

## MODELLING AND TOPOLOGY OF FULLERENES

The dodecahedron  $C_{20}$  structure has been modified to all possible fullerenes up to  $C_{40}$  with the help of simple isoperimetric transformations. The new type of rectangular  $5 \times 12$  matrix has been suggested for fullerenes. It has been shown that all modelled fullerenes have toroidal matrices ( $T$ -matrices). The symmetry character of  $T$ -matrices is correlated with the symmetry of corresponding fullerenes.

The discovery of the  $C_{60}$  fullerene (Buckminsterfullerene) [1,2] and carbon nanotubes [3,4] was preceded by theoretical works [5,6] which discussed possibility of their existence. Scientific journals are publishing yearly more than 2.000 articles devoted to fullerenes and nanotubes. The first book [7] on this topic has been published in 1995. Most of the papers are experimental in character. In our opinion, the fact that theory lags behind practice is due to the insufficiently developed language apparatus of the new field of chemistry. We have proposed the name *surfarenes* (from "surface" and "arenes") [8] for compounds built by surfaces that consist of  $sp^2$ -hybridized carbon atoms forming aromatic cycles. One of the typical difficulties bound up with projecting three-dimensional structures on the plane has been solved with the help of connected graphs. The latter ones have been called Schlegel diagrams [9]. In case of other polycyclic compounds graphs are used for setting up systematic names (according to the IUPAC rules). For that a Hamilton loop has to be constructed on a graph. It is possible to give the systematic name in case of the  $C_{60}$  fullerene which appears as follows:

hentriacontacyclo[29,29,0,0<sup>2,14</sup>,0<sup>3,29</sup>,0<sup>4,27</sup>,0<sup>5,13</sup>,0<sup>6,25</sup>,0<sup>7,12</sup>,0<sup>8,23</sup>,0<sup>9,21</sup>,0<sup>10,18</sup>,0<sup>11,16</sup>,0<sup>15,60</sup>,0<sup>17,58</sup>,0<sup>19,56</sup>,0<sup>20,54</sup>,0<sup>22,52</sup>,0<sup>24,50</sup>,0<sup>26,49</sup>,0<sup>28,47</sup>,0<sup>30,45</sup>,0<sup>32,44</sup>,0<sup>33,59</sup>,0<sup>34,57</sup>,0<sup>35,43</sup>,0<sup>36,55</sup>,0<sup>37,42</sup>,0<sup>38,53</sup>,0<sup>39,51</sup>,0<sup>40,48</sup>,0<sup>41,46</sup>] hexacontane [10].

This name is too bulky (232 signs) for practical use. It is only fit for reconstructing a structure of the compound. That is why it cannot be used for its identification (for example, for computer operations). At last there are fullerenes for which no Hamilton loop can be constructed. Therefore, universality, the obligatory requirement to a nomenclature system, is not satisfied here.

Until recently only two fullerenes,  $C_{60}$  and  $C_{70}$ , have been isolated and identified. Nevertheless a supersonic beam produced by laser vaporization of a carbon target contains a continuous series of carbon clusters with different numbers of carbon atoms, as it follows from the mass-spectrum (See Fig. 1).

Most likely, these clusters possess similar fulleroid structures. They can be hardly modelled and studied in terms of topology for lack of convenient procedures of constructing and comparing structures of possible fullerenes.

Isoperimetric transformations (IT) of fullerene graphs, in particular those that result in an increasing number of cycles, are of use for modelling fullerene structures. One of them consists in formation of an additional edge which divides one of hexagonal cycles into two cycles (two nodes, i.e. two carbon atoms, are added to a fullerene), the

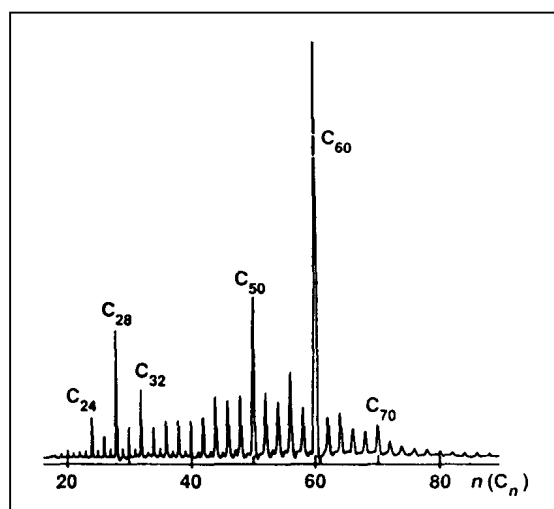


Fig. 1. Mass-spectrum of  $C_n$ -clusters [11].

