Prediction of Fullerene Stability Using Topological Descriptors

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**Abstract.** In recent years, several attempts have been made to characterize the geometric structure of fullerenes by means of topological shape factors in order to predict their physical properties and stability. In this paper, we present a simple method to estimate the stability of fullerenes on the basis of quantitative topological criteria. This approach is based on the concept of the generalized combinatorial curvatures defined on the set of simple graphs embedded on a closed surface without boundary (sphere, torus, projective plane, Klein bottle). It is shown that starting with the computed generalized combinatorial curvatures several novel topological indices can be generated. From computations performed on a set of C\(_{40}\) and C\(_{60}\) fullerenes, we concluded that the four topological shape factors tested (\(\Lambda(-1)\), \(\Omega(-1)\), \(\Lambda(1)\) and \(\Omega(1)\)) could be successfully used to preselect the most stable fullerene isomers.

1. **Introduction**

Methods for topological characterization of fullerene isomers have made steady progress over the past decade and many calculations of stabilities of traditional and non-traditional fullerenes have been reported [1-14]. In this paper, we present a simple method to estimate the thermodynamic stability of fullerenes using novel topological descriptors. This approach is based on the concept of the generalized combinatorial curvatures defined on the set of embedded graphs. It is shown that starting with the computed generalized combinatorial curvatures, various topological shape indices can be generated. The current paper reports systematic calculations performed on C\(_{40}\) and C\(_{60}\) fullerenes. Results obtained confirm that an appropriately selected finite set of novel topological indices appears to be useful for identifying stable fullerene isomers.

2. **Finite cellular systems**

A finite cellular system (FC system) is defined as a tessellation of a closed and orientable, unbounded surface by a finite set of 2D simply connected regions. These regions (combinatorial polygons) are called cells. This implies that a FC system can be represented by an embedded finite
planar graph, where \( V \), \( E \) and \( N \) stand for the number of vertices, edges and faces (cells), respectively.

In a FC system, the number \( E \) of edges is related to the number \( N \) of cells, the number \( V \) of vertices, the average valency \( [r] \) and the mean number of sides per cell \( \langle n \rangle \)

\[
2E = \sum_{n} n N_n = \sum_{n} n p_n = \langle n \rangle N = \sum_r r V_r = V \sum_r q_r = V[r]
\]  

(1)

where \( N_n \) is the number of \( n \)-sided polygons and \( V_r \) is the number of \( r \)-valent vertices. The number \( N \) of cells is \( N = \sum N_n \) where \( n=2,3,..., n_{\text{max}} \), and the number \( V \) of vertices is \( V = \sum V_r \). In Eq.(1), \( p_n = N_n/N \) is the fraction of \( n \)-sided cells, and \( q_r = V_r/V \) is the fraction of vertices of valency \( r \), respectively.

Since the cells are simply connected regions, the Euler’s equation for a closed surface (i.e. surface without boundary) can be formulated as

\[
\chi = N - E + V = \begin{cases} 2 - 2g & \text{for an orientable surface} \\ 2 - g & \text{for a non-orientable surface} \end{cases}
\]

(2)

where \( \chi \) is the Euler-characteristic, \( g \) is the genus of the surface [15,16,17]. In particular, the Euler characteristic is 2 for sphere, 1 for the projective plane, 0 for the torus and Klein bottle, and negative for all other surfaces [16]. Taking into consideration, that for a FC system equalities \( \langle n \rangle = 2E/N \geq 3 \) and \( [r] = 2E/V \geq 3 \) hold, from Eqs.(1 and 2), we have

\[
\frac{1}{[r]} + \frac{1}{\langle n \rangle} = \frac{1}{2} + \frac{\chi}{2E} \leq \frac{1}{2} + \frac{1}{E}
\]

(3)

If all of the vertices of a FC system have the same valency \( \rho \geq 3 \), then such a system is said to be regular, or \( \rho \)-valent.

