Affine Classes of 3-Dimensional Parallelohedra - Their Parametrization -

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Abstract. In addition to the well-known classification of 3-dimensional parallelohedra we describe this important class of polytopes classified by the affine equivalence relation and parametrize representatives of their equivalent classes.

1 Introduction

For each dimension, parallelohedra constitute a very important class of Euclidean polyhedra that have important applications in geometry, especially in geometry of numbers, combinatorial geometry, and in some other fields of mathematics. Three-dimensional parallelohedra play a significant role in geometric crystallography. The concept and the term of a paralleloherdon were introduced by the Russian eminent crystallographer E.S.Fedorov ([1]).

A *d-parallelohedron* is defined as a polyhedron whose parallel copies tile the space R^d in a face-to-face manner. Classical theorems by H. Minkowski [2] and B. A. Venkov [3] are equivalent to the following criterion:

Theorem 1. *([3,4]). A d-dimensional convex bounded polyhedron is a parallelohedron if and only if*
(i) P is centrally symmetric;
(ii) all its faces are centrally symmetric;
(iii) the projection of P along each of its $(d-2)$-faces is either a parallelogram or a centrally symmetric hexagon.

E. S. Fedorov [1] determined all five combinatorial types of convex 3-parallelohedra.

⋆ Supported by the RF goverment grant N 11.G34.31.0053 and the RFBR grant 11-01-00633-a.
⋆⋆ Supported by Grant-in Aid for Scientific Research (No. 23540098), JSPS.
⋆⋆⋆ Supported by Grant-in Aid for Scientific Research (No. 23540160), JSPS.

J. Akiyama, M. Kano, and T. Sakai (Eds.): TJJCCGG 2012, LNCS 8296, pp. 64–72, 2013.

Theorem 2. *([1]) There are five combinatorial types of convex parallelohedra in R^3: the cube, the right hexagonal prism, the rhombic dodecahedron, the elongated dodecahedron, and the truncated octahedron.*

A well-developed, algorithmical theory of a very important subclass of parallelohedra had been elaborated by G.Voronoi [4]. This subclass consists of those parallelohedra which can be represented as Dirichlet-Voronoi domains of points in a integer point lattice. Now such parallelohedra are called *Voronoi parallelohedra*. Not every parallelohedron is a Voronoi parallelohedron. So, for instance in a plane every 2-dimensional parallelohedron (syn. *parallelogon*) is either a parallelogram or a centrally symmetric hexagon. However, a parallelogon is a Voronoi 2-dimensional parallelohedron if and only if it is either a rectangle or a centrally symmetric hexagon inscribed into a circle.

Voronoi introduced a notion of a *primitive parallelohedron* as a parallelohedron to tile a space in such a way that each vertex belongs to the least possible number (for a given dimension d) of tiling cells, namely, $d+1$. In a space of dimension 2 or 3 there is the only combinatorial type of primitive parallelohedra (if $d=2$ it is the hexagon but not the parallelogram, if $d=3$, it is the truncated octahedron only). If $d=4$ or 5, there are 3 or 222 combinatorial types of primitive parallelohedra, respectively. Voronoi proved that *every primitive parallelohedron is affine equivalent to some Voronoi parallelohedron* and suggested a conjecture: *For any parallelohedron there exists an affine equivalent* (for brevity, *a-equivalent*) *Voronoi parallelohedron.* Regardless of serious efforts and significant progresses this centennial conjecture on the *existence* of the a-equivalent Voronoi parallelohedron still remains unsolved. Among recent results we select out so-called *uniqueness* theorems. In [5] it was proved that if a parallelohedron P is primitive, then an a-equivalent Voronoi parallelohedron P' is determined uniquely up to similarity. The uniqueness theorem was proved in [6] in a very elementary way for a wider class of parallelohedra, namely for those parallelohedra whose boundary after the removal of all standard faces (see [6] for definition) remains connected.

The uniqueness theorem easily implies a surprising fact. As already said, Voronoi developed a deep theory of Voronoi parallelohedra ([4]). According to this theory, all Voronoi parallelohedra of a given primitive combinatorial type correspond to lattices which fill a so-called *Voronoi type domain* in the cone of positive quadratic forms. If, instead a Voronoi tiling by primitive parallelohedra, one considers dual Delaunay tiling (in the primitive case by simplexes), in the interior of a given Voronoi type domain *all the Delaunay tilings* are pairwise affine equivalent. The surprising fact to follow from the uniqueness theorem is that *all Voronoi tilings are pairwise affine non-equivalent*, in contrast to the uniqueness of affine classes of Delaunay tilings within the domain.

