The minimal non-fullerene Voronoi polyhedra

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Abstract

When placing n points uniformly on a sphere their associated Voronoi regions define a polyhedron that is for most n a fullerene. In this paper the exceptional minimal non-fullerene polyhedra are discussed.

In this paper we study uniform distributions of points on a unit sphere. To each distribution of n points with unit vectors $\mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_n\}$ on a unit sphere we may associate an energy function

$$E(\mathbf{R}) = \sum_{i<j} \frac{1}{d_{i,j}^2}, \qquad (1)$$

where $d_{i,j} = |\mathbf{r}_i - \mathbf{r}_j|$ is the usual Euclidean distance in 3D space. Distributions with minimal energy are sought. Since finding a global minimum is difficult we used an approximate numerical method. It is based on the standard gradient method [3] combined with the random walk method [15] in order to escape from a local minimum. Thus we use a sort of simulated annealing method.

To each point distribution we may associate a *Voronoi diagram* in the following way: The sphere is cut into n regions, each region f_i being associated with a point $\mathbf{r}_i$. The region f_i contains those points on the sphere that are closer to i than to any other point of the distribution $\mathbf{R}$. The collection of all regions obtained in this way defines the Voronoi diagram $V(\mathbf{R})$ on the sphere. Until now Voronoi diagrams have been usually studied in the plane or in the space. The reader is referred to [13] for further reading.

The Voronoi diagram $V(\mathbf{R})$ is therefore a graph embedded in the sphere. The boundary between two regions f_i anf f_j is a segment of the great circle of a unit sphere perpendicular to and bisecting the one connecting the points $\mathbf{r}_i$ and $\mathbf{r}_j$. Let e denote the number of such segments. These segments are the edges of the Voronoi diagram. There is only a finite number v of points in the sphere where more than two regions meet. These points are the vertices of the Voronoi diagram. The Voronoi diagram has thus v vertices, e edges and n regions (faces). By the Euler polyhedral formula we have

$$v - e + n = 2. \tag{2}$$

Note that Voronoi diagrams can be considered as *topological polyhedra* with *curved* faces.

As in the case of the Voronoi diagrams in the plane the most common situation arises when all of its vertices are trivalent although cases with higher valencies could occur. In the latter case a perturbation of a single point in $\mathbf{R}$ may remove some higher valencies and thus results in a different Voronoi diagram. This means that the higher valencies are "topologically unstable". In the trivalent Voronoi diagram the Euler formula combined with the handshaking lemma $2e = 3v$ gives the following identities:

$$\begin{aligned} v &= 2n - 4, \\ e &= 3n - 6. \end{aligned} \tag{3}$$

The problem of a uniform placing of n points on a unit sphere can now be rephrased in terms of polyhedra. The minimal energy point distribution $\mathbf{R}$ defines the *minimal Voronoi diagram* and thus the *minimal n-face polyhedron.*

In the further text V_n denotes a Voronoi polyhedron with n faces having the minimal energy.

If for a given n a single minimum exists and if the corresponding polyhedron is trivalent we may expect that the numerical calculation will yield a stable solution that will correctly describe the topological type of the polyhedron. This reasoning can be partially reversed. If numerical experiments give always the Voronoi diagrams of the same topological type, we may conclude that the likelihood of this solution of being the correct minimum is high.

Our preliminary experiments indicate an interesting fact that minimal Voronoi polyhedra are indeed trivalent (with a single exception found). Even more, almost all of them are topologically equivallent to fullerenes, i.e. trivalent polyhedra whose faces consist of hexagons and exactly 12 pentagons. We observed only a small number of exceptions. Since no fullerenes with $v = 2, 4, 6, 8, 10, 12, 14, 16, 18, 22$ vertices exist, it is clear that the minimal Voronoi polyhedra will be non-fullerene for $n = 3, 4, 5, 6, 7, 8, 9, 10, 11, 13$. Our experiments indicate that even in the cases of higher n where fullerenes exist we found two cases: $v = 32$ and $v = 38$, for which the minimal Voronoi polyhedra are non-fullerene.

