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On Mathematical Properties of Buckminsterfullerene[#]

*Nenad Trinajstić**, *Milan Randić*** and *Douglas J. Klein*

*Department of Marine Science, Texas A&M University,
Galveston, Texas 77553-1675, USA*

Darko Babić

*The Rugjer Bošković Institute, P.O.B. 1016,
HR-41001 Zagreb, Croatia*

Zlatko Mihalić

*Faculty of Science, The University of Zagreb,
HR-41001 Zagreb, Croatia*

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»The essential fact is simply that *all* the pictures which science now draws of nature, and which alone seem capable of according with observational facts, are *mathematical* pictures«.

Sir James Jeans (1931)¹

Some of the mathematical properties of buckminsterfullerene are considered, that is, geometrical, topological, group-theoretical and graph-theoretical properties. These mathematical properties are used to predict several structural and chemical properties of buckminsterfullerene.

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* Permanent address: The Rugjer Bošković Institute, P.O.B. 1016, HR-41001 Zagreb, Croatia

** Permanent address: Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311, USA

INTRODUCTION

A pure carbon molecule consisting of 60 atoms, C_{60} , was discovered by Kroto, Heath, O'Brien, Curl and Smalley² in 1985 at Rice University in Houston. The molecule was imaginatively named buckminsterfullerene after the American architect Richard Buckminster Fuller (1895–1983). His pavillion in the shape of the geodesic dome was used to house the American exhibition at Expo '67 in Montreal and stimulated Kroto³ to propose the buckminsterfullerene name for C_{60} . It is perhaps interesting to mention here that Kroto almost went to work for Buckminster Fuller, but then the offer came from The University of Sussex and he remained in chemistry for the benefit of the subject. The discoverers of C_{60} were really after something else: They vaporized graphite by laser irradiation in a high-pressure supersonic nozzle in attempting to understand the mechanism by which long carbon-chains are formed in interstellar space and circumstellar shells.^{4–6} Their experiments, however, resulted in C_{60} , a cage molecule of unusual stability. It is clear from all documents that the discovery of C_{60} was serendipitous* (as many discoveries in science are).⁸ In this example one can readily see the vanity of epistemological discourses on the supposedly timeless rules of any »logic of scientific discovery«. The unexpected discovery by Kroto, Heath, O'Brien, Curl and Smalley² is much more online with Pasteur's famous dictum:⁹ »In the field of observation, chance favours the prepared mind« (Louis Pasteur (1822–1895) said this in an official address delivered at the Faculty of Sciences, University of Lille on December 7, 1854, when he became Professor of chemistry and Dean of the Faculty of Sciences there).¹⁰

The work by Kroto, Heath, O'Brien, Curl and Smalley² represents the initial contribution to a fast growing field of chemistry that is now known as fullerene chemistry.¹¹ The generic name *fullerenes* was proposed by Kroto for the family of carbon cages C_n ($n = 20, 24, 26, \dots$) and the decision to use this name was made during his telephone conversation with Alex Nickon when they discussed the problem of naming carbon cages.¹² Fullerenes also represent the third allotropic (and also the first molecular) form of carbon,¹³ the other two carbon allotropes being graphite (the most common form of carbon) and diamond (a sparkling, colorless and extremely hard crystal). In this sense fullerenes are inorganic compounds, but they participate in many typical organic reactions¹⁴ as well as in inorganic reactions.¹⁵

In 1990 buckminsterfullerene finally became available in macroscopic quantities via a remarkably simple procedure developed by Krätschmer *et al.*¹⁶ In spite of the work by Krätschmer *et al.*, the interest in preparation of C_{60} (and other fullerenes) by different routes is still a topic of considerable interest,¹⁷ and a method is also suggested which results in a substantial reduction in the cost of purifying C_{60} and C_{70} .¹⁸ The procedure by Krätschmer *et al.*¹⁶ made C_{60} and fullerenes readily available and caused an explosion of publications on various aspects of fullerene chemistry and physics. Fullerene papers are appearing almost on daily basis in all kinds of chemistry journals, in many physics journals and in journals of general science.¹⁹ Braun called this phenomenon quite appropriately »the epidemic spread of fullerene research«. ²⁰ A new journal has also appeared, entitled: »*Fullerene Science and Tech-*

* Derived from the word *serendipity* ((talent for) making fortunate and unexpected discoveries by chance)⁷ coined by the English writer Horace Walpole (1717–1797) from the Persian fairy tale *The Three Princes of Serendip*.

nology», entirely devoted to fullerenes. The shape of buckminsterfullerene is possibly more familiar now than any other molecular structure, apart perhaps from the hexagon representing benzene and the double helix modeling DNA. The impact of fullerenes on science is tremendous and is still difficult to assess.

Many interesting concepts concerning fullerenes, such as the three-dimensional (spherical) aromaticity²¹ or the »onion-like« soot forming mechanisms,^{4,22} have appeared in the literature.²³ The first clearest and best proposal relating to onion-scrolling around C_{60} -nucleus to form soot appeared in an article by the Rice University Group in 1986.²⁴ Also, within a year or so after this article appeared the very suggestive electron micrograph of Ijima²⁵ (though, actually, the picture was originally published in 1980 in the »*Journal of Crystal Growth*« without any chemical structural interpretation).²⁶ Many properties of C_{60} , ranging from its aromaticity to superconductivity when it is doped by alkali metals, are often discussed in the fullerene literature. However, it is less often mentioned that C_{60} is also highly interesting mathematical object.²⁷ Buckminsterfullerene was referred to by its discoverers as »unusually beautiful« and »uniquely elegant« molecule.² Hoffmann in a series of essays,²⁸ considered what makes a molecule beautiful. He pointed out that there are many factors which may trigger an aesthetic response of an individual chemist to a molecule. These are the shape or the structure of the molecule, the complex biological function that the molecule performs, the quantized motion that the molecule undergoes, the mystery of the mechanism of molecular construction by nature, *etc.* Perhaps the mathematical properties of buckminsterfullerene are part of the source of its beauty?

