# Isoperimetric Quotient for Fullerenes and Other Polyhedral Cages

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The notion of Isoperimetric Quotient (IQ) of a polyhedron has been already introduced by Polya. It is a measure that tells us how spherical is a given polyhedron. If we are given a polyhedral graph it can be drawn in a variety of ways in 3D space. As the coordinates of vertices belonging to the same face may not be coplanar the usual definition of IQ fails. Therefore, a method based on a proper triangulation (obtained from omni-capping) is developed that enables one to extend the definition of IQ and compute it for any 3D drawing. The IQs of fullerenes and other polyhedral cages are computed and compared for their NiceGraph and standard Laplacian 3D drawings. It is shown that the drawings with the maximal IQ values reproduce well the molecular mechanics geometries in the case of fullerenes and exact geometries for Platonic and Archimedean polyhedra.

## INTRODUCTION

Fullerenes, carbon nanotubes, and other polyhedral cages have become a subject of intensive research (see, e.g. ref 1). As in the case of fullerenes the number of possible isomers of such pure carbon cages is roughly some constant times $n^9$, where $n$ is the number of carbon atoms, as shown by W. P. Thurston in his unpublished work;[2] it is highly desirable, after generating (all of) them[3] to sort out the most stable ones. A series of rules has been developed to do such a sorting with the IP (isolated-pentagon) rule[4,5] having a prominent role. By applying the IP and supplementary rules to fullerenes, one is still faced with a huge number of their feasible isomers. In passing we note that an efficient algorithm exists for generating topologies of fullerenes and other trivalent polyhedral cages with prescribed properties.[6]

The stability of a fullerene depends both on the strain of its $\sigma$ skeleton and on the delocalization of its $\pi$-electron network. An interesting theoretical approach to the strain of polyhedral cages can be found in refs 7 and 8. In this paper we deal only with the strain in fullerenes and similar polyhedra, and we propose a new index which is based on the *isoperimetric quotient* (IQ)[9,10] as a measure of the strain in these cages. An initial study of the stability of fullerenes and other polyhedral cages versus IQ is performed in this paper.

## IQ OF SPHEROIDAL OBJECTS

The sphere is an object in which the strain is mostly uniformly distributed. The ratio of the square of its volume, $V^2 = ((4\pi r^3)/3)^2$, and the cube of its surface area, $S^3 = (4\pi r^2)^3$, where $r$ is the radius of the sphere, is a dimensionless quantity which equals $^1/_{36\pi}$. The normalized counterpart of this ratio for a general spheroidal geometrical object M

$$\mathrm{IQ}(M) = 36\pi\frac{V^2}{S^3} \qquad (1)$$

we call *the isoperimetric quotient* of $M$. Obviously, as a sphere has a minimal surface area for a given volume, IQ of an arbitrary spheroidal object obeys the following property

$$0 \le \mathrm{IQ}(M) \le 1 \qquad (2)$$

where the right equality holds only for a sphere see (refs 9 and 10), while the left equality holds only for the degenerate case with $V = 0$.

## CALCULATION OF (3D) GEOMETRIES OF POLYHEDRAL CAGES

Once the connectivity of atoms in a carbon cage is known, the geometry of the cage could be computed in a variety of ways ranging from simplified ones to sophisticated *ab initio* calculations.

Here, the geometries of fullerenes and other polyhedral cages are calculated by two simple graph drawing algorithms. The first one is based on the Fruchterman and Reingold spring-embedding model[11] and is known as the *NiceGraph* algorithm; see refs 12−15. There are several spring-embedders described in the literature. A pioneering example can be found in ref 16. For further references in this field the reader should consult recent publications of D. Harel and co-workers.[17−19] The second one is based on selected triplets of the adjacency or the Laplacian matrix eigenvectors.

Let us explain the method that uses the Laplacian matrix of a molecular graph. Let $G$ be a graph with the vertices labeled by 1, 2, ..., $n$. As usual, let $A(G) = (a_{u,v})$ denote the symmetric adjacency matrix of $G$. The Laplacian matrix $Q(G)$ of $G$ is defined to be $Q(G) = D(G) - A(G)$, where D(G) is the diagonal matrix containing the valencies of vertices of $G$ as the corresponding diagonal elements. In the case of regular graphs, the method for drawing graphs with a Laplacian matrix does not differ from the one that uses an adjacency matrix. For general graphs the Laplacian method gives better results than an adjacency matrix since

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it takes different valencies into consideration explicitly. In the case of heteroatomic molecules one should explore the possibility of assigning different weights to edges and thus exploit the strategy first developed in ref 20.