In the case of d-dimensional primitive parallelohedra the dimension of each Voronoi type domain is equal to $\frac{d(d+1)}{2}$. Thus, from the uniqueness theorem ([5,6]) it follows that the dimension of the space of affine equivalence classes is equal to $d(d+1)/2-1$. So, if $d=2$, for example, in the primitive case (the centrally symmetrical hexagon) the dimension of the space of affine equivalence classes of a primitive parallelohedron is 2. If $d = 3$ the dimension of the space of affine equivalence classes with combinatorial type of the truncated octahedron is equal to 5.

We see that the affine classification of parallelohedra turns out a delicate question relevant to the Voronoi conjecture. In this paper, we classify convex parallelohedra in R^3 by the affine equivalence relation and realize their representatives in geometric formulation. In this way we will find the dimension of the space of affine equivalence classes of all 5 different combinatorial types of parallelohedra in 3-space (Theorems 4-6).

We study on centrally symmetric hexagons in Sect. 2 and truncated octahedrons in Sect. 3. The main theorems are showed in Sect. 3 for primitive parallelohedra and in Sect. 4 for non-primitive parallelohedra. The affine equivalent classes of parallelohedra with the combinatorial type of the truncated octahedron, are parameterized by a 5-tuple $(\alpha, \beta, h, \delta, l)$ which satisfies $0 < \alpha,\ 0 < \beta \leq (\pi - \alpha)/2, 0 \leq h, 0 < \pi - \gamma < \tan^{-1}(\sin(\alpha/2)/h), 0 < \pi - \delta < \tan^{-1}(\sin(\beta/2)/h)$, and the inequalities (4) and (5) given in the section 3 (Theorem 4). The affine classes of parallelohedra with the combinatorial type of the rhombic dodecahedron are parameterized by a 3-tuple $(\alpha,\ \beta, h)$ where $0 < \alpha, 0 < \beta \leq (\pi - \alpha)/2, 0 < h$ (Theorem 5).

2 Two-Dimensional Case

We start with parallelogons, i.e. 2-dimensional parallelohedra. There are two combinatorial types of parallelogons: the quadrangle and the hexagon. Moreover, since parallelohedra are centrally symmetric, a parallelogon is either a parallelogram or a centrally symmetrical hexagon.

All parallelograms are obviously pairwise a-equivalent, i.e. belonging to one affine class. The dimension of the space of affine classes of parallelograms is zero.

Now give a centrally symmetric (c.-s.) hexagon. A c.-s. hexagon is inscribed into an ellipse. By an appropriate affine map the ellipse is transformed on a unit circle. Let O be the center of the unit circum-circle of the hexagon transformed by the affine map, and let $A_1, A_2, A_3, A_4, A_5, A_6$ be vertices of the hexagon. A centrally symmetric hexagon has three pairs of central angles symmetric each other: $\widehat{A_1OA_2} = \widehat{A_4OA_5}$, $\widehat{A_2OA_3} = \widehat{A_5OA_6}$, and $\widehat{A_3OA_4} = \widehat{A_6OA_1}$. Let α, β, γ be the values of these angles. Without loss of generality we can and will consider only the following triples

$$0 < \alpha \leq \beta \leq \gamma, \text{ where } \alpha + \beta + \gamma = \pi. \tag{1}$$

Each triple α, β, γ with (1) determines a unique (up to congruence) a-equivalent c.-s. hexagon inscribed into a unit circle, and vice versa. On the other hand, two inscribed c.-s. hexagons with different triples satisfying (1) $(\alpha, \beta, \gamma) \neq (\alpha', \beta', \gamma')$ are *not* a-equivalent.

Theorem 3. *The configuration space of a-equivalence classes of centrally symmetric (c.-s.) hexagons has dimension 2 and can be parameterized by ordered triples* (α, β, γ) *provided* $0 < \alpha \leq \beta \leq \gamma$, $\alpha + \beta + \gamma = \pi$.

3 The Truncated Octahedron

For a given combinatorial type K of parallelohedra, we denote by $\mathcal{A}(K)$ the set of the affine equivalence classes of parallelohedra combinatorially equivalent to K.