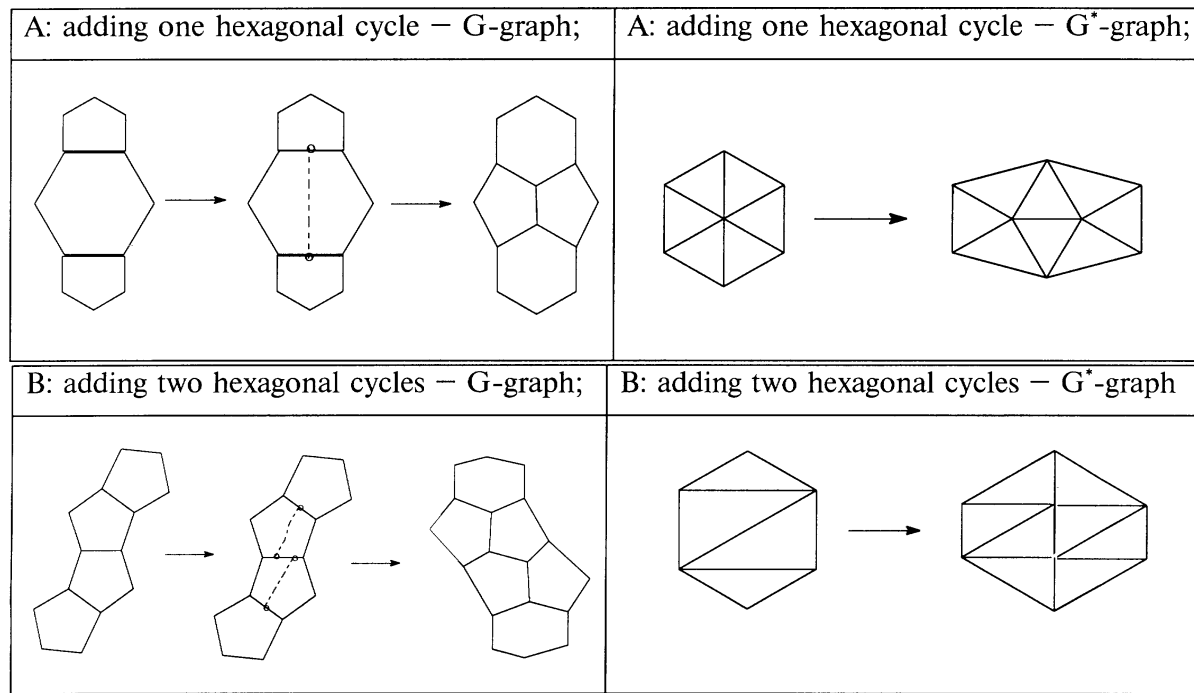


Fig. 2. A- and B-isoperimetric operations of fullerene modification.

Table 1. Fullerene graphs

$C_n$	Spatial fullerene graph	Planar graph – G	Dual graph – G*
$C_{34}$ -I			
$C_{34}$ -II			
$C_{38}$			

number of hexagonal cycles increasing by one (Fig. 2, A operation). As a result of another operation (B), two additional edges are added to neighbour pentagonal cycles, the number of hexagonal cycles increasing at once by two, but the obligatory presence of hexagonal cycles in an initial fullerene is not required.

Isoperimetry of the transformations is more obvious if dual graphs  $G^*$  [12] are used. We took the simplest  $C_{20}$  fullerene as the reference structure for modelling other fullerenes. Indirect evidences of  $C_{20}$  fullerene existence have been found by H. Prinzbach [13]. The B operation on  $C_{20}$  fullerene results in formation of the second member of the "family" –  $C_{24}$  fullerene. The latter is transformed with the help of the A operation into the only possible  $C_{26}$  fullerene. Similarly it is transformed into two isomers of  $C_{28}$  fullerene, the latter ones – into three  $C_{30}$  isomers. The numbers of possible isomers of  $C_{32}$ ,  $C_{34}$ ,  $C_{36}$ ,  $C_{38}$  and  $C_{40}$  fullerenes make up 6, 6, 15, 17 and 40 respectively.