The aim of this article is to review some of the mathematical properties of C_{60} . Furthermore, we also wish to stress that physical and chemical properties of buckminsterfullerene are direct consequences of its mathematical properties.

The article is structured as follows. In the next two sections the geometry and topology of C_{60} are, respectively, discussed. In the fourth section, the symmetry properties of C_{60} are reviewed. The fifth section contains graph-theoretical studies performed on the graph representation of buckminsterfullerene. We end the article with the concluding remarks.

GEOMETRY OF BUCKMINSTERFULLERENE

The geometry of the σ -skeleton of buckminsterfullerene is modeled by the truncated icosahedron which is depicted in Figure 1.

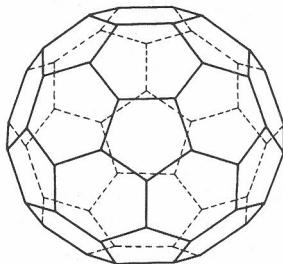


Figure 1. A model of buckminsterfullerene as truncated icosahedron.

The truncated icosahedron has 60 vertices, 90 edges and 32 faces, 12 of which are pentagonal and 20 hexagonal. Each pentagonal face is surrounded by hexagonal faces. Each vertex of the truncated icosahedron is populated by a carbon atom and each carbon atom is σ -bonded to three other carbon atoms along the edges of the truncated icosahedron. There are also 60 π -electrons available, which represent a π -electron quasi-sea in which the σ -skeleton of C_{60} is immersed. The front cover of the issue of »*Nature*« in which the buckminsterfullerene paper by Kroto, Heath, O'Brien, Curl and Smalley² appeared visualizes the above as the truncated icosahedron immersed in a cloud of dots (representing π -electrons).

The truncated icosahedron is one of 13 semiregular polyhedra known as the Archimedean polyhedra or Archimedean solids.²⁹ The first surviving description of Archimedean polyhedra is that by a Greek geometer Pappus of Alexandria who lived during the fourth century (around 320–340 C.E.).³⁰ It should be noted at this point that Archimedean polyhedra are formed by truncating regular polyhedra named Platonic polyhedra (or Platonic solids)²⁹ in various ways. Pappus of Alexandria explicitly attributes the invention of truncated Platonic polyhedra to Archimedes (287–212 B.C.E.). Hence, the name archimedene has also been proposed for C_{60} .³⁰ However, Haymet³¹ earlier proposed this name for a hypothetical carbon cage with 120 atoms C_{120} , modeled by the truncated icosidodecahedron containing 12 ten-membered rings, 20 six-membered rings and 30 four-membered rings.

The Archimedean polyhedra were rediscovered during the Renaissance by the painter and mathematician Piero della Francesca.^{23(c)} It was, however, Johannes Kepler (1571–1630) who catalogued the 13 Archimedean polyhedra in 1619 and gave them their now generally accepted names.³² Kepler also discovered a class of non-convex »semiregular« polyhedra, now known as the Keplerian polyhedra.

It has been already stated that the truncated icosahedron is a semiregular polyhedron. A semiregular polyhedron is a polyhedron whose faces are regular but different polygons and each of its vertices is symmetrically equivalent to every other. The truncated icosahedron can be generated from the icosahedron depicted in Figure 2.

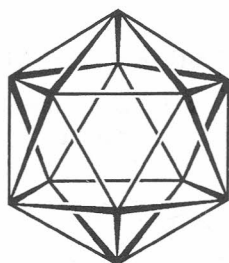


Figure 2. The structure of icosahedron.

The icosahedron is one of the five regular polyhedra and possesses 12 vertices, 30 edges and 20 trigonal faces. (A regular polyhedron is a polyhedron whose faces are identical regular polygons such that each of its vertices is symmetrically equivalent to every other). The icosahedron is truncated by cutting off each vertex along a plane perpendicular to the fivefold axis of symmetry at the vertex. Since each vertex

of the icosahedron is the meeting point of five triangular faces (see Figure 2), the new faces created by the decollation of vertices are necessarily pentagonal faces. Thus, the truncated icosahedron contains exactly 12 pentagons. The above process of vertex decollation forces the 20 trigonal faces of the icosahedron to convert into the 20 hexagonal faces of the truncated icosahedron. This process can easily be visualized in two-dimensions by converting an equilateral triangle into a regular hexagon by cutting off the vertices of the triangle.

But, though the buckminsterfullerene molecule has the symmetry of the semiregular truncated icosahedron, it is not realized to be strictly semiregular. That is,³³ the bonds radiating from pentagons are shorter than those on the sides of the pentagons, so that the hexagonal faces do not form regular hexagons (see discussion later in the text).

Let us end this section by mentioning that the surface structure of the slightly deflated modern soccerball (or football in Europe) resembles to the truncated icosahedron. This is the reason why soccerballene and footballene were also among the proposed names for C_{60} . Incidentally, the IUPAC name for C_{60} is rather clumsy, especially for oral communications:^{23,34}

hentriacontacyclo[29.29.0.0².14.0³.12.0⁴.59.0⁵.10.0⁶.58.0⁷.55.
0⁸.53.0⁹.21.0¹⁰.11.20.0¹³.18.0¹⁵.30.0¹⁶.28.0¹⁷.25.0¹⁹.24.0²².52.
0²³.50.0²⁶.49.0²⁷.47.0²⁹.45.0³².44.0³³.60.0³⁴.57.0³⁵.43.0³⁶.56.
0³⁷.41.0³⁸.54.0³⁹.51.0⁴⁰.48.0⁴².46]hexaconta-1,3,5(10),6,8,11,
13(18),14,16,19,21,23,25,27,29,(45),30,32(44),33,35(43),36,38
(54), 39(51),40(48),41,46,49,52,55,57,59-triacontaene.