Let $0 = \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$ be the sequence of eigenvalues of $Q(G)$ and let $\tau_1$, ..., $\tau_n$ be the sequence of the corresponding eigenvectors. Of course, the eigenvectors corresponding to different eigenvalues are pairwise orthogonal. In the case of eigenvectors corresponding to an eigenvalue of higher multiplicity, the eigenvectors could be orthogonalized, e.g., by using the well-known Gram-Schmidt orthogonalization procedure. Let us select a triplet of eigenvectors, $\tau_i$, $\tau_j$, and $\tau_k$, and define the vertex coordinates $(\tau_i(v), \tau_j(v), \tau_k(v))$ of vertex $v$. In the case of regular graphs, the eigenvector $\tau_1$ is given by $\tau_1 = (1, 1, ..., 1)^t$ and is of little use as source of the first coordinates, since the drawing is then necessarily in the plane $x = 1$, spanned by the other two coordinates. In the papers in refs 20−22 the argument favors small values of indices. That is why we define $i = 2, j = 3, k = 4$ as the *standard triple* and the coordinates defined by $(\tau_2, \tau_3, \tau_4)$ we call the *standard Laplacian drawing* of a graph. In a similar way we define *standard adjacency drawing,* etc.

Note that the standard Laplacian drawing of a graph is determined solely by the pure connectivity properties of the graph itself. It is thus of interest to investigate standard Laplacian drawings of various families of graphs, especially of graphs that are of interest in chemistry-like fullerenes or other polyhedral cages.

## PRACTICAL COMPUTATION OF IQ

The IQ is well-defined for polyhedron (with planar faces). The methods we described above determine 3D coordinates of the vertices of a polyhedron graph but may generally generate nonplanar faces. Let us call a cellular 3D structure with nonplanar faces a *map* (*topological polyhedron*). Maps are generalizations of polyhedra. A map with triangular faces only is necessarily a polyhedron.

Any face of a map other than a triangle may have noncoplanar coordinates. It is thus necessary to generalize the definition of the IQ to maps.

A naive approach is to triangulate a map arbitrarily—without introducing new vertices—and to calculate then the corresponding IQ, expecting that the triangulated map will resemble the starting map. This method is plausible in the case the original faces are almost planar and is exact if all faces are planar. Note that an example of a hexagonal face would be shaped as a benzene ring, while a nonplanar hexagonal face can be shaped as a cyclohexane.

One of the reasons for calculating IQ of polyhedra with triangular faces was of a practical nature. Namely one can compute the surface area of such a polyhedron by adding up the areas of triangles. The volume of such a polyhedron can be computed by adding the algebraic (signed) volumes of irregular tetrahedra spanned by the three vertices of each triangle and by the origin (or any other fixed point in the space) playing the role of the fourth vertex. The analytic geometry formulas for the triangle area and irregular tetrahedron volume can be found in the Appendix.

In the case of highly nonplanar faces this approach may lead to some strange conclusions. Namely, one of us (D.B.) wrote an algorithm that tried to find a coordinate placement of vertices of a map that would maximize its IQ. It is based on genetic approach. It generates a collection of polyhedra with the same topological structure but with randomly selected coordinates. By making small random changes of coordinates of each specimen, keeping only the best IQ candidates, and replacing the worst candidates with newly randomly generated specimens, the "population" evolves in such a way that the IQ of the best specimen never decreases and eventually leads to a (locally) optimal solution.

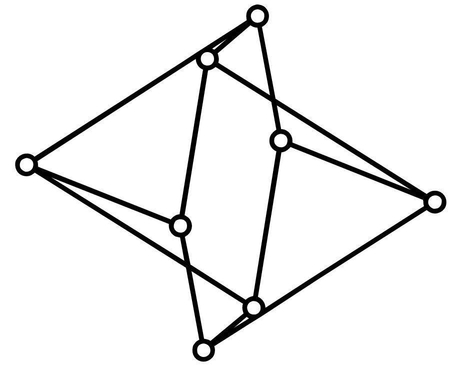

**Figure 1.** The map of a cube with coordinates obtained by genetic algorithm that maximizes the IQ. The computed IQ turns out to be larger than the IQ of a perfect cube.

