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Complexity, sphericity, and ordering of regular and semiregular polyhedra

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Abstract. The five Platonic (regular) polyhedra may be ordered by various numerical indicators according to their complexity. By using the number of their vertices, the solid angle, and information theoretic indices one obtains a consistent ordering for the Platonic polyhedra. For the thirteen semiregular Archimedean polyhedra these criteria provide for the first time an ordering in terms of their complexity.

Introduction

Polyhedral hydrocarbons $(CH)_{2k}$ with k = 2, 4, and 10 are valence isomers of annulenes. Only three of the five Platonic polyhedra fulfill the condition of corresponding to cubic graphs, whose vertices of degree three can symbolize CH groups. Eaton's cubane (k = 4) is stable despite its steric strain, and its nitro-derivatives are highly energetic materials. Paquette's synthesis of dodecahedrane (k = 10) was a momentous achievement, equaled soon afterwards by a different synthesis due to Prinzbach. Tetrahedrane (k = 2) is unstable but Maier's tetra-*tert*-butyltetrahedrane is a stable compound. For details and some literature data, see ref.[1] Other chemically relevant references are collected in the final section of this article.

The complexity concept can be treated scientifically by listing the factors that influence it.[2-7] For graphs and other similar mathematical concepts, these factors include branching and cyclicity. The tetrahedron can be viewed as a three-dimensional geometrical polyhedron or as the K_4 graph (the complete graph with four vertices or the trivalent cage with girth 3). The order of the symmetry group of the tetrahedron graph is higher than that of the tetrahedron as a polyhedron. In the present study we shall discuss polyhedra as geometrical objects in the three-dimensional Euclidean space.

The five regular polyhedra have congruent faces that are regular polygons. When more than one type of regular polygons meets at a vertex, one obtains semiregular polyhedra. These are the 13 Archimedean polyhedra (two of which – the snub polyhedra – are chiral, leading in 3D space to enantiomeric solids), together with the infinity of regular prisms and antiprisms (having two parallel poly-*n*-gons connected by *n* squares or 2*n* triangles, respectively), and the few elongated square gyrobicupolas. All Platonic and Archimedean polyhedra are vertex transitive. Neither the two chiral Archimedean polyhedra, nor prisms, antiprisms, and gyrobicupolas will be considered in detail here.

Results

Several recent studies have been published on the complexity of regular polyhedra, either viewed graph-theoretically or geometrically.[8-11] Together with earlier studies on related topics,[12-15] these papers produced results that allow an ordering of the regular (Platonic) polyhedra according to various numerical criteria. We add to these criteria in the present study another one, termed "sphericity": how closely the polyhedra (viewed as geometrical objects) approach a sphere, again according to various quantitative measures. Just as radians measure angles as the ratio between the length of an arc and the radius of the circle centered at the meeting points of the two straight lines subtending that arc (1 radian = 57.296º), solid angles are measured in steradians defined as the ratio between the area of the sphere delimited by the planes meeting at the center of the sphere, and the square of the sphere radius. [A different definition, which will not be used here, does not consider how "pointed" is a vertex, but looks from the center of a unit sphere at the angle subtended by a surface's projection onto the sphere. Thus, the projection of a face of a cube centered at the origin is the whole area of the sphere divided by the number of cube faces, i. e. $4\pi/6 = 2.094$ steradians, and for a regular tetrahedron a similar calculation yields $4\pi/4 = \pi = 3.14$ steradians].[16]

Several intuitive measures of sphericity are provided by the solid angle (θ) (measured in steradians or in degrees), or by the ratios between the radius of an inscribed (r) or circumscribed sphere (R) and the length (L) of an edge of the regular polyhedron. The last two ratios (r/L and R/L) can be calculated without difficulty. For the solid angle, however, one must use formulas that can be proved with a small effort.[17]

Thus, for a solid angle formed by three incident edges defining three planar angles α_i (i = 1, 2, and 3) we have:

$$\cos(\theta/2) = [2 - \Sigma_i \sin^2(\alpha_i/2)] / 2\Pi_i \cos(\alpha_i/2)], \text{ or}$$

For the maximal solid angle formed by four incident lines of length L [defining four planar angles α_i (i = 1, 2, 3, and 4) with their endpoints resulting in a quadrilateral that is inscribable in a circle] we have:

$$\cos(\theta/2) = [2 - \Sigma_i \sin^2(\alpha_i/2) - 2\Pi_i \sin(\alpha_i/2)] / 2\Pi_i \cos(\alpha_i/2)].$$