3. Generalized combinatorial curvature

Let \( X_j \) an \( r \)-valent vertex \((j=1,2,...,V)\) which is the common vertex of \( r \) different cells. For vertex \( X_j \) the vertex-charge of order \( S \) is defined as

\[
CV_s(X_j) = n_{i,j}^{s} + n_{2,j}^{s} + ... + n_{r(j),j}^{s}
\]

(4)

where \( n_{i,j}, n_{2,j},...n_{r(j),j} \) are the side-numbers of cells meeting at the common vertex \( X_j \) and \( S \) is an arbitrary real number. Now, starting with Eq.(4) we define for vertex \( X_j \) the generalized combinatorial curvature \( \Phi_s(X_j) \) as follows

\[
\Phi_s(X_j) = 1 - \frac{r(X_j)}{2} + CV_s(X_j)
\]

(5)

Let us denote by \( \mu_m(\Phi_s) \) the \( m \)-th moments of generalized curvatures \( \Phi_s(X_j) \), where \( m \) is a positive integer. It is easy to verify that

\[
\mu_1(\Phi_s) = \frac{1}{V} \sum_{j=1}^{V} \Phi_s(X_j) = 1 - \frac{[r]}{2} + \frac{1}{V} \sum_{j=1}^{V} CV_s(X_j) = 1 + [r] \left\{ \frac{\langle n^{S+1} \rangle}{\langle n \rangle} - \frac{1}{2} \right\}
\]

(6)
where \( (n^k) = \sum n^k p_n \) and \([r^k] = \sum r^k q_r \) stand for the k-th moment of side-number n of polygonal cells and of the valency number of vertices, respectively.

If \( S = -1 \), from Eq. ( ), we obtain the traditional combinatorial curvature \( \Phi_{-1}(X_j) \) of vertex \( X_j \)
\[
\Phi_{-1}(X_j) = 1 - \frac{r(X_j)}{2} + \frac{1}{n_{j,1}} + \frac{1}{n_{j,2}} + \ldots + \frac{1}{n_{j,r(j)}}.
\]  
(7)
as a particular case [18-23]. An FC system is called a vertex homogenous system (VH-system) if its traditional combinatorial curvatures \( \Phi_{-1}(X_j) \) are equal in each vertex for \( j = 1, 2, \ldots V \). It should be noted that prisms and antiprisms, the five Platonic polyhedra and the 13 Archimedean polyhedra represent VH-systems. From theoretical considerations [18-23] it follows that
\[
V \mu_1(\Phi_{-1}) = \sum_{j=1}^{V} \Phi_{-1}(X_j) = V - E + N = \chi
\]  
(8)For the case of \( S = 0 \), equality \( \Phi_0(X_j) = 1 + r(X_j)/2 \) is fulfilled. Consequently, one can obtain
\[
\mu_m(\Phi_0) = \frac{1}{V} \sum_{j=1}^{V} \Phi_0^m(X_j) = \frac{1}{2^m} \left( \sum_{i=0}^{m} \binom{m}{i} 2^i r^{m-i} \right) \]  
(9)In particular cases we have
\[
\mu_1(\Phi_0) = \frac{1}{V} \sum_{j=1}^{V} \Phi_0(X_j) = \frac{\chi + 2E - N}{V} = 1 + \frac{[r]}{2}
\]  
(10)\[
\mu_2(\Phi_0) = \frac{1}{V} \sum_{j=1}^{V} \Phi_0^2(X_j) = 1 + [r] + \frac{[r^2]}{4}
\]  
(11)If an FC system is \( \rho \)-valent (i.e. \( \rho \geq 3 \) positive integer) from Eq.(9) it follows
\[
\mu_m(\Phi_0) = \frac{1}{V} \sum_{j=1}^{V} \Phi_0^m(X_j) = \mu_1^m(\Phi_0) = \left(1 + \frac{\rho}{2}\right)^m
\]  
(12)From Eqs.(4-5) inequality \( \Phi_1(X_j) \geq 1 + 5r(X_j)/2 \) can be obtained. The equality \( \Phi_1(X_j) = 1 + 5r(X_j)/2 \) is fulfilled if only triangles are incident with vertex \( X_j \). If an FC-system is composed of triangles only, this implies that
\[
\mu_m(\Phi_1) = \frac{1}{V} \sum_{j=1}^{V} \Phi_1^m(X_j) = \frac{1}{2^m} \left( \sum_{i=0}^{m} \binom{m}{i} 5^i r^{m-i} \right) \]  
(13)Particularly, we obtain
\[
\mu_1(\Phi_1) = \frac{1}{V} \sum_{j=1}^{V} \Phi_1(X_j) = 1 + \frac{5}{2}[r]
\]  
(14)\[
\mu_2(\Phi_1) = \frac{1}{V} \sum_{j=1}^{V} \Phi_1^2(X_j) = 1 + 5[r] + \frac{25}{4}[r^2]
\]  
(15)
When $S = -1$, from Eqs. (14-15) inequality $\Phi_{-1}(X_j) \leq 1 - r(X_j)/6$ can be obtained. As a special case we have $\Phi_{-1}(X_j) = 1 - r(X_j)/6$ if only triangles are incident with vertex $X_j$. Consequently, if an FC-system includes only triangles, we have