Although the complete results on fullerenes obtained with our experiments will appear elsewhere [12], for the sake of completeness we identify the remaining minimal Voronoi polyhedra up to $n = 22$ as the fullerenes: $V_{12} = 20 : 1, V_{14} = 24 : 1, V_{15} = 26 : 1, V_{16} = 28 : 2, V_{17} = 30 : 1, V_{19} = 34 : 5, V_{20} = 36 : 13$, and $V_{22} = 40 : 40$, where notation is the same as in Atlas Tables A.1.- A.4. of reference [6].

Conjecture 1 *Only a finite number of the minimal non-fullerene Voronoi polyhedra exists.*

Here we present the minimal energies and drawings of the above exceptions together with their structure of faces. The results are collected in Table 1. Beside the minimal energies we present there also their normalized values. The *average* (per pair of particles) *energy* $\overline{E}$ is defined as:

$$\overline{E} = \frac{E}{\binom{n}{2}} \tag{4}$$

Table 1. *The list of the minimal non-fullerene Voronoi polyhedra V_n with n faces and v vertices. The numbers n_2, n_3, n_4, n_5 and n_6 denote the numbers of*

2-,3-,4-,5- and 6-gons, respectively. In the next two columns the corresponding minimal (E) (1) and average ($\overline{E}$) (4) energies on the unit sphere are given.

n	v	n_2	n_3	n_4	n_5	n_6	Energy	$\overline{E}$
3	2	3					1.00000000	0.333
4	4		4				2.25000000	0.375
5	6		2	3			4.25000000	0.425
6	8			6			6.75000000	0.450
7	10			5	2		10.25000000	0.488
8	12			8			14.33679108	0.512
9	14			3	6		19.25286878	0.535
10	16			2	8		25.04135972	0.556
11	18			2	8	1	31.83472164	0.579
13	22			1	10	2	47.77330898	0.612
18	32			2	8	8	104.31468528	0.682
21	38			1	10	10	150.32512274	0.716

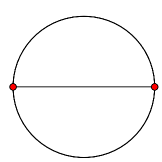
We can observe that the values of the average energy ($\overline{E}$) follow approximately the $\sqrt{n}$ rule. Indeed, the least square fitting has given the approximation:

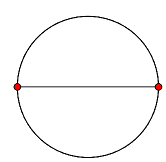
$$\overline{E} = 0.1275n^{0.5116} + 0.1313$$

Therefore, the maximal energy E behaves approximately as $n^{5/2}$ what can be estimated from simple physical arguments as well.

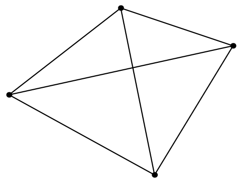
The drawings of the minimal non-fullerene Voronoi polyhedra together with their Schlegel diagrams[11] are given in Figure 1.

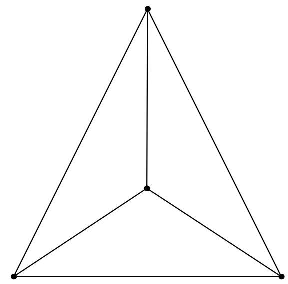
Figure 1. *The drawings of the minimal non-fullerene Voronoi polyhedra together with their Schlegel diagrams.*



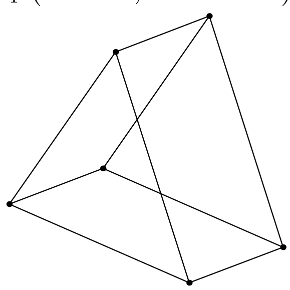


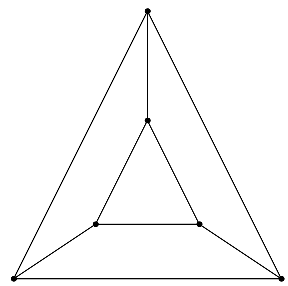
V_3 (3 faces, 2 vertices)