TOPOLOGY OF BUCKMINSTERFULLERENE

The surface of any polyhedron in three-dimensional space is made up of two-dimensional faces, one-dimensional edges and zero-dimensional vertices. Euler's formula relates faces (f), edges (e) and vertices (v) as follows:²⁹

$$f - e + v = 2 . \quad (1)$$

This beautifully simple formula is the first formula in topology. Some have ranked Euler's formula as the second most beautiful mathematical formula.³⁵ Topology (»the rubber sheet geometry«) is the part of mathematics which deals with the way objects are connected, without regard to the straightness and metric.²⁹ There are a number of proofs of Euler's formula in the literature.³⁶

Euler's formula, of course, holds for the truncated icosahedron ($f=32$, $e=90$ and $v=60$):

$$32 - 90 + 60 = 2 . \quad (2)$$

Since each vertex in the truncated icosahedron is a meeting point of three edges, it is a trivalent vertex. Hence, this Archimedean polyhedron belongs to trivalent (or

3-regular) polyhedra. For these polyhedra the number of edges and the number of vertices are related by:

$$2 e = 3 v . \quad (3)$$

We will use this formula and Euler's formula, with an additional constraint that pentagonal and hexagonal faces are the optimum faces for carbon cages.^{27(a)} The number of edges in a polyhedron is also related to the number of n -sided faces (f_n):³⁷

$$2 e = \sum_n n f_n \quad (4)$$

where the summation is over all the faces of the polyhedron. Formulae (3) and (4) can be easily verified for the truncated icosahedron. One can rewrite Euler's formula (1) by equating $f = \sum f_n$

$$\sum_n f_n - e + v = 2 . \quad (5)$$

Variables e and v can be eliminated from Eq. (5) by means of Eqs. (3) and (4):

$$\sum_n (6 - n) f_n = 12 . \quad (6)$$

If we allow only pentagonal faces (f_5) and hexagonal faces (f_6) faces (based on the chemical stability arguments which suggest restrictions on ring sizes and preferences of sizes 5 and 6 over rings of sizes 3,4,7 and 8),^{38,39} then:

$$f_5 = 12 \quad (7)$$

and from Eqs. (3) and (5):

$$f_6 = v/2 - 10 . \quad (8)$$

In the case of buckminsterfullerene:

$$f_6 = 20 . \quad (9)$$

The importance of the above result is that Euler's theorem does not restrict the number of hexagonal faces on the surface of a polyhedral fullerene, but requires exactly 12 pentagons. The position of pentagonal faces on the surface of large fullerenes (C_n , $n \geq 60$) determines their stability because cages with abutting (adjacent) five-membered rings are less stable than those in which no two pentagonal rings abut.^{27(a),40} For example, among 1812 isomers⁴¹ of C_{60} , only buckminsterfullerene has no abutting five-membered rings and it is, consequently, predicted to be the most stable of all C_{60} -isomers.^{41(a)-(c)} Buckminsterfullerene is the first fullerene in which pentagons are completely surrounded by hexagons. All lower fullerenes (C_n , $n=20, 24, \dots, 58$) are destabilized to a certain degree by having two or more (depending on size) adjacent pentagonal rings, as are also^{41(a)} all other fullerenes of sizes 68, 66, 64, 62 or 60.

SYMMETRY OF BUCKMINSTERFULLERENE

We have already stated that the aesthetic appeal of buckminsterfullerene can perhaps be attributed to its symmetry characteristics. This section will be devoted to some of the symmetry properties of C_{60} . Symmetry is an attribute of a body's shape and does not depend on its size or its position in space. The theory of groups is the appropriate mathematical framework for formalizing symmetry.⁴²

Buckminsterfullerene belongs to the I_h point group,⁴³ with elements E , 12 C_5 , 12 C_5^2 , 20 C_3 , 15 C_2 , i , 12 S_{10} , 12 S_{10}^3 , 20 S_6 and 15 σ_h . Therefore, the order of the buckminsterfullerene symmetry group is 120. The irreducible representation, of the I_h group associated to the π -MO eigenvectors of buckminsterfullerene, are as follows:⁴⁴

$$\Gamma = a_g(1) + t_{1g}(3) + t_{2g}(3) + 2g_g(4) + 3h_g(5) + 2t_{1u}(3) + 2t_{2u}(3) + 2g_u(4) + 2h_u(5) . \quad (10)$$

The numbers in the parentheses indicate degeneracies, that is:

$$1 \times 1 + 1 \times 3 + 1 \times 3 + 2 \times 4 + 3 \times 5 + 2 \times 3 + 2 \times 3 + 2 \times 4 + 2 \times 5 = 60 .$$

Their use in factoring the adjacency matrix and the Laplacian matrix will be demonstrated in the next section.

As we have already stated, there are 1812 C_{60} -isomers. They differ considerably in their symmetry characteristics.^{43(d),45} These 1812 isomers may be classified according to their symmetries in the following groups:

$$C_1 (1508), C_s (67), C_2 (189), C_{2v} (9), C_{3v} (1), C_{2h} (4), D_2 (19), D_3 (3), D_5 (1), D_{2h} (1), D_{6h} (2), D_{2d} (4), D_{5d} (1), S_4 (2), I_h (1).$$

In the parentheses, numbers of C_{60} -isomers belonging to a given point group are given.

CONNECTIVITY IN BUCKMINSTERFULLERENE

The connectivity in a molecule is defined by the neighbourhood relationship, *i.e.*, atoms in the molecule are either bonded or not.⁴⁶ When considering connectivity, the actual bond lengths do not play a role, only the existence of a chemical bond is important. The mathematical tool that underlies connectivity is the theory of graphs.⁴⁷

Schlegel graphs

Projections of polyhedral objects are known as Schlegel diagrams.⁴⁸ Graphs which are used to depict polyhedra can be called Schlegel graphs if all vertices are at a finite distance from one another.⁴⁹ These are planar graphs. (A graph is planar if it can be drawn in the plane in such a way that no two edges intersect or, in other words, a graph is planar if it can be embedded in the plane). A graph in which every vertex has the same valency is called a regular graph. If every vertex in graph G has valency D , then G is said to be a regular graph of valency D or a D -regular graph. The Schlegel graphs representing regular (Platonic) and semiregular (Archimedean) polyhedra are D -connected graphs, with $D=3$ for C_{60} . The Schlegel graph of buckminsterfullerene is shown in Figure 3.