It turned out that such an algorithm deliberately selects nonplanar faces that make the IQ of the selected triangulation as large as possible. For instance, for a cube the map given in Figure 1 is obtained. This map has faces that are far from being planar. We should perhaps stress that this behavior is not a property of the algorithm but of the problems itself. Any algorithm that would maximize the IQ under the same definition would lead to the same anomalies.

It is therefore clear that one has to define IQ in a such way that will "punish" nonplanar faces and be independent of the choice of face triangulation.

Here is a solution we propose.

Let $F$ be a face with vertices $v_1$, $v_2$, ..., $v_k$ whose coordinates are given by vectors $\vec{v}_1, \vec{v}_2, ..., \vec{v}_k$, respectively. The vector $\vec{\bar{v}} = (\vec{v}_1 + \vec{v}_2 + ..., + \vec{v}_k)/k)$ defines the position of the barycenter of the face $F$. Now triangulate the face $F$ by replacing it with $k$ triangles $\Delta i$, $i = 1, 2, ..., k$. The position of vertices of $\Delta i$ are given by $\vec{\bar{v}}, \vec{v}_i, \vec{v}_{i+1}$ with $\vec{v}_{k+1} = \vec{v}_1$. If we do this for every face, we obtain what is known to be *a two-dimensional subdivision* $S_2(M)$[23] of map $M$. (A two-dimensional subdivision is also known as *omnicapping*.[24]) We should warn the reader that this operation is usually defined in a purely topological way without specifying the coordinates of new vertices. Each new vertex can be viewed as the apex of a "pyramid" above the face. In the case where the face is planar (i.e., all vertices of the face lie in the same plane) we select the "degenerate pyramid" of zero height and volume. Our choice of new coordinates ensures that the coordinates of the barycenter of a planar face stay in the same plane.

Since $S_2(M)$ is a triangulation it is a polyhedron and its IQ is well-defined. Obviously, when $M$ itself is a polyhedron (has planar faces) $\mathrm{IQ}(M) = \mathrm{IQ}(S_2(M))$. In this respect the proposed method is stable since we always have $IQ(S_2(M)) = IQ(S_2(S_2(M)))$.

Let us define the *nonplanarity ratio* $\nu(M)$ of a map as the ratio between the sum of volumes of convex hulls of all faces of the map and the volume of $S_2(M)$. Clearly $\nu(M)$ is a

**Table 1.** IQ Results for Trivalent Polyhedral Clusters

| method | IQ | $v$ |
|---|---|---|
| NiceGraph | 0.277 | 0.56 |
| Laplace234 | 0.309 | 0.896 |
| Genetic Algorithm | 0.571 | 0.050 |

**Table 2.** IQ Results for Platonic Polyhedra

| polyhedron | IQ(Nice) | $v$(Nice) | IQ(Lap) | $v$(Lap) | $n$ | $e$ | $f$ |
|---|---|---|---|---|---|---|---|
| tetrahedron | **0.3023** | 0 | **0.3023** | 0 | 4 | 6 | 4 |
| octahedron | 0.6046 | 0 | 0.6046 | 0 | 6 | 12 | 8 |
| cube | 0.5236 | 0.005323 | 0.5236 | 0 | 8 | 12 | 6 |
| dodecahedron | 0.7547 | 0.002587 | 0.7547 | 0 | 20 | 30 | 12 |
| icosahedron | **0.8288** | 0 | **0.8288** | 0 | 12 | 30 | 20 |

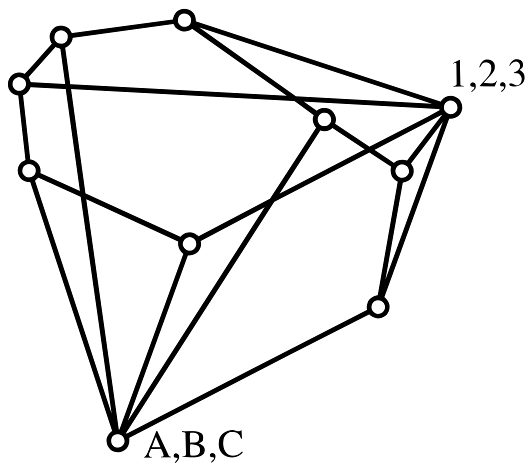


**Figure 2.** The map of a cubic polyhedron $P_{14,8}$ on 14 vertices, 21 edges, and 9 faces with coordinates obtained by a genetic algorithm that maximizes the IQ of $S_2(P_{14,8})$. Vertices 1, 2, and 3 are clearly mapped in the same 3D point. So are the vertices A, B, and C.

measure of nonplanarity of faces. In the special case of Figure 1, $v$ turned out to be equal to $^2/_3$ within numerical precision used.