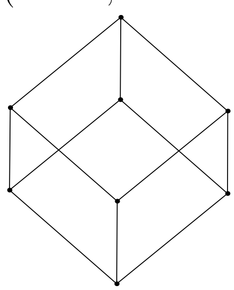


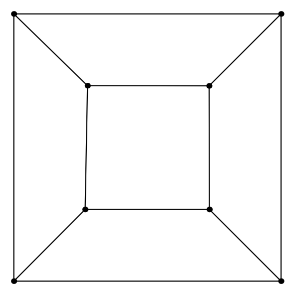
V_4 (4 faces, 4 vertices)



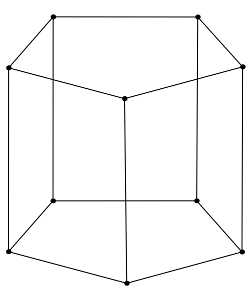


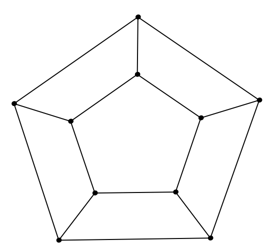
V_5 (5 faces, 6 vertices)



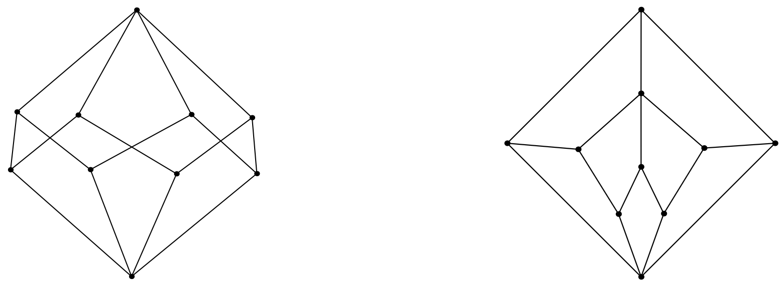


V_6 (6 faces, 8 vertices)

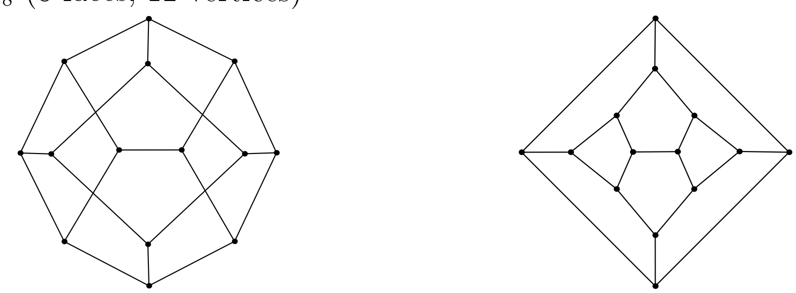




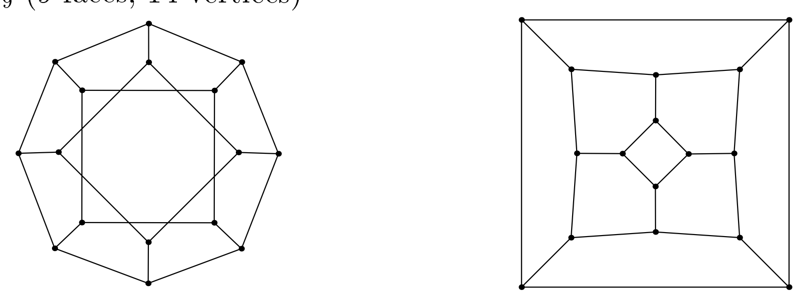
V_7 (7 faces, 10 vertices)



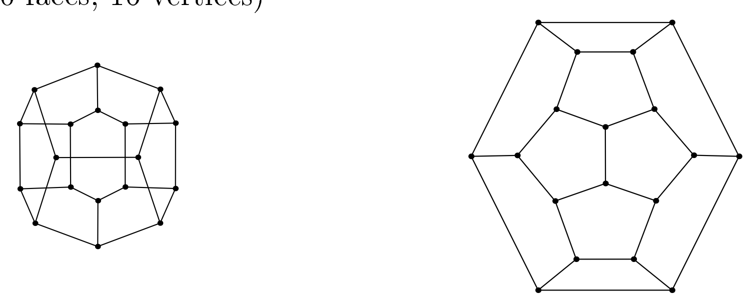
V_8 (8 faces, 12 vertices)