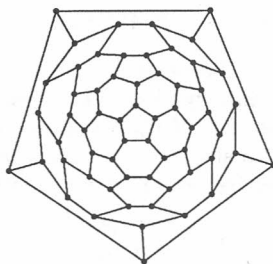
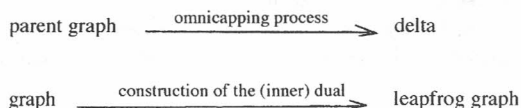


Figure 3. The Schlegel graph of buckminsterfullerene.

The leapfrog technique for generating higher fullerenes

A powerful graph-theoretical technique, called the leapfrog technique, was introduced by Fowler and coworkers^{43(d),50} for a systematic generation of certain fullerenes. The leapfrog technique consists of two steps: (1) the omnicapping process and (2) the construction of the dual (or perhaps the inner dual). The initial polycyclic (polygonal) graph is called the parent graph. The omnicapping process consists of putting a vertex in the center of each face (polygon) of the polycyclic graph and then connecting each newly created vertex with the vertices on the face boundary. This process generates a fully triangulated polycyclic graph, called the delta graph, from the parent graph. All faces in the delta graph are triangles. The dual of the delta graph is created in the following way. A vertex is placed in the center of each triangle of the delta graph (including the »outer« one) and, if two triangles have a common edge e , then these are joined by an edge e^* crossing only e . Alternatively one can cap the »outer« face and make an inner dual. This technique can also be used to generate many different classes of polycyclic graphs.⁵¹ The overall operation gives a novel polycyclic graph, called the leapfrog graph. An important point to emphasize is that the symmetry characteristics of the parent graphs and leapfrog graphs are the same.⁵² The leapfrog technique can be schematized as follows:



In the case of fullerenes the simplest example for the application of the leapfrog technique is generation of buckminsterfullerene from the smallest fullerene C_{20} modeled by the dodecahedron. The dodecahedron has 12 pentagonal faces. To simplify presentation, the dodecahedron will be represented by the corresponding Schlegel graph. The omnicapping process of the dodecahedral graph leads to the 32-vertex 60-face delta graph. Its 32 vertices are partitioned, according to their degrees, into twelve 5-valent and twenty 6-valent vertices. In the next step the dual of the delta graph is constructed by replacing each triangle by a vertex. In this process each 5-valent vertex becomes the center of a pentagonal face and each 6-valent vertex be-

comes the center of a hexagonal face of the delta graph. The final graph is a Schlegel graph of the truncated icosahedron, a geometric model of buckminsterfullerene. The above is diagrammatized in Figure 4. The construction of the inner dual of the delta is shown in Figure 5.

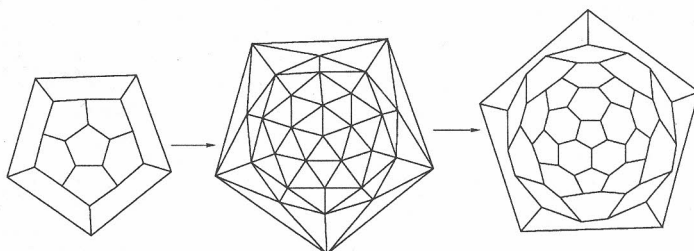


Figure 4. The construction of the Schlegel graph representing buckminsterfullerene from the Schlegel graph depicting dodecahedron by the leapfrog technique.

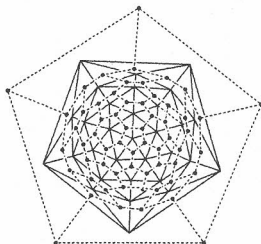


Figure 5. The dual graph obtained from the 32-vertex 60-face delta graph. The five outermost triangles are missing in order to avoid the abstruseness of the picture.

Another, fully equivalent, way of performing the leapfrog transformation is by taking first a dual of the fullerene graph and then truncating the vertices of the dual.⁵³ If we denote truncation, dualization and capping by T, D and C, then we evidently have $TD = DC$ (where as often done for operators to act on a space (here of polyhedra) we order from right-to-left). That is, there is an »algebra« (or actually a semigroup) of operations, which might also be extended, say to include the Archimedean operations of edge truncation and of »snubbing«.

Canonical labeling of the Schlegel graph corresponding to buckminsterfullerene

The (vertex-)adjacency matrix A of buckminsterfullerene is a 60×60 sparse matrix reflecting the connectivity of the structure. This matrix is shown in Table I. The entries in the matrix are 1's for the adjacent vertices and 0's for non-adjacent vertices.

TABLE II
 Canonical adjacency list for buckminsterfullerene.

Atom label	Labels of the adjacent atoms	Atom label	Labels of the adjacent atoms	Atom label	Labels of the adjacent atoms
1	60 59 58	21	44 29 28	41	50 40 12
2	60 57 56	22	38 27 26	42	28 14 12
3	59 57 55	23	32 27 22	43	46 20 11
4	60 54 53	24	29 26 25	44	52 21 10
5	58 54 52	25	31 24 23	45	30 11 10
6	59 51 50	26	28 24 22	46	43 33 9
7	55 51 49	27	37 23 22	47	55 35 8
8	57 48 47	28	42 26 21	48	17 9 8
9	56 48 46	29	30 24 21	49	39 16 7
10	54 45 44	30	45 29 20	50	58 41 6
11	53 45 43	31	25 20 19	51	13 7 6
12	52 42 41	32	23 19 18	52	44 12 5
13	51 40 39	33	46 19 17	53	56 11 4
14	42 40 38	34	35 18 17	54	10 5 4
15	39 38 37	35	47 34 16	55	47 7 3
16	49 36 35	36	37 18 16	56	53 9 2
17	48 34 33	37	36 27 15	57	8 3 2
18	36 34 32	38	22 15 14	58	50 5 1
19	33 32 31	39	49 15 13	59	6 3 1
20	43 31 30	40	41 14 13	60	4 2 1

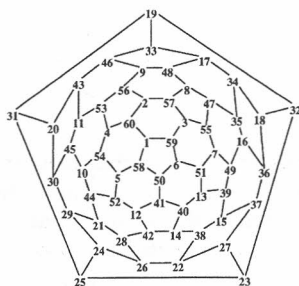


Figure 6. Canonical labeling of the Schlegel graph corresponding to buckminsterfullerene.

malized» form of the Hückel π -molecular theory (HMO).⁵⁷ In fact, the graph-spectral theory and Hückel theory are isomorphic theories.⁵⁸ Hence, one should refer to HMO as topological molecular orbitals (TMOs), which they indeed are.