In order to have a method that would work in all cases we need the following fact that we tested experimentally for several small cases:

Given a map $M$ there is an equivalent polyhedron $M'$ (with planar faces) such that $\mathrm{IQ}(M) \leq \mathrm{IQ}(M')$.

We modified the genetic algorithm so that it maximizes the IQ of $S_2(M)$ and tested it on various polyhedra. For instance, when we ran it on the selected subset of small cubic polyhedra that were first used in ref 25, we found out that sometimes, when a polyhedron has an intrinsic nonplanar face, the IQ is maximized by contracting certain sets of vertices. Let $P_{n,i}$ denote the $i$th trivalent polyhedron on $n$ vertices given in ref 25.

The genetic algorithm had to punish the inherent nonplanarity of the polyhedron by clustering some vertices together and essentially turning a trivalent polyhedron with 1 octagon, 4 pentagons, 2 quadrilaterals, and 2 triangles into a polyhedron with 8 trivalent vertices and 2 five-valent vertices having 7 quadrilaterals and 2 triangles.

Table 1 shows what happens to $P_{14,8}$ for various coordinatization methods. Both NiceGraph and Standard Laplace method point out intrinsic nonplanarity of its faces. The modified genetic algorithm found largest IQ but collapsed two sets of vertices in order to replace large faces by smaller ones (triangles and quadrilaterals.)

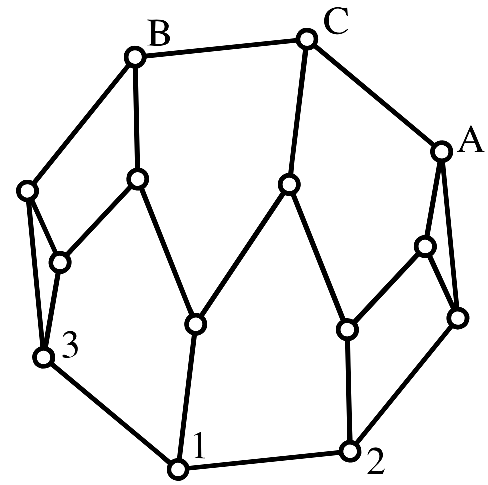


**Figure 3.** Schlegel diagram of polyhedron $P_{14,8}$ from Figure 2.

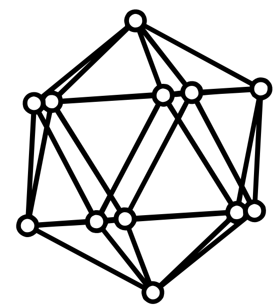

**Figure 4.** Icosahedron. Maximal IQ for Platonic: IQ(Lap): **0.8288**.

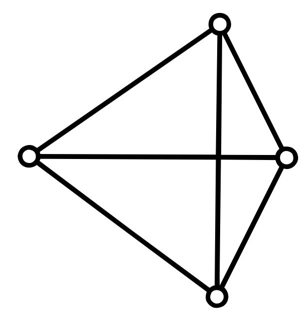

**Figure 5.** Tetrahedron. Minimal IQ for Platonic: IQ(Nice): **0.3023** (=IQ(Lap)).

Our method is able to reproduce experimentally the results from ref 10 for Platonic polyhedra. We carried out our tests for other Archimedean polyhedra. We also investigated all small trivalent polyhedral clusters, see ref 25. The bold numbers in Tables 2−4 represent extreme values. "Nice" refers to NiceGraph method, "Lap" to standard Laplace, and "MM3" to Molecular Mechanics. Finally, $n$ represents the number of vertices, $e$ the number of edges, and $f$ the number of faces.

In Table 2 we can see that both methods reproduce theoretical values within numerical precision used, although NiceGraph produces nonplanar faces for both nontriangular Platonic solids: the cube and dodecahedron. Extreme cases are shown in Figures 4 and 5.

In Table 3 we can read that snub dodecahedron is the most spherical Archimedean polyhedron. The fact that standard Laplace produces nonplanar faces in truncated cuboctahedron and truncated icosidodecahedron has a plausible explanation. These two solids cannot be obtained by geometrical truncation: topological truncation is needed. Extreme cases are shown in Figures 6 and 7.