When a incident edges belonging to poly-n-gons meet at a vertex forming equal planar angles α, the maximal solid angle may also be calculated from the formula:

$$\theta = 2\pi - 2a \arccos[\cos(\pi/a) / \cos(\alpha/2)] = 2\pi - 2a \arccos[\cos(\pi/a) / \sin(\pi/n)].$$

For the five Platonic polyhedra we may also use other relationships. Their solid angle θ may be computed with the aid of the dihedral angles, δ, which may be found from a related relationship.

$$\sin(\delta/2) = \cos(\pi/a) / \cos(\alpha/2) = \cos(\pi/a) / \sin(\pi/n)$$

$$\theta = a\delta - (a - 2)\pi$$

Finally, we denote by γ the angle between two lines emerging from the center of the polyhedron: one line connects it to a vertex, and the other line is normal to a face having this vertex.

We present in Table 1 the five Platonic polyhedra and the thirteen Archimedean semiregular polyhedra with a few characteristic details, including the number F of faces, V of vertices, and E of edges.[18] The truncated cuboctahedron is also called the great rhombicuboctahedron, and the truncated icosidodecahedron is also called the great rhombicosidodecahedron, and these last names are preferred, therefore their smaller namesakes are named with the “small” prefix. The symbol indicates the size and the number of regular polygons that are the faces of the polyhedron, e. g. polyhedron 16 (small rhombicosidodecahedron) with the symbol $3^{20}\ 4^{30}\ 5^{12}$ has 62 faces: 20 triangles, 30 quadrilaterals and 12 pentagons.

One may check that Euler' relationship is satisfied in all cases from Table 1:

$$V + F = E + 2$$

Further numerical characteristics of the five Platonic polyhedra and the thirteen Archimedean polyhedra are presented in Tables 2 and 3.

Ordering of Platonic and Archimedean polyhedra according to their complexity

The two pairs of dual regular polyhedra (cube and octahedron, dodecahedron and icosahedron) have the property that a member of the pair is converted into the other member by connecting centers of faces. For each pair of dual regular polyhedra, the number of edges is the same. Also the ratios of the inscribed and circumscribed spheres are equal for the two pairs of dual Platonic polyhedra. The names of the regular polyhedra are derived from the number of their faces, but it would be misleading to consider that this number orders Platonic polyhedra according to their complexity. One can see that the sphericity is not increasing with the number of faces, but with the number of vertices and with the other characteristics (sum of planar angles at a vertex, solid angle at each vertex, and the angle γ). The duals of semiregular polyhedra are Catalan polyhedra, and they will not be discussed here. One can note in Table 1 that there are also two pairs of Archimedean solids which share triplets of the numbers V, E, F: the truncated cube and the truncated octahedron form one such pair; the truncated dodecahedron and the truncated icosahedron form another pair.

In Table 1 one can also see the sum of planar angles at each vertex. On subtracting this sum from 360º = 2π steradians, one obtains the deficit of the solid angle. According to the theorem of Descartes, the sum of these deficits for all vertices equals 4π steradians.

The sum of planar angles has the same high degeneracy as the number of vertices. However, the number of edges has a lower degeneracy: it is not able to discriminate between the pairs of dual polyhedra and truncated analogs, but otherwise also this numerical indicator E orders the Platonic and Archimedean polyhedra according to their numbers of vertices, not their numbers of faces.

A highly discriminating and reliable measure of sphericity of polyhedra is the solid angle. It has no degeneracy among the 16 polyhedra from Table 1 that have values for their solid angle (we do not have these values for the two chiral snub polyhedra).The solid angle θ and the sum of planar angles at each vertex have a non-linear correlation (Fig. 1). If a linear correlation is attempted, the r^2 value is modest: $r^2 = 0.856$. Thus, Platonic and Archimedean polyhedra can be ordered according to their sphericity in a unique sequence based on the solid angle θ of their vertices. It will be observed from Table 1, which is ordered according to increasing numbers of edges, that the new ordering according to θ leads to an inversion between Archimedean polyhedra 13 and 14, and intercalates Archimedean polyhedra 6 and 7 between the Platonic polyhedra 3 and 4.