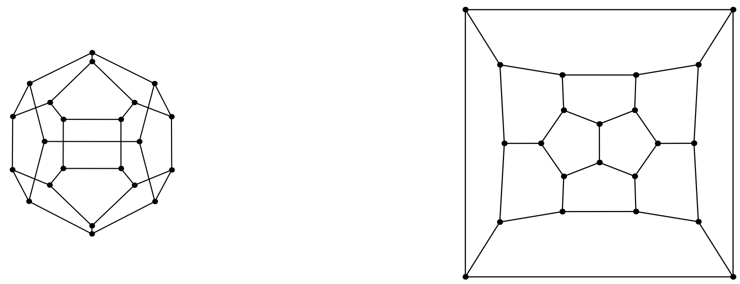
V_9 (9 faces, 14 vertices)



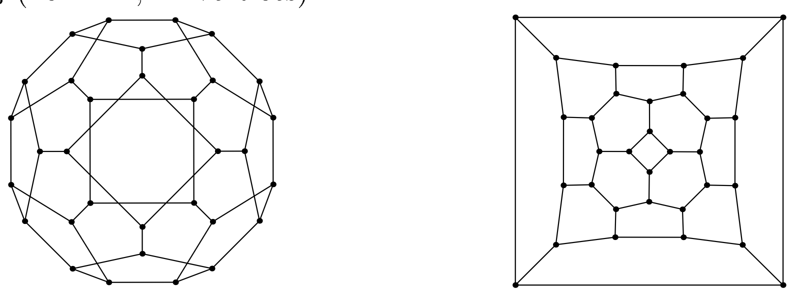
V_{10} (10 faces, 16 vertices)



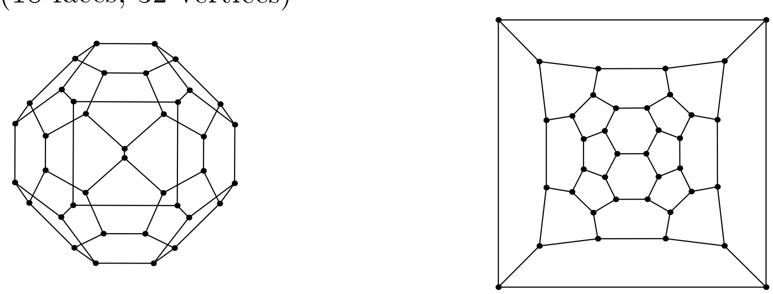
V_{11} (11 faces, 18 vertices)



V_{13} (13 faces, 22 vertices)



V_{18} (18 faces, 32 vertices)



V_{21} (21 faces, 38 vertices)

From the above drawings the following properties of the above minimal polyhedra are deduced.

- V_3 is the well-known Θ-graph. It has two vertices on the poles and three parallel edges as meridians.
- V_4 is the complete graph K_4 on the sphere as the regular tetrahedron.
- V_5 is the trigonal prism. Its graph is the Cartesian product $K_2 \times C_3$.
- V_6 is the cube $K_2 \times K_2 \times K_2$.

- V_7 is the pentagonal prism $K_2 \times C_5$
- The next graph, V_8 is the only non-trivalent graph among *all* minimal polyhedra. It can be obtained from a bichromatic cycle C_8 by adding two vertices b and w and 8 edges in such a way that 4 white vertices of C_8 are joined to w and all black vertices of C_8 are joined to b.
- V_9 has a pronounced pair of antipodal vertices surrounded by three pentagons, defining a 3-fold axis of rotation.
- V_{10} is a generalized Petersen graph $GP(8, 2)$. It can be also obtained from V_8 by truncating both of its four-valent vertices.
- V_{11} is showing a lower symmetry than the previous polyhedra.
- V_{13} is the largest in the series of non-fullerenes "by mathematical argument". Namely, for $n = 2, 3, ..., 11$ the fullerenes are ruled out since the smallest fullerene is the dodecahedron which happens to be V_{12}. Since fullerenes on v vertices exist for $v = 20 + 2k, k \geq 0, k \neq 1$, see for instance [9], a fullerene on 22 vertices does not exist hence V_{13} cannot be a fullerene.
- V_{18} has two opposite twisted quadrilaterals whose centers define a 4-fold alternating axis of improper rotation. This property is also valid for V_{10}. Note that V_{18} is of lower energy as defined in (1) than all 6 non-isomorphic fullerenes on 32 vertices[6].
- There are 17 non-isomorphic fullerenes on 38 vertices[6]. It turns out that a non-fullerene V_{21} is obtained when minimizing the function (1). This and the previous polyhedron are the only known polyhedra where non-fullerenes "beat" fullerenes of the same size. V_{21} has a distinguished edge whose midpoint is fixed by each of the symmetries of the polyhedron. The distinguished edge lies on the border of two pentagons, and each of its endpoints is surounded by three pentagons. This property can also be found in other two cases V_{11} and V_{13} with the same point group C_{2v}. Note that the face opposite to the distinguished edge is a quadrilateral in V_{18} and V_{21} but is a hexagon in V_{11}.

