Isoperimetric quotient for fullerenes and other polyhedral cages

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The notion of isoperimetric quotient (IQ) of a polyhedron was introduced by Polya [1]. It is a measure that tells how spherical is a given polyhedron. If one is given a polyhedral graph, it can be drawn in a variety of ways in three-dimensional (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 extending the definition of IQ and compute it for any 3D drawing. The IQs of fullerenes and other polyhedral cages are computed.

Fullerenes, nanotubes and other polyhedral cages were a subject of intensive research. 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 C atoms; it is highly desirable, after generating (all of) them to sort out the most stable ones. A series of rules were developed to do such a sorting with the isolated-pentagon (IP) rule 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, notice that an efficient algorithm exists for generating topologies of fullerenes and other trivalent polyhedral cages with prescribed properties. The stability of a fullerene depends both on the strain of its σ skeleton and on the delocalisation of its π-electron network. Pisanski *et al.* dealt only with the strain in fullerenes and similar polyhedra, and they proposed an index, which is based on the *isoperimetric quotient* (IQ) as a measure of the strain in these cages [2]. They also performed an initial study of the stability of fullerenes and other polyhedral cages *vs*. IQ.

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

$$S_T = \frac{1}{2}\left|(\mathbf{a}-\mathbf{c})\times(\mathbf{b}-\mathbf{c})\right| \qquad (1)$$

and to the *signed* volume

$$V_T = \frac{1}{6}\begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \qquad (2)$$

of an irregular tetrahedron with four vertices: **a**, **b**, **c**, and the origin **0**. Therefore,

$$S = \sum_T S_T \qquad (3)$$

$$V = \left|\sum_T V_T\right| \qquad (4)$$

and

$$\mathrm{IQ} = 36\pi V^2 / S^3 \qquad (5)$$

In both sums index T runs over all triangular faces. Notice that each term in the sum for S is non-negative, while the terms for V may be either positive or negative. Obviously, as a sphere has a minimal surface area for a given volume, IQ of an arbitrary spheroidal object obeys the following property

$$0 \le \mathrm{IQ} \le 1 \qquad (6)$$

where the right equality holds only for a sphere [3], while the left equality holds only for the degenerate case with $V = 0$.

Table 1 shows the results for C_{12} (I_h) and some IP fullerenes with up to 82 vertices. It is clear that all fullerenes in Table 1 have high IQ. They are spherical and all faces are almost planar.

Table 1. Isoperimetric Quotient (IQ) results for polyhedra.

Polyhedron	Vertices	Edges	Triang. faces	Pentag. faces	Hexag. faces	Total faces	Surface (Å²)	Volume (Å³)	IQ
C_{12} (I_h)	12	30	20	–	–	20	17.22	6.1	0.8288
C_{60} (I_h)	60	90	–	12	20	32	147.52	160.2	0.9037
C_{70} (D_{5h})	70	105	–	12	25	37	173.73	204.1	0.8982
C_{80} (C_2)	82	123	–	12	31	43	195.45	244.0	0.9016

References

1. G. Polya, *Introduction and Analogy in Mathematics*, Princeton University, Princeton, 1954.
2. T. Pisanski, M. Kaufman, D. Bokal, E. C. Kirby and A. Graovac, *J. Chem. Inf. Comput. Sci.*, **37** (1997) 1028.

3. A. Deza, M. Deza and V. Grishukhin, *Discrete Math.*, **192** (1998) 41.