For a given parallelohedron P and each $(d-2)$-face of P, there is a cycle of four or six $(d-1)$-faces by Theorem 1 (iii). We call this cycle a *belt* of P.

In the rest of this section, we consider P a parallelohedron with its combinatorial type of the truncated octahedron. So, P has six different belts. Each belt consists of six faces (two parallelograms and four centrally symmetric hexagons) and it has six parallel edges by Theorem 1 (iii).

Lemma 1. *Six centers of faces on a belt and the center of P are coplanar.*

Proof. Let the center of P be the origin O in R^3, and G_i be centers of six consecutive faces $F_i\,(1 \le i \le 6)$ of a belt of P. Since P is centrally symmetric, $\overrightarrow{OG_i} = -\overrightarrow{OG_{i+3}}$ for $1 \le i \le 3$. Since P is a parallelohedron, P tiles the space by its parallel copies in a face-to face manner. Let P_1 and P_2 be the copies of P obtained by the parallel translations along $2\overrightarrow{OG_1}$ and $2\overrightarrow{OG_2}$ respectively. Since P is primitive, the edge $F_1 \cap F_2$ belongs to exactly three parallel copies of P (including itself) in its tiling. So, P_2 is obtained by the parallel translation of P_1 along $2\overrightarrow{OG_3}$. Hence $\overrightarrow{OG_3} = \overrightarrow{OG_2} - \overrightarrow{OG_1}$. Therefore, $G_i\,(1 \le i \le 6)$ and the origin are coplanar.

Now we fix a belt of P, and define a reduced parallelohedron P_r of P corresponding to the belt, which is described in R^3 with the origin O as the center of P.

Step 1. We can assume all centers of the faces of the belt is on the xy-plane by Lemma 1 and the center of P is the origin. The orthogonal projection of P to the xy-plane is a centrally symmetric hexagon by Theorem 1 (iii).

Step 2. There is an affine transformation which satisfies the following conditions:
i) the c.-s. hexagon in the xy-plane is mapped to a c.-s. hexagon inscribed in the unit circle with center O in xy-plane, by Theorem 3, and
ii) the parallel six edges of the belt are mapped to edges with unit length, which are parallel to the z-axis.

We denote such transformation by $f_a = f_{a,\mathcal{B}}$ which depends on the belt $\mathcal{B}$. We call the image P_r of P by f_a a *reduced parallelohedron* of P. Now we show that P_r is uniquely determined by the following five parameters.

Definition of Parameters. Let $\pm F_1$ be two parallelograms and $\pm F_i\,(i = 2, 3)$ be four hexagons in the belt of P_r, where F_1, F_2 and F_3 are consecutive in order. Let α (resp. β) be $\angle A_1OA_2$ (resp. $\angle A_2OA_3$) where the line segment A_1A_2 (resp. A_2A_3) is the projection of F_1 (resp. F_2) to the xy-plane. We can assume $\beta \le (\pi - \alpha)/2$ by considering $-F_3$ instead of F_2 if necessary.

Let B_1, B_2, B_3, B_4, B_5 and B_6 be consecutive vertices of F_2, where the line segment B_1B_2 is the common edge of F_1 and F_2 and the z-coordinate of B_2 is greater than the one of B_1. Notice that we can assume the z-coordinate of the midpoint of the edge B_1B_2, denoted by h, satisfies $h \geq 0$, by considering $-F_1$ and $-F_2$ instead of F_1 and F_2 if necessary. Denote $\angle B_1B_2B_3$ and $\angle B_3B_4B_5$ by γ and δ respectively (see Fig. 2).

Let C_1 and C_2 be vertices of F_1 so that $F_1 = B_1B_2C_2C_1$. By $|A_1A_2| = 2\sin(\alpha/2)$, $\angle B_1B_2C_2 = \tan^{-1}(|A_1A_2|/2h) = \tan^{-1}(\sin(\alpha/2)/h)$, where $|XY|$ means the Euclidean distance of X, $Y \in R^3$. Since P is convex, $\triangle B_2B_3C_2$ is upper than the parallelogram $B_2C_2(-B_1)(-C_1)$, and so $\gamma > \pi - \tan^{-1}(\sin(\alpha/2)/h)$. Since F_2 is convex, $\gamma < \pi$. Hence