$$\mu_m(\Phi_{-1}) = \frac{1}{V} \sum_{j=1}^{V} \Phi_{-1}^m(X_j) = \frac{1}{6^m} \left( \sum_{i=0}^{m} \binom{m}{i} (-1)^i 6^i r^{m-i} \right).$$  \hspace{1cm} (16)

In particular, for triangular FC-systems

$$\mu_i(\Phi_{-1}) = \frac{1}{V} \sum_{j=1}^{V} \Phi_{-1}^i(X_j) = \frac{1}{6} \left( 6 - [r] \right) = \frac{X}{V}$$  \hspace{1cm} (17)

$$\mu_2(\Phi_{-1}) = \frac{1}{V} \sum_{j=1}^{V} \Phi_{-1}^2(X_j) = \frac{1}{36} \left( 36 - 12[r] + [r^2] \right)$$  \hspace{1cm} (18)

$$\mu_3(\Phi_{-1}) = \frac{1}{V} \sum_{j=1}^{V} \Phi_{-1}^3(X_j) = \frac{1}{216} \left[ 216 - 108[r] + 18[r^2] - [r^3] \right].$$  \hspace{1cm} (19)

In the following we will show that the moments $\mu_m(\Phi_{S})$ calculated from generalized combinatorial curvatures $\Phi_{S}(X_j)$ can be efficiently used to characterize the topological structures of fullerene-like molecules.

### 4. Topological descriptors defined on the basis of generalized combinatorial curvatures

Based on the concept outlined in Refs. [14,24], a fullerene is considered as a finite cellular system defined on an unbounded, closed and orientable or non-orientable surface, and composed of a finite set of combinatorial polygons (cells), where cells are simply connected regions and all common edges are shared only by two different neighboring cells. Fullerenes of such types will be referred to as cellular fullerenes.

Taking into consideration the decisive role of the Euler characteristic ($\chi$) in the topological analysis, cellular fullerenes with $\chi = 2$ are called spherical fullerenes. In the following we consider only spherical fullerenes which can be classified into two families: Spherical fullerenes represented by convex polyhedra (characterized by 3-connected planar graphs) are called polyhedral fullerenes, while the others, which cannot be represented by convex polyhedra, are called non-polyhedral fullerenes. According to the Steinitz’s theorem, a finite graph is polyhedral if and only if it is planar and 3-connected [16]. This implies that a non-polyhedral spherical fullerene can be represented only by a connected planar graph with a vertex connectivity number less than 3.

In order to characterize the local topological structure of cellular fullerenes, we defined the topological descriptors $\Lambda(S)$ and $\Omega(S)$ calculated on the basis of the moments of the generalized combinatorial curvatures $\Phi_{S}(X_j)$

$$\Lambda(S) = 100 \left( \frac{1 + \sqrt{\mu_2(\Phi_{S})}}{1 + \sqrt{\mu_1^2(\Phi_{S})}} - 1 \right)$$  \hspace{1cm} (20)
and

\[
\Omega(S) = \begin{cases} 
0 & \text{for } \mu_2(\Phi_S) = 0 \\
100 \left( \frac{\mu_3(\Phi_S)}{\mu_{3/2}^2(\Phi_S)} - 1 \right) & \text{for } \mu_2(\Phi_S) > 0
\end{cases}
\] (21)

where \( S \) is an appropriately selected real number different from zero. (If \( S=0 \), it follows that \( \Lambda(0)=\Omega(0)=0 \) for any \( \rho \)-valent, regular FC system where \( \rho \geq 3 \) positive integer.) It is easy to see that \( \Lambda(S) \) is always a non-negative number, but \( \Omega(S) \) can be negative, as well. Another consequence is that \( \Lambda(-1)=\Omega(-1)=0 \), if and only if the FC system is vertex homogenous.