**Table 3.** IQ Results for Archimedean Polyhedra

| polyhedron | IQ(Nice) | $v$(Nice) | IQ(Lap) | $v$(Lap) | $n$ | $e$ | $f$ |
|---|---|---|---|---|---|---|---|
| truncated tetrahedron | 0.4534 | 0 | **0.3966** | 0 | 12 | 18 | 8 |
| truncated octahedron | 0.749 | 0.002816 | 0.7302 | 0 | 24 | 36 | 14 |
| truncated cube | 0.6056 | 0 | 0.5764 | 0 | 24 | 36 | 14 |
| truncated dodecahedron | 0.7893 | 0.0006683 | 0.7779 | 0 | 60 | 90 | 32 |
| truncated icosahedron | 0.9027 | 0.000691 | 0.901 | 0 | 60 | 90 | 32 |
| cuboctahedron | 0.7412 | 0 | 0.7412 | 0 | 12 | 24 | 14 |
| icosidodecahedron | 0.8601 | 0.0001663 | 0.8602 | 0 | 30 | 60 | 32 |
| snub cube | 0.8955 | 0.000207 | 0.8734 | 0 | 24 | 60 | 38 |
| snub dodecahedron | **0.9406** | 6.176e-05 | 0.9194 | 0 | 60 | 150 | 92 |
| rhombicuboctahedron | 0.8669 | 4.084e-05 | 0.8515 | 0 | 24 | 48 | 26 |
| truncated cuboctahedron | 0.8186 | 0.03118 | 0.8204 | 0.01844 | 56 | 84 | 30 |
| rhombicosidodecahedron | 0.9357 | 0.0002102 | 0.9174 | 0 | 60 | 120 | 62 |
| truncated icosidodecahedron | 0.9053 | 0.0002607 | 0.8852 | 0.003704 | 120 | 180 | 62 |

**Table 4.** IQ Results for IP Fullerenes up to 80 Atoms

| Id. | point group | IQ(Nice) | $v$(Nice) | IQ(Lap) | $v$(Lap) | MM3 | $v$(MM3) | $n$ | $e$ | $f$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 60:1 | $I_h$ | 0.9027 | 0.0009936 | 0.901 | 0 | 0.9038 | 4.242e-05 | 60 | 90 | 32 |
| 70:1 | $D_{5h}$ | 0.9009 | 0.01177 | 0.912 | 0.00725 | 0.8987 | 0.01418 | 70 | 105 | 37 |
| 72:1 | $D_{6d}$ | 0.8795 | 0.02378 | 0.9133 | 0.01289 | **0.8649** | 0.03569 | 72 | 108 | 38 |
| 74:1 | $D_{3h}$ | 0.9145 | 0.01203 | 0.9121 | 0.009421 | 0.9098 | 0.01862 | 74 | 111 | 39 |
| 76:1 | $D_2$ | 0.8954 | 0.02171 | 0.915 | 0.01403 | 0.8887 | 0.0303 | 76 | 114 | 40 |
| 76:2 | $T_d$ | 0.9194 | 0.01101 | 0.9164 | 0.008864 | 0.9152 | 0.01759 | 76 | 114 | 40 |
| 78:1 | $D_3$ | 0.892 | 0.02186 | 0.9162 | 0.01501 | 0.8878 | 0.02986 | 78 | 117 | 41 |
| 78:2 | $C_{2v}$ | 0.9019 | 0.0174 | 0.9142 | 0.01153 | 0.8944 | 0.02593 | 78 | 117 | 41 |
| 78:3 | $C_{2v}$ | 0.9126 | 0.01363 | 0.9178 | 0.01015 | 0.9075 | 0.02041 | 78 | 117 | 41 |
| 78:4 | $D_{3h}$ | 0.8891 | 0.02136 | 0.9102 | 0.01433 | 0.8792 | 0.03306 | 78 | 117 | 41 |
| 78:5 | $D_{3h}$ | 0.9208 | 0.0107 | 0.9209 | 0.009473 | 0.9178 | 0.01577 | 78 | 117 | 41 |
| 80:1 | $D_{5d}$ | 0.8707 | 0.01914 | 0.9174 | 0.01399 | 0.8728 | 0.02318 | 80 | 120 | 42 |
| 80:2 | $D_2$ | 0.8899 | 0.02308 | 0.9134 | 0.01538 | 0.884 | 0.03141 | 80 | 120 | 42 |
| 80:3 | $C_{2v}$ | 0.9123 | 0.01494 | 0.9184 | 0.01057 | 0.9071 | 0.02253 | 80 | 120 | 42 |
| 80:4 | $D_3$ | 0.9003 | 0.02128 | 0.9168 | 0.01328 | 0.8889 | 0.03041 | 80 | 120 | 42 |
| 80:5 | $C_{2v}$ | 0.9205 | 0.01233 | 0.9202 | 0.01065 | 0.9161 | 0.01923 | 80 | 120 | 42 |
| 80:6 | $D_{5h}$ | 0.9251 | 0.01072 | 0.9236 | 0.0103 | 0.9239 | 0.0164 | 80 | 120 | 42 |
| 80:7 | $I_h$ | **0.9256** | 0.009388 | 0.9242 | 0.01076 | 0.9253 | 0.01587 | 80 | 120 | 42 |