A plot of the number of edges in the Platonic and Archimedean polyhedra versus the solid angle is presented in Fig. 2. It will again be seen that this is nonlinear variation, which has an even smaller coefficient (one obtains $r^2 = 0.734$ for a linear correlation).

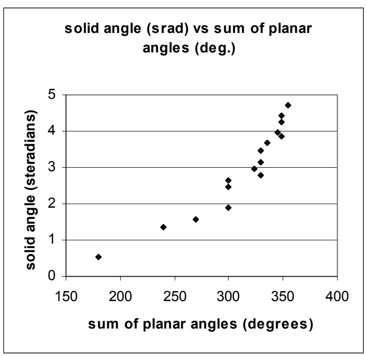

Fig. 1. Plot of the solid angle (steradians) versus the sum of planar angles for polyhedra.

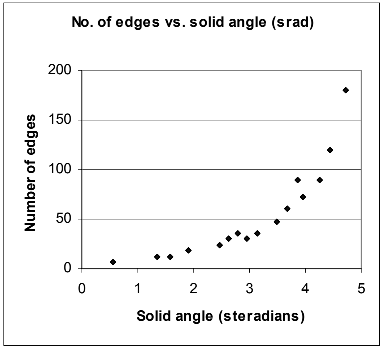

Fig. 2. Plot of the number of edges versus the solid angle at a vertex for polyhedra.

Both in Fig. 1 and Fig. 2 one can see that unlike the solid angle that has no degeneracy, the sum of planar angles and the number of edges have several degenerate values, as observed also in Table 1.

Three other geometric descriptors in Table 1 measure the relative sphericity within the 0 to 1 range as a ratio between one-, two-, and three-dimensional parameters of the polyhedron and the corresponding circumscribed sphere. The first of these measures, which might be called *radial* sphericity, is defined as the ratio of the radii of the inscribed and circumscribed sphere, r/R. While generally increasing with sphericity, this descriptor shows degenerate values for the two pairs of dual Platonic bodies. The ordering of the Archimedean polyhedra that this measure provides differs with four inversions from that based on the solid angle, with two of the inversions corresponding to polyhedra having the same number of edges. S*urface sphericity* ($A_{polyhedron}/A_{sphere}$) and *volume sphericity*, ($V_{polyhedron}/V_{sphere}$), in contrast, are nondegenerate and increase in a regular manner within the 0 to 1 range and follow very closely the ordering produced by the solid angle with a single inversion at polyhedra # 13 and # 14. All measures constructed classify the great rhombicosidodecahedron as the most spherical one, with the radial, surface, and volume sphericity values, equal to 0.983, 0.963, and 0.898, respectively.

The last column in Tables 2 and 3 shows the values of the polyhedra information content (I_{fd}). The latter is defined on the distribution of polyhedra vertices into the respective faces. More specifically, this is a distribution of polyhedra vertices into individual polygons into which the polyhedron is considered decomposed. For example, the cuboctahedron with eight triangular and six quadratic faces is characterized by the distribution of 48 (not 12!) vertices: I_{fd}(cuboctahedron) = 48lb48 – 8x3lb3-6x4lb4 = 182.0 bits, where lb stands for the logarithm at a base two for measuring information in binary units. The information sphericity measure induces an Archimedean polyhedra ordering very close to that produced by the solid angle. The single exception shows # 11 (snub cube) as more spherical than # 12 and 13 (icosidodecahedron and truncated cubooctahedron, respectively). For the Platonic bodies however, the ordering produced differs from the solid angle ordering and matches the one of Bonchev's 2-D complexity measures.

Discussion of the results

In a series of papers using resistance distances in graphs, Lukovits, Nikolić and Trinajstić have compared the ordering of the graphs corresponding to the five Platonic solids (or the ordering of their Schlegel diagrams), concluding that the number V of vertices provides the best natural order, in agreement with the resistance distance between all pairs of vertices (polyhedra 1<2<3<4<5). Three other criteria based on topological indices provide the same ordering: Wiener's index, Hosoya's Z-index and Randić's connectivity index. Other criteria have degenerate values for the two pairs of dual polyhedra (cube/octahedron and icosahedron/dodecahedron): the number of edges, of spanning trees, and Estrada's first-order edge-connectivity index.