5. Topological characterization of traditional fullerene isomers

For testing purposes, four topological descriptors \( \Lambda(-1) \), \( \Omega(-1) \), \( \Lambda(1) \) and \( \Omega(1) \) derived from Eqs.(20-21) have been chosen. In order to evaluate their discriminating power, we used the sets of \( C_{60} \) and \( C_{40} \) isomers. This is explained by the fact that several topological descriptors have been already calculated for \( C_{60} \) and \( C_{40} \) isomers: the pentagon adjacency index \( N_P \) [1,6,9,14], the Wiener index \( W_I \) [10], the resistance distance \( R_T \) [10], the isolation index \( IS \) [25], the Aboav parameter \( A_R \) [26], the Kekulé structure count [11], the graph independence number [12], the number of spanning trees [13].

For traditional fullerenes, topological descriptors \( \Lambda(S) \) and \( \Omega(S) \) can be easily computed. Because only pentagons (5-gons) and hexagons (6-gons) meet at each trivalent vertex, there exist only four types of vertex configurations which are denoted by \( C_{5,5,5}, C_{5,5,6}, C_{5,6,6} \) and \( C_{6,6,6} \) respectively [23, 25, 27].

From Eqs.(4 and 5) it follows that the corresponding generalized combinatorial curvatures are:

\( \Phi_S(C_{5,5,5}) = 5^{S} + 5^{S} + 5^{S} -1/2 \), \( \Phi_S(C_{5,5,6}) = 5^{S} + 5^{S} + 6^{S} -1/2 \), \( \Phi_S(C_{5,6,6}) = 5^{S} + 6^{S} + 6^{S} -1/2 \) and \( \Phi_S(C_{6,6,6}) = 6^{S} + 6^{S} + 6^{S} -1/2 \).

It is important to note that on basis of the four vertex configurations \( (C_{5,5,5}, C_{5,5,6}, C_{5,6,6} \) and \( C_{6,6,6} ) \) the traditional fullerenes can be partitioned into subclasses. Balaban et al verified that the 1812 \( C_{60} \) isomers can be classified into 42 equivalence classes [27]. It is easy to see that among the traditional fullerene isomers there are only two, namely the Buckminster fullerene and the dodecahedron \( C_{20} \) for which equalities \( \Lambda(S) = 0 \) and \( \Omega(S) = 0 \) hold for any \( S \neq 0 \).

We will compare the selected topological indices \( \Lambda(-1), \Omega(-1), \Lambda(1) \) and \( \Omega(1) \) with other predictors of fullerene stability, including the pentagon adjacency index \( N_P \). The pentagon adjacency index is one of the most important topological descriptors which is identical to the number of pentagon-pentagon fusions [1,5,6,9]. It is known that \( N_P \leq 30 \) for any classical fullerene, and the most stable fullerenes are characterized by the smallest pentagon adjacency indices. (For a fullerene with isolated pentagons, \( N_P = 0 \) holds.)
5.1 Characterization of \(C_{60}\) isomers

Each \(C_{60}\) isomer includes 12 pentagonal and 20 hexagonal faces, exactly. Among them, the smallest pentagon adjacency index \((N_P=0)\) belongs to the Buckminster fullerene which is considered as the most stable one, (Fig. 1a), while the greatest pentagon adjacency index \((N_P=20)\) characterizes the least stable isomer shown in Fig. 1b. [27].