$$0 < \pi - \gamma < \tan^{-1}(\sin(\alpha/2)/h). \tag{2}$$

Since $\angle B_2B_4B_5 < \delta < \pi$ and $\angle B_2B_4B_5 = \pi - \tan^{-1}(\sin(\beta/2)/h)$, δ satisfies

$$0 < \pi - \delta < \tan^{-1}(\sin(\beta/2)/h). \tag{3}$$

For a point Q and a set S in R^3, we denote by $-Q$ the symmetric point of Q about the origin, and by $-S$ the set $\{-Q : Q \in S\}$. For three points P_1, P_2 and P_3 in R^3 which are not collinear, we denote by $\Pi(x, y, z;\, P_1, P_2, P_3) = 0$ the equation of the plane including those three points and by $\Pi(Q;\, P_1, P_2, P_3)$ the value $\Pi(q_x, q_y, q_z;\, P_1, P_2, P_3)$ for a point $Q = (q_x, q_y, q_z)$.

Since the plane including $\triangle B_2B_3C_2$ (resp. $\triangle(-B_1)(-B_6)(-C_1)$) does not intersect with the edge $(-B_1)(-B_6)$ (resp. $(B_2)(B_3)$),

$$\Pi(A_2;\, B_2, B_3, C_2) \cdot \Pi(-B_6;\, B_2, B_3, C_2) > 0 \tag{4}$$

and

$$\Pi(A_2;\, -B_1,\, -C_1,\, -B_6) \cdot \Pi(B_3;\, -B_1,\, -C_1,\, -B_6) > 0 \tag{5}$$

hold , where

(i) $A_1A_2 \cdots A_6$ is the hexagon centrally symmetric about the origin with vertices $A_1 = (\cos\alpha, \sin\alpha, 0)$, $A_2 = (1, 0, 0)$, $A_3 = (\cos\beta,\, -\sin\beta, 0)$,

(ii) $B_1B_2 \cdots B_6$ is the hexagon centrally symmetric about the midpoint of A_2A_3 with vertices $B_1 = (1, 0,\, -1/2 + h)$, $B_2 = (1, 0,\, 1/2 + h)$ and the point B_3 determined by $\angle B_1B_2B_3 = \gamma$ and $\angle B_3B_4B_5 = \delta$, and

(iii) C_1 and C_2 are the points symmetric to B_2 and B_1 respectively about the midpoint of A_1A_2 (see Figs. 1, 2 and 4).

We call such 5-tuple $(\alpha, \beta, h, \delta, l)$ a *parameterization of* P_r. We show that for each 5-tuple satisfying the above conditions, there exists a unique parallelohedron with the given parametrization and the combinatorial type of the truncated octahedron.

Theorem 4. *The affine equivalent classes $\mathcal{A}(K)$ of parallelohedra with the combinatorial type K of the truncated octahedron are parameterized by a 5-tuple $(\alpha, \beta, h, \delta, l)$ which satisfies the following:*

$$0 < \alpha,\ 0 < \beta \leq (\pi - \alpha)/2,\ 0 \leq h,$$

$$0 < \pi - \gamma < \tan^{-1}(\sin(\alpha/2)/h),$$
$$0 < \pi - \delta < \tan^{-1}(\sin(\beta/2)/h),$$

and the conditions (4) and (5).

Proof. Let $(\alpha, \beta, h, \delta, l)$ be a 5-tuple satisfying all conditions in the theorem.

Step 1. Take a c.-s. hexagon $A_1A_2\cdots A_6$ in R^3 satisfying the following conditions (1)-(4): (1) inscribed in the unit circle with the center of the origin O, (2) included in the xy-plane, (3) $\angle A_1OA_2 = \alpha$ and $\angle A_2OA_3 = \beta$, and (4) the point A_2 is in the positive x-axis (see the left figure in Fig. 1).