The above polyhedra could be characterized by their point groups and related graphs by their automorphisms groups. The connection between geometrical symmetry and graph automorphisms is an involved problem, but the first results appeared recently[7, 10, 2]. In the Table 2 the point groups and the orders $|Aut(V_n)|$ of the automorphisms groups of the minimal non-fullerene Voronoi polyhedra V_n are given. Further, the numbers of vertex, edge and face orbits of the automorphisms groups $Aut(V_n)$ are given. Let us recall, that a vertex orbit of $Aut(G)$ of a graph G is the subset of vertices of G which is invariant under the action of $Aut(G)$. In an analogous way the edge and face orbits are defined.

Table 2. *The orders $|Aut(V_n)|$ of the automorphism groups, numbers of vertex, edge and face orbits, and point groups of the minimal non-fullerene Voronoi polyhedra V_n with n faces and v vertices.*

n	v	$\|Aut(V_n)\|$	vertex orbits	edge orbits	face orbits	Point group
3	2	12	1	1	1	D_{3d}
4	4	24	1	1	1	T_d
5	6	12	1	2	2	D_{3d}
6	8	48	1	1	1	O_h
7	10	20	1	2	2	D_{5d}
8	12	16	2	2	1	S_4
9	14	12	3	3	2	D_{3h}
10	16	16	2	3	2	S_4
11	18	4	6	9	5	C_{2v}
13	22	4	7	11	6	C_{2v}
18	32	16	3	5	3	S_4
21	38	4	10	18	9	C_{2v}

Although the problem of finding the minimal configuration of points on a unit sphere is as old as the Thompson model of the atom, and since then has been studied in such diverse fields as stereochemistry, botany, virology, information theory, office assignment problem, etc. [4, 14, 8, 5, 1], resulting in large number of papers, here we focused for the first time attention to a situation in which the points are associated with the faces of the polyhedra.

As our computer experiments indicate that fullerenes minimize the energy function (1) in almost all cases, we restricted our attention here to the 12 known exceptions to this finding. The smallest 10 exceptions arise from the mathematical arguments of non-existence of corresponding fullerenes. The last two exceptions, although not being prohibited by mathematical arguments to be fullerenes, turned out to be non-fullerenes.

All V_n except V_8 are trivalent polyhedra. It is easy to see that trivalent polyhedra are maintaining their topological properties even when the minimal configuration of points are slightly distorted due to numerical errors. No V_n contains a face of size larger than 6. For $n \geq 6$ only quadrilaterals, pentagons and hexagons are candidates for the faces.

It would be interesting to know topological properties of the minimal polyhedra in advance, without actually computing them, at least for some cases. It would be also interesting to know which topological properties remain invariant under numerical errors, type of surface on which the points are placed, etc. Especially, it would be interesting to study the influence of the choice of the energy function. For instance, instead of the $1/r^2$ potential, a more usual Coulomb $1/r$ potential or even more general function $1/r^\alpha$ can be considered. The work on these questions is in the progress.

Finally, the most important question that we address in a follow-up paper [12] is the systematic study of larger minimal polyhedra V_n, their relation to fullerenes and especially to those experimentally detected up to now in chemical laboratories.

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