If we need the HMO π -energy levels, we need only to diagonalize the adjacency matrix. However, the adjacency matrix of buckminsterfullerene is invariant under the action of the icosahedral symmetry group I_h , and thus it can be reduced to the block-diagonal form.^{44,59} Each block is associated with an irreducible representation of I_h and the block sizes are the multiplicities of such representations (see above). The factored Hückel determinant for buckminsterfullerene is given in Table III.

TABLE III

The subdeterminants resulting from the action of the icosahedral symmetry point group I_h on the Hückel determinant for buckminsterfullerene. Note ϕ is equal to $(\sqrt{5} + 1)/2$

Symmetry lable	Hückel subdeterminant
a_g	$ x + 3 $
t_{1g}	$ x - \phi^{-2} $
t_{2g}	$ x - \phi^2 $
g_g	$\begin{vmatrix} x + 1/2 & \sqrt{5}/2 \\ \sqrt{5}/2 & x - 3/2 \end{vmatrix}$
h_g	$\begin{vmatrix} x + 9/5 & 0 & 2\sqrt{6}/5 \\ 0 & x + 1/2 & \sqrt{5}/2 \\ 2\sqrt{6}/5 & \sqrt{5}/2 & x - 3/10 \end{vmatrix}$
t_{1u}	$\begin{vmatrix} x + \phi^2 & -\phi^{-1} \\ -\phi^{-1} & x \end{vmatrix}$
t_{2u}	$\begin{vmatrix} x & -\phi \\ -\phi & x + \phi^{-2} \end{vmatrix}$
g_u	$\begin{vmatrix} x & 2 \\ 2 & x - 1 \end{vmatrix}$
h_u	$\begin{vmatrix} x & 1 \\ 1 & x - 1 \end{vmatrix}$

There are also graph-theoretical approaches described in the literature for a simple computation of eigenvalues for buckminsterfullerene. Such approaches, like that of Davidson,⁴⁴ Dias,⁶⁰ and Hosoya and Tsukano,⁶¹ are based on the clever fragmentation of the Schlegel graph of buckminsterfullerene.

The HMO π -energy levels (corresponding to the graph-spectrum of buckminsterfullerene) in β units are diagrammatized in Figure 7. We note that the lowest eigenvalue is equal to -3.00 . This is a characteristic of regular graphs, for which the lowest eigenvalue is equal in magnitude to the valency of their vertices.

Hückel π -electron energy $E_\pi(\text{HMO})$ of buckminsterfullerene is equal to twice the sum of the occupied orbital energy levels, that is $E_\pi(\text{HMO}) = 93.168 \beta$. A simple type of Hückel resonance energy,⁶² HRE, for C_{60} is then given by:

$$\text{HRE}(C_{60}) = E_\pi(\text{HMO}) - 2 n_{C=C} = 33.17 \beta \quad (11)$$

where $n_{C=C}$ is the number of carbon-carbon double bonds in the molecule. Additionally the HRE per π -electron, HRE/e, is:

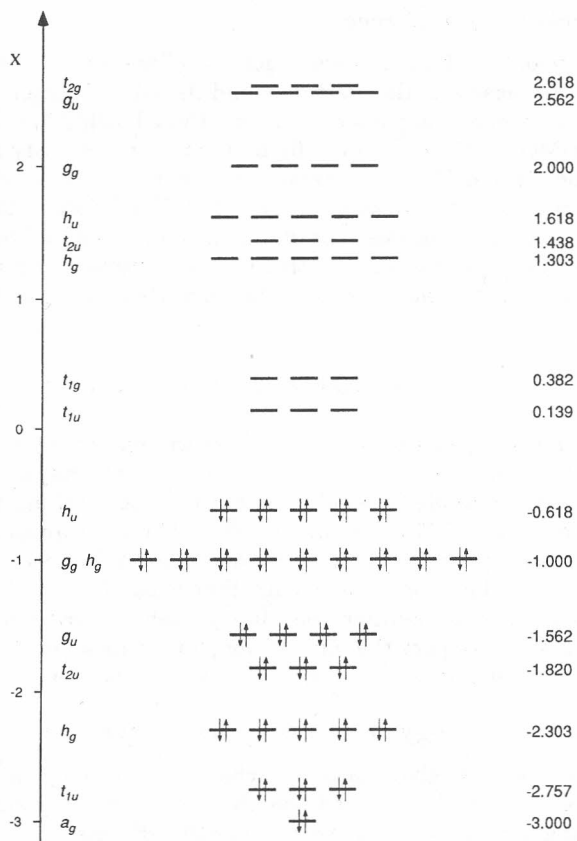


Figure 7. Hückel energy levels in units of the parameter β of buckminsterfullerene.