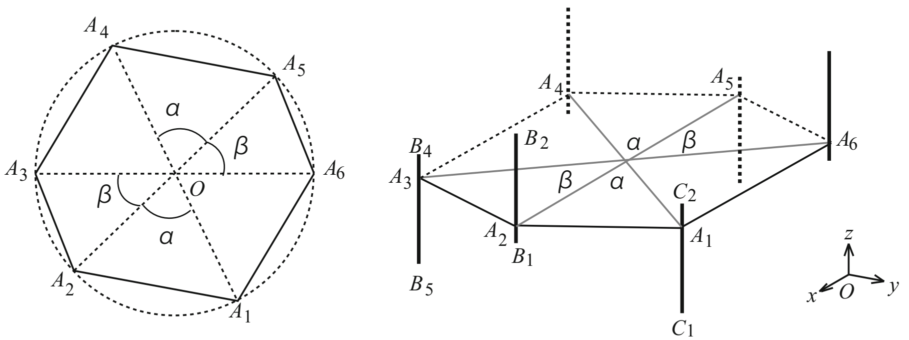

Fig. 1. Steps to obtain a truncated octahedron

Step 2. Let e_1 be the line segment with unit length included in the line passing through A_1, and orthogonal to the xy-plane, whose midpoint has the z-coordinate $-h$. Draw five edges $e_i\,(i = 2, \cdots, 6)$ with unit length parallel to e_1 such that e_{i+1} is symmetric to e_i about the midpoint of A_iA_{i+1} for each $i = 1, \cdots, 6$, where e_7 means e_1. Denote by $e_1 = C_1C_2$, $e_2 = B_1B_2$, and $e_3 = B_4B_5$, where the z-coordinate of B_2 (resp. B_4) is greater than the one of B_1 (resp. B_5) (see the right figure in Fig. 1).

Step 3. Let F_1 be the parallelogram $C_1C_2B_2B_1$ spanned by e_1 and e_2. Let F_2 be a c.-s. hexagon $B_1B_2\cdots B_6$ with angles $\angle B_1B_2B_3 = \gamma$ and $\angle B_3B_4B_5 = \delta$ (see Fig. 2).

Step 4. Let Π_1 be the plane including the edges B_2B_3 and B_2C_2 . Let Π_2 be the plane including the edges $(-C_1)(-B_1)$ of $-F_1$ and $(-B_1)(-B_6)$ of $-F_2$.

By the conditions (2) and (3), B_3 and $-B_6$ are higher than the plane including the parallelogram $B_2C_2(-B_1)(-C_1)$.

Since Π_1 and Π_2 include parallel lines B_2C_2 and $(-C_1)(-B_1)$ respectively, and cannot be parallel planes from the existence of B_3 (upper than B_2) and $-B_6$ (upper than $-B_1$), the two planes Π_1 and Π_2 intersect in a line (denoted by l) which is parallel to B_2C_2 and $(-C_1)(-B_1)$.

By the assumption (4), two points $-B_6$ and A_2 are in the same half-space divided by the equation $\Pi(x, y, z;\, B_2, B_3, C_2) = 0$. So, l does not intersect with the

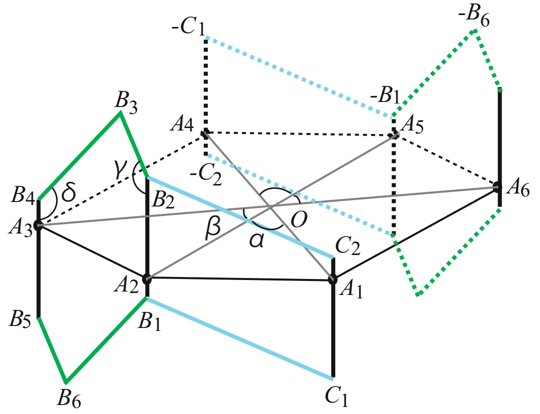

Fig. 2. Construction of four faces for the given parameters

edge $(-B_1)(-B_6)$, Similarly, by the assumption (5), $\Pi(A_2; -B_1, -C_1, -B_6) \cdot \Pi(B_3; -B_1, -C_1, -B_6) > 0$, the line l does not intersect with B_2B_3 (see the left figure in Fig. 3 which is the orthogonal projection to the xy-plane).

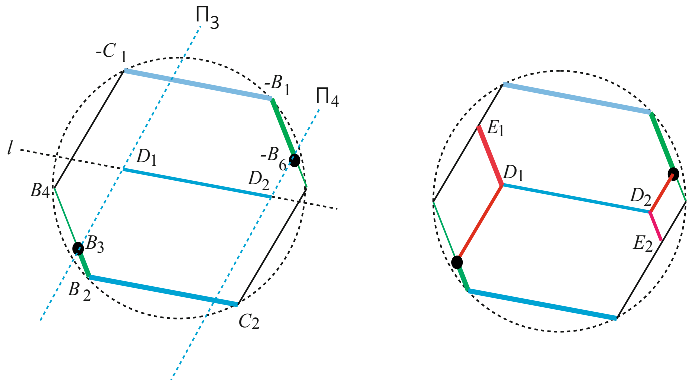

Fig. 3. The orthogonal projection to the xy-plane

Step 5. Let Π_3 (resp. Π_4) be the plane which is orthogonal to the xy-plane, parallel to A_3A_4, and which includes the point B_3 (resp. $-B_6$). Denote by D_1 (resp. D_2) the intersection point of the line l and Π_3 (resp. Π_4) (see the left figure in Fig. 3).