Table 1 gives some examples of modelled fullerenes. It is important that one graph type can be easily transformed into the other one with the help of HyperChem computer program [14]. Such a procedure is assuming ever greater importance as the number of carbon atoms of a fullerene is increasing.

Similarly to other organic compounds, the structure of fullerenes can be represented as connectivity matrix. Such a matrix cannot be reduced to its canonical form, therefore, it cannot be used for comparison and identification. Using the fact that all (5,6)-fullerenes contain 12 pentagonal cycles, we have proposed a new matrix presentation which should describe fullerene structure. At first a Hamilton loop of go-round of the nodes of degree 5 is chosen on a dual  $G^*$  graph. Starting in each node from the ray which connects it to the previous node (a ray passes only through the node of degree 6 unimpeded), one has to go round all remaining rays clockwise. Each ray is

Table 2. Full fullerene T-matrices

<i>T-matrix of fullerene <math>C_{34-I}</math></i>											
5	65	65	5*	5	65	65	5*	5	65	65	5*
5*	5	65	65	5*	5	65	65	5*	5	65	65
65	5	5*	5	65	5	5*	5	65	5	5*	5
665	665	665	665	665	665	665	665	665	665	665	665
65	5*	5	5	65	5*	5	5	65	5*	5	5

<i>T-matrix of fullerene <math>C_{34-II}</math></i>											
65	65	65	65	6665	5*	5	6665	65	65	65	65*
65	5	5	5*	5	65	65	5*	5	5	5	65
65	5*	5	65	6665	65	65	6665	65	5*	5	65
5*	5	5*	5	5*	5	5*	5	5*	5	5*	5
5	65	6665	5	65	65	65	65	5	6665	65	5

<i>T-matrix of fullerene <math>C_{38}</math></i>											
5	65	65	5*	5	65	665	5*	5	65*	65	5*
65*	65	5	5	65*	65	5	665	65	666665	5*	5
65	665	5	5	65	65	5*	5	5*	5	5	6665
5	65	665*	665	665	65	665	5	65	65	5	665
5	5*	5	665	5	5*	5	665	65	666665	5	665

Table 3. Simplified T-matrix of  $C_{34}$ -II fullerene

-	I	I	*	-	I	2	*	-	I*	I	*
I*	I	-	-	I*	I	-	2	I	5	*	-
I	2	-	-	I	I	*	-	*	-	-	3
-	I	2*	2	2	I	2	-	I	I	-	2
-	*	-	2	-	*	-	2	I	5	-	2

characterized by degree of the nodes it passes through. The notation corresponding to a node takes up a column. Neighbour columns are conformed by a column of a common ray. Thus we obtain a rectangular 5x12 matrix for fullerene of any complexity.

We have been constructed matrices of 50 fullerenes. Each of them has such a Hamilton loop which enables to conform the first and the last columns. Thus a vertically cylindric matrix is obtained (See Tables 2-3). Because of a horizontally cylindrical character of the construction of columns, matrices have a toroidal symmetry and, therefore, can be called as toroidal matrices, or T-matrices.

Just a toroidal character makes matrices canonical, i.e. those that can be used for comparison and identification of fullerenes. T-matrices can be easily transformed back into graphs ( $G$  and  $G^*$ ) that belongs to their positive features.

Tables 2-3 present T-matrices of  $C_{34}$ -I,  $C_{34}$ -II and  $C_{38}$  fullerenes, the graphs of which are shown in Table 1. Nodes corresponding to next columns are marked with an asterisk. In the latter ones the designations of the same rays are set out opposite to an asterisk (but on the opposite side). Matrices are presented in a complete form, i.e. all nodes on rays are designated. A column containing node numbers makes a matrix more obvious but it can be omitted. All cells of matrices contain fives which can be also omitted by mutual agreement. Furthermore, sixes can be replaced by the numbers of them. A simplified form of a T-matrix is presented in Table 3. T-Matrices have the elements of the symmetry which is correlated with the symmetry of corresponding fullerenes.

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