Bonchev has discussed in much detail this ordering of the five Platonic polyhedra in the context of complexity, arriving at a different conclusion: except for the total walk count, many criteria investigated by Bonchev point out that the icosahedron (with the highest vertex degree) and not the dodecahedron appears to be the most complex, yielding the following ordering: 1<3<2<5<4.

Both of the above comparisons were made for the Platonic polyhedra viewed as graphs or as Schlegel diagrams. The present discussion, however, takes into consideration the geometry by basing the ordering of both Platonic and Archimedean polyhedra in a combined set on the solid angle of their vertices. One should note that these polyhedra are vertex transitive in the Euclidean three-dimensional space, except for the antipodes in the two pairs of enantiomeric snub Archimedean solids which are not superimposable (although their solid angles have the same value for each enantiomeric pair).

In conclusion, the solid angle of vertex-transitive regular and semiregular polyhedra viewed as geometrical objects can be used for ordering such polyhedra according to their sphericity, along with the newly introduced surface and volume sphericities, and the information sphericity index. For the five Platonic polyhedra, this geometrical ordering according to their sphericity agrees in some cases with the graph-theoretical ordering based on a few topological indices such as the Wiener, Randić, and Hosoya indices, but in many other cases the graph-theoretical ordering for complexity and the geometrical ordering for sphericity differ, as argued by Bonchev. Apparently, the ordering for Archimedean polyhedra according to their sphericity has not yet been discussed in the literature. This study demonstrates that the four sphericity measures mentioned above order in a similar way the thirteen Archimedean bodies from cubooctahedron and truncated tetrahedron to snub dodecahedron and large rhombicosidodecahedron.

Selected bibliography for "chemistry and Platonic and Archimedean polyhedra"

In addition to Platonic solids as valence isomers of annulenes mentioned in the introductory paragraph, inorganic compounds also have such structures. Only a few will be selected in what follows,[19] and then several chemical examples with Archimedean polyhedral structures will be presented.

Tetrahedron. The white allotropic form of phosphorus contains tetrahedral P_4 molecules, which persist in all three phases (solid, liquid, and vapor up to 800º C). Interestingly and counter-intuitively, its conversion into a cube-shaped P_8 molecule is disfavored both enthalpically and entropically. Arsenic and antimony also are known as As_4 and Sb_4 molecules. Polynuclear transition metal carbonyls with Co, Ir, Fe, Re tetrahedral clusters have been identified. Boron atoms in the chloride $(BCl)_4$ are connected tetrahedrally.

Cube. In addition to cubane, Si, Ge, and Sn analogues have been reported. Transition metals such as nickel connected to phosphines give rise to empty cubes and cooper to cube cages with a sulfur atom in the center and other external ligands. The nitrogenase enzymes contain two interpenetrating tetrahedra of iron and sulfur atoms (Fe_4S_4) arranged alternately at the corners of a cube. Many other such systems are known.

Octahedron. Octahedral cages and clusters exist in Rh and Co carbonyls, and many transition metal halides M_6X_8 or M_6X_{12} with M = Zr, Nb, Ta, Mo, QW and Re. Only a few boranes and carboranes have octahedral structures: $(BH)_6^{2-}$ and $B_4C_2H_6$.

Icosahedron. In contrast to octahedral molecules, icosahedral ones play a dominant role in boron chemistry, including the most common $(BH)_{12}^{2-}$ dianion and the three isomeric carboranes $B_{10}C_2H_{12}$. Viral proteins that form capsids (virus coats) form quaternary structures (supramolecular assemblies) with icosahedral structure, e. g. in human poliovirus.

Dodecahedron. This structure achieved in Paquette's and Prinzbach's spectacular syntheses of dodecahedrane is not common for inorganic compounds. However, in crystallography it appears as splendid crystals of pyrite.