$$\text{HRE}(\text{C}_{60})/e = 0.55 \beta . \quad (12)$$

This value is higher than the HRE/e value (0.33β) for benzene, the prototype of an aromatic molecule. Other models of aromaticity, which are also based on the Hückel π -energies but have more elaborate reference structures, give the opposite result, that is, that buckminsterfullerene is less aromatic than benzene. Thus, the Zagreb group model,⁶³ in which the reference structure is approximated by two parameters, gives $\text{HRE}(\text{C}_{60})/e = 0.033 \beta$ and $\text{HRE}(\text{benzene})/e = 0.073 \beta$ and the Hess-Schaad model,⁶⁴ in which the reference structure is given in terms of six independent parameters, gives $\text{HRE}(\text{C}_{60})/e = 0.031 \beta$ and $\text{HRE}(\text{benzene})/e = 0.065 \beta$, though a more carefully parametrized version⁶⁵ gives $\text{HRE}(\text{C}_{60})/e = 0.0459 \beta$ and $\text{HRE}(\text{benzene})/e = 0.0706 \beta$. The above is seen even better if we consider, that the ratio $\text{HRE}(\text{C}_{60})/\text{HRE}(\text{benzene})$ for the considered models, that is, the Hückel model, the Zagreb model, the Hess-Schaad and the Galveston model, respectively, is as follows: 1.67, 0.45, 0.48 and 0.65.

Hardness of buckminsterfullerene

The Hückel theory for large systems such as fullerenes is a useful initial theoretical approach. For example, the inertness, and the vibronic interaction and intrinsic conductivity of buckminsterfullerene were studied using the Hückel theory.⁶⁶ Similarly, the HOMO-LUMO gap (0.757β), a qualitative reactivity index,⁶⁷ was also obtained from the Hückel MOs of buckminsterfullerene.⁶⁸ This index is also much smaller for buckminsterfullerene than benzene (HOMO-LUMO = 2β). Buckminsterfullerene and benzene also considerably differ in their absolute chemical hardness. The absolute hardness η has been introduced by Pearson, Parr and collaborators.⁶⁹⁻⁷¹ For the conjugated molecule it can be calculated using the following expression:^{72,73}

$$\eta = (\text{HOMO} - \text{LUMO})/2 \quad (13)$$

Absolute hardness appears to be a valuable reactivity criterion since it is defined in terms of frontier orbitals. The bigger the values of η , the harder a molecule, that is, it is a less reactive molecule. The values of hardness for buckminsterfullerene and benzene, respectively, are $0.378 (-\beta)$ and $1.000 (-\beta)$. These values show both molecules to be hard, but benzene to be much harder than buckminsterfullerene. Translated into the chemical language, this means that buckminsterfullerene is more reactive than benzene. Thus, neither the simple stability criteria nor the simple reactivity criteria fully support the supposition, sometimes encountered in the literature, that buckminsterfullerene is the 3D version of benzene.

Topological resonance energy of buckminsterfullerene

The adjacency matrix gives also the characteristic polynomial of a graph. Balasubramanian and Liu⁷⁴ computed the characteristic polynomial for buckminsterfullerene using the classical Le Verrier-Faddeev-Frame method,⁷⁵ adopted for use on the modern computers.⁷⁶ The Le Verrier-Faddeev-Frame method is a very convenient method for computing the characteristic polynomial of any matrix,⁷⁷ though it has historically been introduced for obtaining the characteristic polynomial of the adjacency matrix. The characteristic polynomial of buckminsterfullerene is shown in Table IV. Its zeros are, of course, identical to the Hückel eigenvalues reported in Figure 7.

Hosoya⁷⁸ has computed the matching⁷⁹ (alternatively called reference⁸⁰ or acyclic⁸¹) polynomial of buckminsterfullerene. This polynomial contains only contributions from qualified acyclic subgraphs of G (these are the same subgraphs that enter Sachs' construction of the characteristic polynomial,⁸² but only acyclic components make a contribution). Thus, the characteristic polynomial and the matching polynomial are closely related polynomials for any graph. They are, of course, identical for acyclic graphs. The matching polynomial of buckminsterfullerene is shown in Table V. Its zeros, because of the connection between the Hückel theory and graph-spectral theory, can also be presented as the energy levels of the reference structure corresponding to buckminsterfullerene. They are given in Figure 8. Note that the roots of the buckminsterfullerene matching polynomial do not show any degeneracies unlike its characteristic polynomial. Here we also point out that since the smallest face of C_{60} is pentagonal, its characteristic polynomial and the matching polynomial necessarily have the third coefficient identical.

TABLE IV

The characteristic polynomial of buckminsterfullerene

$$\begin{aligned}
& x^{60} - 90x^{58} + 3825x^{56} \\
& + 24x^{55} - 102160x^{54} \\
& - 1920x^{53} + 1925160x^{52} \\
& + 72240x^{51} - 27244512x^{50} \\
& - 1700640x^{49} + 300906380x^{48} \\
& + 28113600x^{47} - 2661033600x^{46} \\
& - 347208896x^{45} + 19180834020x^{44} \\
& + 3327625680x^{43} - 114118295000x^{42} \\
& - 25376437920x^{41} + 565407465144x^{40} \\
& + 156652575440x^{39} - 2346799508400x^{38} \\
& - 792175427520x^{37} + 8189116955350x^{36} \\
& + 3308173115904x^{35} - 24056403184260x^{34} \\
& - 11466942645600x^{33} + 59443188508110x^{32} \\
& + 33076275953760x^{31} - 123163094844616x^{30} \\
& - 79417625268960x^{29} + 212712221820840x^{28} \\
& + 158412719276240x^{27} - 303315997028160x^{26} \\
& - 261359090670624x^{25} + 351861389316780x^{24} \\
& + 354145195147200x^{23} - 324375523213200x^{22} \\
& - 390055074762240x^{21} + 228227031040884x^{20} \\
& + 344185906596720x^{19} - 122654402736360x^{18} \\
& - 238553091055200x^{17} + 29617003666920x^{16} \\
& + 126428882536240x^{15} + 4679380503120x^{14} \\
& - 49433493646080x^{13} - 8131429397135x^{12} \\
& + 13627897407360x^{11} + 3576552321006x^{10} \\
& - 2527365617120x^9 - 831616531095x^8 \\
& + 310065067080x^7 + 108565938200x^6 \\
& - 26034025632x^5 - 7440712560x^4 \\
& + 1566501120x^3 + 186416640x^2 \\
& - 54743040x + 2985984
\end{aligned}$$

