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On the real crystal octahedra

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A real crystal octahedron is defined as any polyhedron bounded, at least, by some of four pairs of parallel planes being in a standard crystallographic orientation with arbitrary distances between them. All the combinatorially non-equivalent shapes (30 in total) are found and characterized by 2-subordination symbols, automorphism group orders and symmetry point groups. The results are discussed with respect to the diamond crystal morphology.

1. Introduction

All facets of a crystal form are equally developed in an ideal crystal. But real morphology is known to be highly dependent on the conditions under which a crystal grows. An interesting thing we often see is decrease in area or even lack of some facets of a crystal form. To generalize, we define a real crystal form as any polyhedron bounded, at least, by some of the planes of a given ideal crystal form in a standard orientation with arbitrary distances from the origin of coordinates. In principle, all the real crystal forms related to a given ideal crystal form can be enumerated in a combinatorial approximation, *i.e.* with respect to the number and combination of different (3-, 4-, 5-, ..., n-gonal) facets. For example, a real crystal cube is nothing but the variety of rectangular parallelepipeds combinatorially equivalent to each other. As for the real crystal octahedron, it is not so trivial. This variety is generated and characterized in the paper.

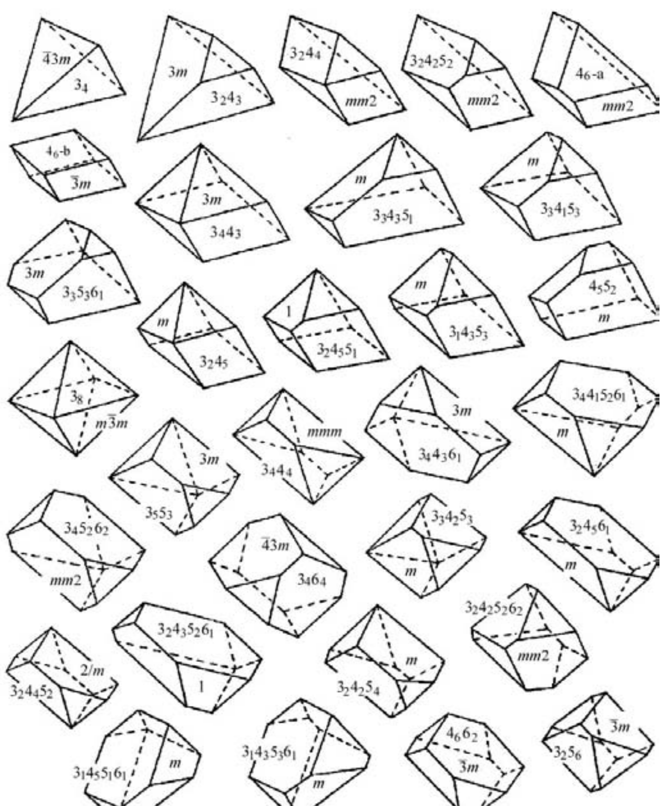

Figure 1
The real crystal octahedra. See text for the symbols.

2. Generation and characterization of polyhedra

In accordance with what was said above, we define a real crystal octahedron as any polyhedron bounded, at least, by some of four pairs of parallel planes in a standard crystallographic orientation with arbitrary distances between them. A generating algorithm consists of five steps:

1. We take a plane from each of four pairs to get the tetrahedron as the simplest 3D polyhedron.
2. The remaining four planes are in an equal orientation to the tetrahedron. Hence, we take any of them to cut it.
3. The remaining three planes are in an equal orientation to the intersected tetrahedron. So we take any of them to intersect the latter, thus obtaining three combinatorially different 6-hedra.
4. Because of the same reason, we take any of the two remaining planes to cut each of the 6-hedra, thus obtaining eight combinatorially different 7-hedra.
5. Finally, we cut each of the 7-hedra to get 17 combinatorially different 8-hedra.

Afterwards, we characterize the shapes by 2-subordination symbols and symmetry point groups. The 2-subordination symbols show the numbers of 3- to 6-gonal facets in a sequence. The symmetry point groups relate to the most symmetrical polyhedra of the same combinatorial types. This is justified by the known theorem: every combinatorial automorphism of a 3D polyhedron is affinely realizable. That is, there exists for a polyhedron of a given combinatorial type a metrical realization such that its symmetry point group is isomorphic to the automorphism group of its edge graph. The only restriction that should be emphasized once again is that the facets of the real crystal octahedra must be in a standard orientation to each other.