Step 6. Let E_1 (resp. E_2) be the point such that the line segment D_1E_1 (resp. D_2E_2) is parallel and congruent to the edge B_3B_4 (resp. B_2B_3) (see the right figure in Fig. 3). Now we obtain a belt (see the left figure in Fig. 4). By drawing

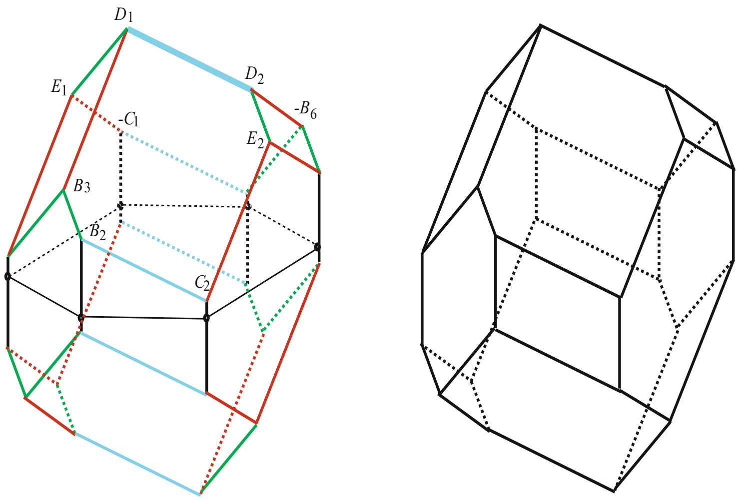

Fig. 4. Process to obtain a truncated octahedron

edges, we obtain the unique parallelohedron with its combinatorial type K of the truncated octahedron and the given parameters.

Remark. For each parallelohedron with its combinatorial type of the truncated octahedron, there are six belts. So, at most six different 5-tuples of parameters may correspond to a-equivalent parallelohedra in Theorem 4.

4 Non-primitive Parallelohedra

By applying the method used in the proof of Theorem 4, we get the following results.

Theorem 5. *The set of affine classes $\mathcal{A}(K)$ with the combinatorial type K of the rhombic dodecahedron are parameterized by a 3-tuple (α, β, h) where*

$$0 < \alpha, 0 < \beta \leq (\pi - \alpha)/2, 0 < h.$$

Proof. Since all faces of parallelohedra with the combinatorial type K of the rhombic dodecahedron are parallelograms, Step 3 in the proof of Theorem 4, we take a parallelogram $B_1B_2B_4B_5$ instead of the hexagon $B_1B_2 \cdots B_6$. Then we get a figure of the orthogonal projection to the xy-plane showed in Fig. 5. By drawing edges, we obtain the unique parallelohedron with combinatorial type K and the given parameters.

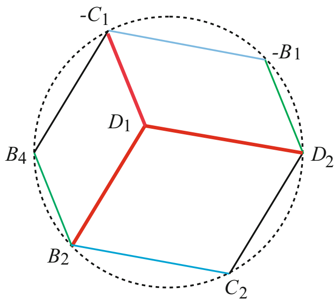

Fig. 5. The orthogonal projection of a parallelohedron with the combinatorial type of the rhombic dodecahedron to the xy-plane

Theorem 6. *The set of affine classes* $\mathcal{A}(K)$ *where* K *is the combinatorial type of the elongated dodecahedron is parameterized by a 4-tuple* (α, β, h, l) *where*

$$0 < \alpha,\, 0 < \beta \leq (\pi - \alpha)/2, 0 < h, 0 < l$$

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Proof. It is proved by Theorem 6.

Acknowledgement. The authors would like to express their thanks to the referee for his careful reading and valuable suggestions. Especially he pointed out the lack of conditions in a preliminary version of Theorem 4.

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