![Schlegel diagrams of the most stable C60:1812 (a) and of the least stable C60:1 (b) isomers](image)

**Fig. 1** Schlegel diagrams of the most stable C60:1812 (a) and of the least stable C60:1 (b) isomers

To perform a comparative analysis, for all \(C_{60}\) isomers we calculated the topological descriptors \(N_P, \Lambda(-1), \Omega(-1), \Lambda(1)\) and \(\Omega(1)\), respectively. Relations between them are illustrated in Fig.2. Analysis of computed results leads to the following conclusions:

On the basis of the pentagon adjacency index \(N_P\), the 1812 \(C_{60}\) isomers can be classified into 12 subclasses. Values of \(N_P\) vary from 20 down to 0 within the \(C_{60}\) set [1]. The diagrams in Fig.1 suggest that the topological index \(\Omega(-1)\) seems to be the most selective one, consequently, \(\Omega(-1)\) has a better discriminating power than \(N_P, \Lambda(-1), \Lambda(1)\) and \(\Omega(1)\).

Comparing the computed values of \(\Lambda(-1), \Omega(-1), \Lambda(1)\) and \(\Omega(1)\), we found the same tendency: their minimum values (i.e. \(\Lambda(-1)=\Omega(-1)=\Lambda(1)=\Omega(1)=0\)) belong to the Buckminster fullerene, while the maximum values (i.e. \(\Lambda(-1)= 0.5155, \Omega(-1)= 5.818, \Lambda(1)= 0.4108\) and \(\Omega(1)= 1.3080\)) correspond to the least stable isomer depicted in Fig. 1b.
From the results obtained it is conjectured that the topological indices $\Lambda(-1)$, $\Omega(-1)$, $\Lambda(1)$ and $\Omega(1)$ are algebraically independent quantities. However, some of them are highly correlated. The calculated correlation coefficients, $(R)$ are given in Fig. 2, as well. As can be stated, there is very
strong correspondence of a linear type between \( N_P \) and \( \Lambda(1) \), the correlation coefficient practically equals 1. (See Fig. 2)

5.2 Characterization of \( C_{40} \) isomers

There are forty \( C_{40} \) isomers; all of them have 12 pentagonal and 10 hexagonal faces, exactly. It is believed that \( C_{40}:38 \) is the most stable, this is followed by \( C_{40}:39 \). Isomer \( C_{40}:38 \) is predicted to be the \( C_{40} \) fullerene of lowest energy by many methods [5-9]. In Table 1 we summarized the computed values of \( \Lambda(-1) \), \( \Omega(-1) \), \( \Lambda(1) \) and \( \Omega(1) \) for some \( C_{40} \) isomers.

<table>
<thead>
<tr>
<th>Fullerenes</th>
<th>( N_P )</th>
<th>( W_I )</th>
<th>( R_T )</th>
<th>IS</th>
<th>( A_R )</th>
<th>( \Lambda(-1) )</th>
<th>( \Omega(-1) )</th>
<th>( \Lambda(1) )</th>
<th>( \Omega(1) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{40}:1 )</td>
<td>20</td>
<td>3035</td>
<td>955,15</td>
<td>3,6363</td>
<td>-1.8788</td>
<td>1,177</td>
<td>37,450</td>
<td>0,229</td>
<td>0,7262</td>
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<td>( C_{40}:2 )</td>
<td>16</td>
<td>3008</td>
<td>936,88</td>
<td>2,9090</td>
<td>-0,4121</td>
<td>0,828</td>
<td>31,910</td>
<td>0,156</td>
<td>0,4952</td>
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<td>( C_{40}:5 )</td>
<td>14</td>
<td>2997</td>
<td>931,10</td>
<td>2,5454</td>
<td>0,3212</td>
<td>0,644</td>
<td>30,610</td>
<td>0,119</td>
<td>0,3755</td>
</tr>
<tr>
<td>( C_{40}:7 )</td>
<td>15</td>
<td>2998</td>
<td>930,14</td>
<td>2,7272</td>
<td>-0,0454</td>
<td>0,737</td>
<td>29,900</td>
<td>0,138</td>
<td>0,4372</td>
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<td>( C_{40}:9 )</td>
<td>13</td>
<td>2995</td>
<td>926,89</td>
<td>2,3636</td>
<td>0,6879</td>
<td>0,550</td>
<td>28,060</td>
<td>0,101</td>
<td>0,3174</td>
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<tr>
<td>( C_{40}:17 )</td>
<td>13</td>
<td>3000</td>
<td>924,15</td>
<td>2,3636</td>
<td>0,6879</td>
<td>0,550</td>
<td>28,060</td>
<td>0,101</td>
<td>0,3174</td>
</tr>
<tr>
<td>( C_{40}:26 )</td>
<td>11</td>
<td>2996</td>
<td>922,13</td>
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<td>0,357</td>
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<td>0,2046</td>
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<td>12</td>
<td>2993</td>
<td>924,07</td>
<td>2,1818</td>
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<td>0,455</td>
<td>21,710</td>
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<td>( C_{40}:31 )</td>
<td>11</td>
<td>2995</td>
<td>921,36</td>
<td>2,0000</td>
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<td>0,357</td>
<td>21,650</td>
<td>0,064</td>
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<td>1,7879</td>
<td>0,258</td>
<td>13,840</td>
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<td>3000</td>
<td>921,47</td>
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Table 1. Calculated values of topological indices for \( C_{40} \) isomers

