equivalence, the k-subordination symbol  $n_1 f_1 n_2 f_2 \dots n_r f_r$ , with  $f_1 < f_2 < \dots < f_r$ , was used, where each  $n_i$ ,  $i = 1, \dots, r$ , gives the number of those k-faces that have subordinated  $f_i$  (k - 1)-faces. As subordination symbols for  $k = (d - 1), \dots, 2$ .

Such a classification is sufficient for parallelohedra in dimensions d < 5 but, beginning with dimension d = 5, a finer classification into contraction types is required because edges of various length may be arranged in different ways within a closed zone. Therefore, parallelohedra of the same combinatorial type may show different behaviour under zone contractions.

Two polytopes P and P' are called *affinely equivalent*, P'  $\cong$  P if there exists an affine mapping  $\varphi$ : P' =  $\varphi$ P. Parallelohedra of the same affine type must have isomorphic zonecontraction lattices. The distinct contraction lattices are used to classify the parallelohedra into contraction types. For a parallelohedron P<sub>s</sub> with s closed zones, all its directly subordinated zone-contracted parallelohedra P<sub>(s-1),i</sub> = P\_s^{\downarrow\_{(i)}},  $i = 1, \ldots, s$ , are determined, and their subordination schemes are ordered lexicographically. As *contraction scheme*, we denote the concatenation of the different subordination schemes in their lexicographic order. We say that two parallelohedra P and P' are of the same *contraction type*, P'  $\cong$  P if (i) they have identical subordination schemes; (ii) they have identical contraction schemes; (iii) they belong to the same zone-contraction family.

#### 5. Results

The combinatorial types of relatively and totally zonecontracted parallelohedra are crucial in the derivation of the contraction types of parallelohedra. In  $E^5$ , there exist 2 rela-

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tively and 82 totally zone-contracted combinatorial types of parallelohedra, which have been described in detail in Engel (1998). Most of them were found by contracting the 1620 contraction types of maximal parallelohedra already known and the final list was obtained by carefully investigating their polyhedral cones in C. We have again verified this list by extending all combinatorial types of totally zone-contracted parallelohedra by zone vectors t\* having components  $h_i \in \{-1, 0, 1\}$ , followed by successive zone contractions in order to obtain a totally zone-contracted parallelohedron again. By this, the completeness of that list was confirmed. The combinatorial types of relatively or totally zone-contracted parallelohedra are denoted by the symbol  $N_{(d-1)}$ .  $N_0$ , where  $N_{(d-1)}$  and  $N_0$  give the numbers of facets and vertices, respectively. In cases where distinct types have the same numbers  $N_{(d-1)}$  and  $N_0$ , the symbol is completed by an order number. In Table 1, the structures of the polyhedral cones  $\Phi_0^+$ for the combinatorial types of totally zone-contracted parallelohedra are described. In  $E^5$ , there exist seven types of cones having maximal dimension k = 5. Most of them are simplicial or have few facets. An exception is the cone of 42.240, which was given in Engel (1998) by a representative Gram matrix of the root lattice  $\mathbf{D}_5^*$ . It was realized from its complete zonecontraction family that the cone  $\Phi_0^+(42.240)$  has dimension k = 5. It is bounded by 10 cones  $\Phi_0^+(42.204)$  of dimension k = 4, 30 cones  $\Phi_0^+(42.168)$  of dimension k = 3, 30 cones  $\Phi_0^+(42.132-1)$  and  $\Phi_0^+(42.132-2)$ , respectively, of dimension k = 2, and has 10 extreme edge forms  $\Phi_0^+(42.96)$  and  $\Phi_0^+(\mathbf{U}_{24,24})$ , respectively. The type  $\mathbf{U}_{24,24}$  is the unique totally zone-contracted parallelohedron in  $E^4$ , corresponding to the four-dimensional root lattice  $\mathbf{F}_4$ . It is contained in a subspace U of dimension ten that intersects the cone C. The base polytope of the cone  $\Phi_0^+(42.240)$  is of combinatorial type 10.10 and has a group of combinatorial automorphisms of order 120. The base polyhedron of the subcone  $\Phi_0^+(42.204)$  is a trigonal bypyramid. For each one-dimensional edge form, a representative Gram matrix is given in Table 1.

For each combinatorial type of relatively or totally zonecontracted parallelohedron  $P_0$ , we have calculated its zonecontraction family  $F(P_0)$  by considering all combinations of extensions by zone vectors from its minimal set  $M(P_0)$  of extendable zone vectors. By this, all 1871 contraction types of maximal parallelohedra were found in a systematic way. In Table 2, the numbers of contraction types of parallelohedra for each zone-contraction family with respect to the numbers of closed zones are given, the numbers of maximal parallelohedra  $P_m$  of which are shown in parentheses. The zone-contraction families are denoted by the symbols of their combinatorial types of relatively or totally zone-contracted parallelohedra, The symbols 10.32 and 26.48 denote the two combinatorial types of relatively zone-contracted parallelohedra. The zone-contraction family 10.32 contains all the contraction types of zonohedral parallelohedra in  $E^5$  (they coincide with the combinatorial types).

As a final result, we obtained: In  $E^5$ , there exist 179372 contraction types of parallelohedra, of which 1871 are maximal. They belong to 84 different zone-contraction families. The number of contraction types of primitive parallelohedra is 792, of which 590 are principal primitive having the maximal number of vertices given by (d + 1)!. The number of combinatorial types of parallelohedra is 103769. The number of combinatorial types of primitive parallelohedra is 222, of which 201 are principal primitive.

### References

- Baranovskii, E. P. & Ryškov, S. S. (1973). Sov. Math. Dokl. 14, 1391–1395.
- Delaunay, B. N. (1929a). Izv. Akad. Nauk SSSR Otd. Fiz. Mater. Nauk, pp. 79–110.
- Delaunay, B. N. (1929b). Izv. Akad. Nauk SSSR Otd. Fiz. Mater. Nauk, pp. 145–164.
- Dirichlet, P. G. L. (1850). J. Reine Angew. Math. 40, 209–227. [Oeuvre, Vol. II, pp. 41–59.]
- Engel, P. (1988). Comput. Math. Appl. 16, 425-436.
- Engel, P. (1998). Proc. Inst. Math. Acad. Sci. Ukraine, 21, 22-60.
- Erdahl, R. M. (1998). Proc. Inst. Math. Acad. Sci. Ukraine, 21, 61–74.
- Erdahl, R. M. & Ryškov, S.S. (1994). Eur. J. Comb. 15, 459-481.
- Fedorov, E. S. (1885). Verh. Russ. Kais. Mineral. Ges. St. Petersburg, 21, 1–279. [Reprint: Akad. Nauk SSSR, 1953.]
- Fedorov, E. S. (1893). Z. Kristallogr. 21, 679-694.
- McMullen, P. (1980). Mathematica, 27, 113-121.
- Minkowski, H. (1897). Nachr. Akad. Wiss. Göttingen. Math. Phys. Kl. 218–219. [Gesammelte Abhandlungen, Vol. II, pp. 120–121.]
- Štogrin, M. I. (1973). Proc. Steklov Inst. Math. 123.
- Venkov, B. A. (1954). Vestn. Leningr. Univ. Ser. Mater. Fiz. Him. 9, 11–31.
- Voronoï, G. M. (1908a). J. Reine Angew. Math. 134, 198-287.
- Voronoï, G. M. (1908b). J. Reine Angew. Math. 135, 67-181.