TABLE V

The acyclic polynomial of buckminsterfullerene

$$\begin{aligned}
& x^{60} - 90x^{58} \\
& + 3825x^{56} - 102120x^{54} \\
& + 1922040x^{52} - 27130596x^{50} \\
& + 298317860x^{48} - 2619980460x^{46} \\
& + 18697786680x^{44} - 109742831260x^{42} \\
& + 534162544380x^{40} - 2168137517940x^{38} \\
& + 7362904561730x^{36} - 20949286202160x^{34} \\
& + 49924889888850x^{32} - 99463457244844x^{30} \\
& + 165074851632300x^{28} - 227043126274260x^{26} \\
& + 256967614454320x^{24} - 237135867688980x^{22} \\
& + 176345540119296x^{20} - 104113567937140x^{18} \\
& + 47883826976580x^{16} - 16742486291340x^{14} \\
& + 4310718227685x^{12} - 783047312406x^{10} \\
& + 94541532165x^8 - 6946574300x^6 \\
& + 269272620x^4 - 4202760x^2 \\
& + 12500
\end{aligned}$$

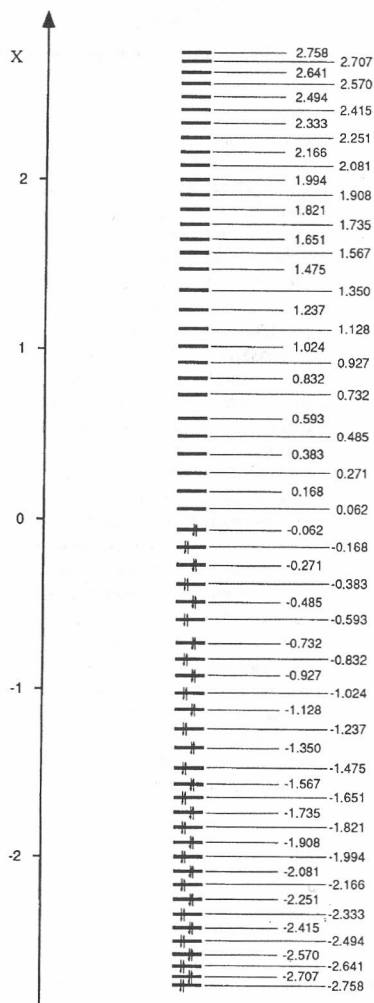


Figure 8. Energy levels in units of the parameter β corresponding to a reference structure for buckminsterfullerene.

The topological resonance energy (TRE) is a very useful measure of aromatic stability.^{80,81,83} It is defined as:

$$\text{TRE} = \sum_i g_i (x_i - x_i^{ac}) \quad (13)$$

where g_i is the number of π -electrons populating each bonding energy level of a molecule, the x_i 's are solutions of the Hückel determinant corresponding to the π -energy levels depicted in Figure 7 and x_i^{ac} 's are solutions of the matching polynomial (cor-

responding to a reference structure, see Figure 8). The TRE/e value of buckminsterfullerene is 0.027β , while TRE/e for benzene is 0.045β .⁸³ The ratio $\text{TRE}(\text{C}_{60})/\text{TRE}(\text{benzene}) = 0.60$ is in this case, much closer to the Galveston model than to the Hückel model as reported above. These results again confirm that buckminsterfullerene is an aromatic molecule, but less stable than benzene. After the initial experimental results suggested that buckminsterfullerene was indeed an aromatic molecule, there doubts were expressed in the literature about its aromaticity.⁸⁴ There are also, of course, other opinions expressed in the literature.⁸⁵ However, one of the reviewers of this paper pointed out quite strongly that C_{60} is an ethylene-like molecule and that chemical and physical evidences now agree that this is not an aromatic molecule in any conventional sense.

VB model of C_{60}

The last coefficient of the matching polynomial is equal to the number of Kekulé structures (K) of buckminsterfullerene, that is $K = 12,500$. The principal Kekulé structure (having every double bond in the maximum number, *i.e.*, 2, of conjugated circuits) of buckminsterfullerene is shown in Figure 9.

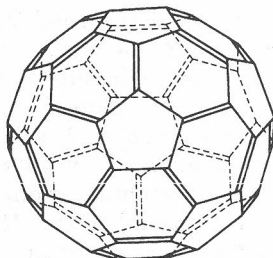


Figure 9. The principal Kekulé structure of buckminsterfullerene.

In this Kekulé structure of buckminsterfullerene every hexagonal face is represented by a Kekulé structure of benzene. This valence structure has the maximum number (20) of Kekulé benzene rings. It should be the most important Kekulé structure of buckminsterfullerene according to the Fries rule,^{53(b),86} which precedes the early VB method. The Fries rule is an empirical rule which states that the Kekulé structures with the largest number of Kekulé benzene rings are dominant. The principal Kekulé structure of buckminsterfullerene possesses the full symmetry of the molecule. Cyvin and co-workers studied recently the characteristics of the buckminsterfullerene Kekulé structures.⁸⁷

There are two types of bonds in buckminsterfullerene: bonds inside pentagonal faces and bonds between six-membered rings. Using Pauling's bond orders⁸⁸ and Pauling-Brockway-Beach's bond order-bond length relationship,⁸⁹ one obtains⁹⁰ a bond order of 0.28 for a bond separating pentagonal and hexagonal rings, and a bond order of 0.44 for a bond separating two hexagonal rings. The associated carbon-carbon bond lengths are 1.433 Å and 1.403 Å. Therefore, buckminsterfullerene is predicted to have 30 bonds of length 1.403 Å and 60 bonds of 1.433 Å. The Kekulé structure of buckminsterfullerene shown in Figure 9 is in accord with the above geometry.