Archimedean polyhedra. To start with organic compounds, an early review by Schultz was published in 1965, before dodecahedrane or buckminsterfullerene were synthesized, and listed several geometric characteristics of polyhedra and regular prisms, including the total angular strain per carbon atom, expressed in angle degrees.[20] A more recent review by Earley lists strain energies of polyhedranes $(CH)_{2k}$ with $k = 2, 3, 4, 5, 6, 8, 10$, and 12, expressed in kcal/mol per carbon atom, and cites relevant references. Strain energies per carbon atom (as angle and kcal/mol) are: for tetrahedrane $(CH)_4$, 254º, 35.4; cubane $(CH)_8$, 106º, 19.8; dodecahedrane $(CH)_{20}$, 9º, 2.2; and truncated octahedron $(CH)_{24}$, 77º, 8.6; strain energies are also given for the Si, Ge, and Sn analogues.[21]

Two enticing synthetic hydrocarbon targets are the valence isomers of $(CH)_{12}$ with angular strain 88º (with one more cyclopropane ring than the known diademane, which rearranges easily to the unsaturated triquinacene), and $(CH)_{24}$, having structures of a truncated tetrahedron and truncated octahedron, respectively, both with lower angular strain than cubane. By contrast, the truncated cube $(CH)_{24}$ has a slightly higher total angular strain, 110º because it has six octagons and eight triangles.

The most important chemical structure corresponding to an Archimedean polyhedron is buckminsterfullerene, C_{60}, whose structure corresponds to the truncated icosahedron. The 1996 Nobel Prize for Chemistry was awarded to Curl, Kroto, and Smalley for its discovery. In addition to graphite and diamond, fullerenes, nanotubes and nanocones – nanohorns constitute new carbon allotropes, and a wide area of research has been opened in an unsuspected vast field. The literature is too vast to cite, but relevant books and reviews are quoted in a recent book chapter.[22] We shall mention only two groups of contributors to this topic: Krätschmer and Huffman who prepared for the first time larger amounts of C_{60},[23] and Scott who designed a rational synthesis of C60.[24,25] Also, early speculations on C_{60} should be mentioned.[26-28]

A paper by Fowler and coworkers extends the notion of *d*-codes to polyhedra including all Platonic and Archimedean polyhedra, and discusses applications to fullerenes and carboranes.[29] Although not involving a regular or semiregular polyhedral structure, mention may be made of another paper by Fowler et al. which gives results of theoretical calculations for small hydrogenated fullerenes $C_{24}H_{2m}$:[30] the authors found that one $C_{24}H_{12}$ isomer with two parallel hexagons and all hydrogens attached to the carbons shared by three pentagons (but not by pentagons and hexagons) has an exceptional stability. This agrees with calculations on "pillow" partly hydrogenated fullerenes.[31]

Cuboctahedral boron structures have been found in several metal borides MB_{12} with M = Sc, Ni, Y, Zr, Hf, W.[19]

One paper of Coulombeau and Rassat, and two papers of Schleyer and coworkers should be mentioned: in the first one, vibrational frequencies are calculated for regular and semiregular polyhedral $(CH)_{2k}$ systems;[32] in the second one, nucleus-independent chemical shifts for such molecules are calculated,[33] and in the third various "sea-urchin" carborane structures are predicted, some of which have relevant polyhedral structures.[34]

Returning to organic compounds with the structure of regular polyhedra, this section will be concluded with bibliography on tetrahedral $(CH)_4$ derivatives,[35] cubane,[36] and "the Mount Everest of alicyclic chemistry" dodecahedrane.[37,38] Finally, a list of articles will be included on perhydro-buckminsterfullerene or buckminsterfullerane, and its perhalo-derivatives $(CX)_{60}$.[39-45]

Table 1. Data for Platonic and Archimedean polyhedra

No.	Platonic regular polyhedron	Symbol	Faces meeting at a vertex	V	E	F	Sum of planar angles (º)	Solid angle sterad
1	Tetrahedron	3^3	3 triangles	4	6	4	180	0.55
2	Octahedron	3^4	4 triangles	6	12	8	240	1.36
3	Cube	4^3	3 squares	8	12	6	270	1.57
4	Icosahedron	3^5	5 triangles	12	30	20	300	2.63
5	Dodecahedron	5^3	3 pentagons	20	30	12	324	2.96