3. Results and discussion

The real crystal octahedra variety is found to consist of 30 combinatorially different shapes with one of them (4_6) having two affinely

Table 1
Simple and non-simple real crystal octahedra with different numbers (n) of facets.

n	Simple	Non-simple
4	3_4	–
5	3_24_3	–
6	$3_24_25_2$, 4_6	3_24_4
7	$3_35_36_1$, $3_14_35_3$, 4_55_2	3_44_3, $3_34_35_1$, $3_34_15_3$, 3_24_5, $3_14_55_1$
8	3_46_4, $3_24_25_26_2$,$3_14_35_36_1$, 4_66_2, 3_25_6	$3_44_15_26_1$, $3_44_36_1$, 3_44_4, 3_55_3, 3_8, $3_45_26_2$, $3_34_25_3$,$3_24_56_1$, $3_24_45_2$, $3_24_35_26_1$, $3_24_25_4$, $3_14_55_16_1$

Table 2
Automorphism group orders (a.g.o.), symmetry point groups (s.p.g.) and 2-subordination symbols of real crystal octahedra.

a.g.o.	s.p.g.	2-subordination symbols
1	1	$3_14_55_1$, $3_24_35_26_1$
2	m	$3_34_35_1$, $3_34_15_3$, 3_24_5, $3_14_35_3$, 4_55_2, $3_44_15_26_1$, $3_34_25_3$, $3_24_56_1$, $3_24_25_4$, $3_14_55_16_1$, $3_14_35_36_1$
4	$mm2$	3_24_4, $3_24_25_2$, 4_6-a, $3_45_26_2$, $3_24_25_26_2$
	$2/m$	$3_24_45_2$
6	$3m$	3_24_3, 3_44_3, $3_35_36_1$, 3_55_3, $3_44_36_1$
8	mmm	3_44_4
12	$\bar{3}m$	4_6-b, 4_66_2, 3_25_6
24	$\bar{4}3m$	3_4, 3_46_4
48	$m\bar{3}m$	3_8

non-equivalent variants. They are shown in Fig. 1. The statistics of simple (*i.e.* only 3 edges meet at each vertex) and non-simple shapes with different numbers of facets are given in Table 1 while their statistics of automorphism group orders and symmetry point groups are in Table 2. Let us consider two examples to explain the procedure of symmetry point-group determination.

1. Being considered as graphs, polyhedra 4_6-a and 4_6-b are combinatorially equivalent to the cube with automorphism group of order 48. But, taking into account the mutual orientations of facets, the maximum symmetry point groups that may be observed for polyhedra of such combinatorial types are $mm2$ and $\bar{3}m$, respectively.

2. Polyhedron 4_66_2 is combinatorially equivalent to a hexagonal prism with $6/mmm$ symmetry point group of order 24. But, taking into account the same reason, it has $\bar{3}m$ symmetry point group of order 12.

In general, the most interesting thing is that, with the exception of the 4_6 shape, each real crystal octahedron is uniquely defined by its 2-subordination symbol. As can also be seen, the real crystal octahedra belong to nine symmetry point groups, mostly to m, $mm2$ and $3m$. How does this fact relate to natural crystals? In crystal morphology, the symmetry of a crystal form is defined by the symmetry of the facet vectors and not by the symmetry of the crystal shape. But the latter can be interpreted in accordance with the Curie principle: only those symmetry elements remain in the morphology of a crystal that do not contradict the symmetry of the environment. The above results can thus be applied to crystals for which the octahedron is a common crystal form.

For example, according to Goldschmidt (1897, pp. 114–115), there are 15 crystal forms of diamond. According to Fersman (1955, pp. 48–49), there exist 29 such forms. But only eight of them are common and only three of the latter are initial. They are the cube, the octahedron and the rhombododecahedron. That is why Harris *et al.* (1975) distinguish between seven morphological types of plane-faced diamonds: cube, octahedron, rhombododecahedron, cube + octahedron, cube + rhombododecahedron, octahedron + rhombododecahedron and cube + octahedron + rhombododecahedron. Our general idea is to significantly extend this taxonomy by combinatorially different combinations of the real crystal cubes, octahedra and rhombododecahedra.

Besides, we have found 12 real crystal octahedra among a great number of diamonds published in Fersman & Goldschmidt (1911), Goldschmidt (1916), Fersman (1955), Kukharenko (1955), Shafranovsky (1964), Orlov (1973) and Afanasiev *et al.* (2000). These are shapes (Goldschmidt, 1916): 3_4 (Fig. 1), 3_24_3 (Figs. 2, 91), 3_8 (Figs. 4, 15, 106), 3_44_4 (Fig. 5), $3_14_35_36_1$ (Fig. 18), 3_46_4 (Fig. 19), 4_6-a (Fig. 93), $3_44_36_1$ (Fig. 135), 3_55_3 (Fig. 229); and (Orlov, 1973, Fig. 24): 4_66_2 (No. 2), $3_14_55_16_1$ (No. 5), $3_24_45_2$ (No. 6).

As follows from Table 2, they belong to all symmetry point groups with the exception of the trivial one. Therefore, in accordance with the Curie principle, we can assert a wide range of local growth conditions for natural diamonds. They can be interpreted in detail as discussed, for example, in Kirchmayer (1965, 1971).

4. Conclusions

All the combinatorially different real crystal octahedra (30 in total) are generated and characterized by 2-subordination symbols and symmetry point groups in the paper. With the exception of the 4_6 shape of two affinely non-equivalent types, the shapes can be uniquely defined by 2-subordination symbols. This fact makes their taxonomy easy. In total, the real crystal octahedra belong to nine symmetry point groups. At least 12 shapes belonging to eight symmetry point groups have previously been published. In accordance with the Curie principle, this fact bears testimony to a wide range of local growth conditions for natural diamonds. As the next step, it makes sense to find the real crystal rhombododecahedra and their combinations with the real crystal cube and octahedra.

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