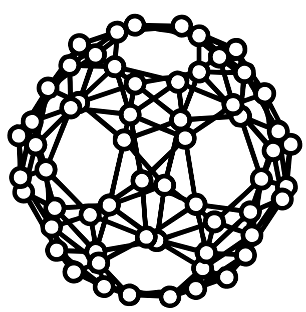

**Figure 6.** Snub dodecahedron. Maximal IQ for Archimedean: IQ(Nice): **0.94064**.

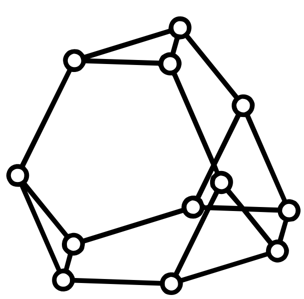

**Figure 7.** Truncated tetrahedron. Minimal IQ for Archimedean: IQ(Nice): **0.4534**.

Table 4 shows the results for all isolated pentagon (IP) fullerenes with up to 80 vertices. The identification of IP fullerenes follows the one of Table A.10 on p 254 of ref 26. In addition to the NiceGraph and standard Laplace we also include their coordinates obtained by Molecular Mechanics MM3 method from ref 27. It is clear that all fullerenes in

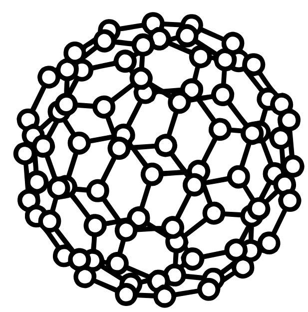

**Figure 8.** $C_{72}$, $D_{6d}$. Maximal IQ for fullerenes: IQ(Nice): **0.92791**.

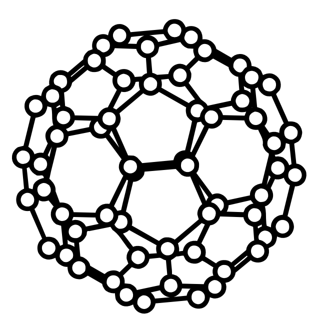

**Figure 9.** $C_{80}$, $I_h$. Minimal IQ for fullerenes: IQ(Nice): **0.90265**.

Table 4 have high IQ and small $v$. They are spherical and all faces are almost planar. It is perhaps surprising that the standard Laplace method produces on average the largest IQ and the smallest $v$. A feasible explanation for nonidealistic behavior of MM3 may be the fact that it is unable to treat $\pi$-electrons which prefer planarity. Extreme cases are shown in Figures 8 and 9.

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## APPENDIX

When calculating the IQ of a polyhedron with triangular faces we need to compute its surface area $S$ and its volume $V$. Each triangular face $T$ with vertices $\vec{a} = (a_x, a_y, a_z)$, $\vec{b} = (b_x, b_y, b_z)$, and $\vec{c} = (c_x, c_y, c_z)$ contributes to the surface area of the triangle $T$

$$S_T = \frac{1}{2}|(\vec{a} - \vec{c}) \times (\vec{b} - \vec{c})| \tag{3}$$

and to the signed(!) volume

$$\mathrm{V_T} = \frac{1}{6}\begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \tag{4}$$

of a irregular tetrahedron with four vertices: $\vec{a}, \vec{b}, \vec{c}$, and the origin $\vec{0}$. Therefore

$$S = \sum_T S_T \tag{5}$$

$$V = |\sum_T V_T| \tag{6}$$

and

$$\mathrm{IQ} = V/S \tag{7}$$

In both sums index $T$ runs over all triangular faces. Note that each term in the sum for $S$ is non-negative, while the terms for $V$ may be either positive or negative.

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