No.	Archimedean semiregular polyhedron	Symbol	Faces meeting at a vertex	V	E	F	Sum of planar angles (º)	Solid angle sterad
6	Truncated tetrahedron	$3^4\,6^4$	2 hexagons + 1 triangle	12	18	8	300	1.91
7	Cuboctahedron	$3^8\,4^6$	2 squares + 2 triangles	12	24	14	300	2.47
8	Truncated cube	$3^8\,8^6$	2 octagons + 1 triangle	24	36	14	330	2.80
9	Truncated octahedron	$4^6\,6^8$	1 square + 2 hexagons	24	36	14	330	3.14
10	Small rhombicuboctahedron	$3^8\,4^{18}$	1 triangle + 3 squares	24	48	26	330	3.48
11	Snub cube*	$3^{32}\,4^6$	4 triangles + 1 square	24	60	38	330	
12	Icosidodecahedron	$3^{20}\,5^{12}$	2 triangles + 2 pentagons	30	60	32	336	3.67
13	Great rhombicuboctahedron	$4^{12}\,6^8\,8^6$	1 square + 1 hexagon + 1 octagon	48	72	26	345	3.95
14	Truncated dodecahedron	$3^{20}\,10^{12}$	1 triangle + 2 decagons	60	90	32	348	3.87
15	Truncated icosahedron	$5^{12}\,6^{20}$	1 pentagon + 2 hexagons	60	90	32	348	4.25
16	Small rhombicosidodecahedron	$3^{20}\,4^{30}\,5^{12}$	1 triangle + 2 squares + 1 pentagon	60	120	62	348	4.44
17	Snub dodecahedron*	$3^{80}\,5^{12}$	4 triangles + 1 pentagon	60	150	92	348	
18	Great rhombicosidodecahedron	$4^{30}\,6^{20}\,10^{12}$	1 square + 1 hexagon + 1 decagon	120	180	62	354	4.71

* Chiral polyhedron

Table 2. Platonic polyhedra and some of their numerical characteristics

No.	Polyhedron	r/L	R/L	r/R	δ (º)	sinγ	γ (º)	A_p/A_s	V_p/V_s	I_{fd}
1	Tetrahedron	1/2√6	√2/2√2	1/3 = 0.333	70.5	1√3	35.3	0.368	0.122	24.0
2	Octahedron	1/√6	1/√2	1/√3 = 0.577	109.5	1/√2	45.0	0.551	0/318	72.0
3	Cube	1/2	√3/2	1/√3 = 0.577	90.0	√(2/3)	54.6	0.637	0.368	62.0
4	Icosahedron	(3+√5)/4√3	√[(5+√5)/8]	$(10+2/\sqrt{5})^{3/2}/40\sqrt{3}$ = 0.795	138.2	√[(1+√5)/2√5]	58.3	0.762	0.605	259.3
5	Dodecahedron	√[(11+5√5)/8√5]	√3(√5+1)/4	$(10+2/\sqrt{5})^{3/2}/40\sqrt{3}$ = 0.795	116.5	(1+√5)/2√3	69.1	0.837	0.665	215.1

Table 3. Archimedean polyhedra and some of their numerical characteristics

No.	Polyhedron	δ (º)	R/L	r/L	r/R	A_p/A_s	V_p/V_s	I_{fd}
6	Truncated tetrahedron	70.5; 109.5	1.173	0.959	0.818	0.702	0.401	105.1
7	Cuboctahedron	125.3	1.000	0.750	0.750	0.753	0.563	182.0
8	Truncated cube	90; 125.3	1.779	1.638	0.921	0.816	0.577	262.2
9	Truncated octahedron	109.5; 125.3	1.581	1.423	0.900	0.853	0.683	272.2
10	Small rhombicuboctahedron		1.399	1.220	0.872	0.873	0.760	450.1
11	Snub cube[a]	135.0	1.343	1.158	0.862	0.875	0.776	628.7
12	Icosidodecahedron	142.6	1.618	1.464	0.905	0.891	0.780	594.4
13	Great rhombicuboctahedron		2.318	2.210	0.953	0.920	0.802	608.4
14	Truncated dodecahedron	116.5; 142.6	2.969	2.885	0.972	0.912	0.775	854.8
15	Truncated icosahedron	138.2; 142.6	2.478	2.377	0.959	0.941	0.867	899.0
16	Small rhombicosidodecahedron		2.233	2.121	0.950	0.947[b]	0.892	1423.2
17	Snub dodecahedron[a]		2.156	2.040	0.946	0.947[b]	0.896	1948.9
18	Great rhombicosidodecahedron		3.802	3.737	0.983	0.963	0.898	2108.2

[a] Chiral polyhedron

[b] These two values are not degenerate: Ap/As(#16) = 0.94655 ; Ap/As(#17) = 0.94666.

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