Table 1 also includes some other predictors of fullerene stability taken from Refs. [10,25,26]: the pentagon adjacency index \( N_P \), the Wiener index \( W_I \), the resistance distance \( R_T \), the isolation index \( IS \) and the Aboav parameter \( A_R \). A comparative analysis of results leads to the following conclusions:

\( C_{40}:38 \) and \( C_{40}:39 \) isomers are characterized by the smallest pentagon adjacency index (\( N_P=10 \)). Moreover, \( C_{40}:38 \) fullerene has the lowest resistance-distance in the set (\( R_T=920,27 \)), whereas its Wiener index of 2994 is shared by two isomers (\( C_{40}:24 \) and \( C_{40}:30 \)) [10]. It seems that \( W_I \) is less efficient from the point of view of isomer discrimination. Considering the computed values of \( \Lambda(-1) \), \( \Omega(-1) \), \( \Lambda(1) \) and \( \Omega(1) \), we can conclude that all of them have the same minimum values for the isomers \( C_{40}:38 \) and \( C_{40}:39 \), namely, \( \Lambda(-1)=0.258 \), \( \Omega(-1)=13.840 \), \( \Lambda(1)=0.046 \) and \( \Omega(1)=0.1462 \). The maximum values belong to isomer \( C_{40}:1 \), namely, \( \Lambda(-1)=1.177 \), \( \Omega(-1)=37.450 \), \( \Lambda(1)=0.229 \) and \( \Omega(1)=0.7276 \). Moreover, the isomer \( C_{40}:1 \) has the highest pentagon adjacency index (\( N_P=20 \)), the highest Wiener index, (\( W_I=3035 \)), the highest resistance distance (\( R_T=955.15 \)), the highest isolation index (\( IS=3,6363 \)) and the lowest Aboav parameter (\( A_R=-1,8788 \)).

For stability prediction purposes, topological indices \( \Lambda(-1) \) and \( \Omega(-1) \) seem to be more efficient than \( \Lambda(1) \) and \( \Omega(1) \). In order to find a proper parameter choice for \( S \), further investigations are needed.
6. Conclusions

A simple method to estimate the stability of fullerenes on the basis of quantitative topological criteria has been presented. This approach is based on the concept of the generalized combinatorial curvatures defined on the set of simple graphs embedded on a closed surface without boundary (sphere, torus, projective plane, Klein bottle). The main conclusions are as follows:

a) By using the moments of the computed generalized combinatorial curvatures novel topological indices can be generated.

b) As a result of comparative tests performed on a set of $\text{C}_{40}$ and $\text{C}_{60}$ fullerenes, we concluded that the four topological shape factors ($\Lambda(-1)$, $\Omega(-1)$, $\Lambda(1)$ and $\Omega(1)$) could be successfully used to preselect the most stable fullerene isomers.

c) In order to find a proper choice of free parameter $S$ included in topological indices $\Lambda(S)$ and $\Omega(S)$, further detailed investigations are needed.

References


