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A formula to estimate the size of a fullerene

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A formula to estimate the radius of an equiareal sphere for any C_n fullerene as a function of n is suggested. It asymptotically characterizes the series of C_n fullerenes with increasing n and is mostly adapted to the symmetric shapes. The estimated radius may also be a reasonable approximation if the shape is not too elliptic.

1. Introduction

All the combinatorial types of C_{20} to C_{60} fullerenes have been enumerated and characterized by the symmetry point groups in Voytekhovsky & Stepenshchikov (2001). As their variety rapidly grows with the number of vertices, C_{62} to C_{70} shapes with pairs of adjacent 5-gonal facets only were reported in the same way in Voytekhovsky & Stepenshchikov (2002). Maximum symmetry and minimum number of adjacent 5-gonal facets are known to increase their stability (Kroto, 1987; Schmalz *et al.*, 1988). But more precise predictions need some energetic potentials and, therefore, metric parameters to be calculated. The latter are dependent on the metric implementation of a fullerene even with its combinatorial type being known. We suggest here an averaging parameter that estimates the size of a C_n fullerene as a function of n only.

2. Derivation of the formula

Let a_m be the edge of a regular m-gon. Then, its perimeter, radii of inscribed and circumscribed circles equal, respectively,

$$P = ma_m, \quad r = a_m/2\tan(\pi/m) \quad \text{and} \quad R = a_m/2\sin(\pi/m).$$

For any m, we have

$$r < \rho < R,$$

where $\rho = P/2\pi$ is the radius of a circle with length P. But

$$r/R \to 1 \quad \text{as} \quad m \to \infty.$$

Hence,

$$\rho/r \to 1 \quad \text{and} \quad \rho/R \to 1 \quad \text{as} \quad m \to \infty,$$

i.e. ρ simultaneously estimates r and R.

The most symmetric fullerenes C_{60} ($\bar{3}\bar{5}m$) and C_{70} ($\overline{10}m2$) are usually characterized by the radii of inscribed and circumscribed spheres. It follows from what was said above an idea to use the radius $\wp$ of an equiareal sphere to characterize any C_n fullerene as an almost 'regular' polyhedron of 12 nearly regular 5-gonal and $n/2 - 10$ 6-gonal facets. Let us consider a fullerene with all vertices being on a sphere. Then,

$$R^2 = r^2 + r_6^2,$$

where r and R are the radii of inscribed and circumscribed spheres while

$$r_6 = a/2\sin(\pi/6) = a$$

is the circumradius of a 6-gonal facet of fixed finite edge length a. Then,

$$r/R = [1 - (a/R)^2]^{1/2} \to 1$$

as $R \to \infty$ caused by $n \to \infty$. Hence, $\wp$ asymptotically estimates r and R.

The areas of 5- and 6-gonal facets equal

$$S_m = ma^2 \cot(\pi/m)/4,$$

where $m = 5$ or 6. So the surface area of a C_n fullerene equals

$$S_{\rm ful} = a^2[15\cot(\pi/5) + 3(n/2 - 10)\cot(\pi/6)/2].$$

Finally, it follows from the equation $S_{\rm ful} = 4\pi\wp^2$ that

$$\begin{aligned} \wp &= a\{[15\cot(\pi/5) + 3(n/2 - 10)\cot(\pi/6)/2]/4\pi\}^{1/2} \\ &\simeq a(0.103374n - 0.424548)^{1/2} \\ &= a\varphi(n). \end{aligned}$$

3. Results and discussion

It follows from the above formula that a is nothing but a scaling coefficient while $\varphi(n)$ non-linearly defines $\wp$ as a function of n. It is tabulated for n = 60 to 100 in Table 1.

Let us compare our results with previous data. It is known for the ideal truncated icosahedron that $R = 2.478a$, $h_5 = 2.327a$ and $h_6 = 2.267a$, where a, R, h_5 and h_6 are the edge, radius of circumscribed sphere and apothems (*i.e.* distances from the centre to 5- and 6-gonal facets), respectively. Our estimate $\varphi(60) \simeq 2.404$ is in good agreement with this model. Haymet (1986) reported for the real C_{60} fullerene that a = 0.14 and R = 0.35 nm. Yeletsky & Smirnov (1995) reported for this case that partial double and double C=C bonds equal 0.144 and 0.139 nm with R = 0.357 nm. It follows from our formula that R = 0.346 and 0.344 nm for a = 0.144 and 0.139 nm, respectively.

So our estimates are close to both an ideal model and experimental data even for the small n = 60 value. We believe they are getting much more precise with increasing n even with C—C bonds being slightly different. This is true in particular for the most symmetric shapes which can be characterized in addition along the symmetry axes. If the shape is not too elliptic, the estimated radius may also be a reasonable approximation.

Table 1
$\varphi(n)$ values for n = 60 to 100.

n	$\varphi(n)$	n	$\varphi(n)$	n	$\varphi(n)$
60	2.403725	74	2.687960	88	2.944888
62	2.446352	76	2.726147	90	2.979784
64	2.488250	78	2.763806	92	3.014276
66	2.529454	80	2.800959	94	3.048378
68	2.569997	82	2.837626	96	3.082103
70	2.609910	84	2.873825	98	3.115462
72	2.649222	86	2.909573	100	3.148468

4. Conclusions

A formula to estimate the radius of an equiareal sphere for any C_n fullerene as a function of n is suggested in the paper. It asymptotically, with increasing n, characterizes the most symmetric C_n fullerenes which can be additionally specified along the symmetry axes. The estimated radius may also be a reasonable approximation if the shape of a fullerene is not too elliptic.

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