Kekulé structures can be also used to compute the resonance energy of buckminsterfullerene by means of the simple VB model named the conjugated-circuit model.⁹¹ A graph-theoretical analysis of Kekulé structures leads to the concept of conjugated circuits. The conjugated circuits are those circuits within the Kekulé structure in which there is a regular alternation of carbon-carbon formal single and double bonds. Hence, the conjugated circuits are necessarily of even length. The circuit decomposition of an individual Kekulé structure gives conjugated circuits of sizes $4n + 2$ (denoted by R_n) and/or $4n$ (denoted by Q_n). The conjugated circuits may be enumerated in a number of ways,⁹² but in the case of molecules with rotational or translational symmetry the method based on the transfer-matrix represents a very efficient and elegant procedure for obtaining the number of conjugated circuits for a molecule.⁹³ The conjugated circuits can be used to generate REs using the following expression:

$$RE = \sum_n (r_n R_n + q_n Q_n) / K \quad (14)$$

where K is the Kekulé-structure count for the molecule, R_n and Q_n are, respectively, oppositely signed parameters corresponding to $4n + 2$ and $4n$ conjugated circuits and r_n and q_n are, respectively, the total counts of R_n and Q_n circuits in all Kekulé structures of the molecule. The parameter R_n measures the extent by which a specific conjugated circuit of size $4n + 2$ influences positively the thermodynamic stability of a conjugated molecule and, thus, it contributes toward the aromatic stability of the system. On the other hand, the parameter Q_n measures the extent by which a specific conjugated circuit of size $4n$ influences negatively the thermodynamic stability of a molecule and, thus, has a destabilizing effect on the aromatic stability of the molecule. In practical computations of the REs for fullerenes, the set of conjugated circuits may often be truncated at circuits of size ten.⁹⁰ The parametric values taken from Randić *et al.*^{91,94} ($R_1 = 0.869$ eV, $R_2 = 0.247$ eV, $Q_1 = -0.781$ eV and $Q_2 = -0.222$ eV) lead to:

$$RE = (83160 R_1 + 59760 R_2) / 12500 = 6.6528 R_1 + 4.7808 R_2 \quad (16)$$

$$RE = 6.96 \text{ eV} \quad (17)$$

$$RE/60 = 0.12 \text{ eV} . \quad (18)$$

Thus, the conjugated-circuit model also predicts benzene to be more aromatic ($RE/6 = 0.14$ eV) than buckminsterfullerene. However, the ratio $RE(C_{60})/RE(\text{benzene}) = 0.86$ is higher than for any of the above MO aromaticity models, but for the original HMO model.

The number of spanning trees in buckminsterfullerene

The final point we wish to discuss in this section concerns the Laplacian matrix of buckminsterfullerene and the computation of the spanning trees in buckminsterfullerene. A spanning tree of a graph G is a connected acyclic subgraph containing all the vertices of G . The concept of spanning tree underlies McWeeny's method⁹⁵ for computing π -electron »ring-current« magnetic properties of conjugated molecules⁹⁶

and has also been used in attempts to quantify the complexity of a molecule.⁹⁷ One way to compute the number of the spanning tress of buckminsterfullerene is the procedure based on the spectrum of the Laplacian matrix.⁹⁸

The Laplacian matrix L of a graph (molecule) is defined as:^{97(a)}

$$L = V - A \quad (19)$$

where V is the degree (valency) matrix and A is the adjacency matrix of the graph. The degree matrix V is a diagonal matrix whose entries are vertex degrees.

The number $t(G)$ of spanning trees of a graph G can be computed from the spectrum $x_i(L)$ of the Laplacian matrix:^{97(a)}

$$t(G) = (1/N) \prod_{i=2}^N x_i(L) \quad (20)$$

(where i labels the eigenvectors in order of increasing eigenvalue).

Since all vertices in buckminsterfullere are of degree 3, its Laplacian matrix is simply the adjacency matrix with negative entries and 3's on the diagonal.

The diagonalization of the Laplacian matrix again can be considerably simplified by utilizing the irreducible representations of the I_h point group. Hence, the determinant of the 60×60 Laplacian matrix can be broken into blocks in the same way as it was done with the adjacency matrix. The spectrum of the Laplacian matrix of buckminsterfullerene is closely related to the spectrum of the adjacency matrix because the graph of C_{60} is regular. The eigenvalues of the Laplacian matrix can be obtained simply by subtracting the eigenvalues of the adjacency matrix from the common degree of vertices in buckminsterfullerene, that is 3. The spectrum of the Laplacian matrix of buckminsterfullerene is given in Table VI.

It should be noted that the first Laplacian eigenvalue is always zero. This can be easily seen if we write down the expression for the first Laplacian eigenvalue of a D -regular graph:

$$x_1(L) = D - x_1(A) \quad (21)$$

and then substitute $D=3$ and $x_1(A)=3$.

Using Eq. (20) and the Laplacian spectrum given in Table VI we obtain the following value for the number of spanning tress in buckminsterfullerene by hand computation:⁹⁹

$$t(G) = 2^{27} \times 3^5 \times 5^4 \times 11^5 \times 19^3 / 2^2 \times 3 \times 5 = 2^{25} \times 3^4 \times 5^3 \times 11^5 \times 19^3 \quad (22) \\ = 375,291,866,372,898,816,000 .$$

This number agrees with the value obtained by more involved machine computations.¹⁰⁰

The mechanism of formation of buckminsterfullerene

The mechanism of formation of buckminsterfullerene is not yet understood.¹⁰¹ One may examine the possibility of assembling the molecule from a set of identical fragments. Although it might seem unrealistic to suppose that in chaotic conditions, as they are in carbon plasma,¹⁰² only a single type of fragment adds into a growing

TABLE VI

The spectrum of the Laplacian matrix of buckminsterfullerene

Eigenvalue	Multiplicity
0	1
$[9\sqrt{2} - \sqrt{10} - 2\sqrt{(19-\sqrt{5})}]/4\sqrt{2}$	3
$(5 - \sqrt{13})/2$	5
$[9\sqrt{2} + \sqrt{10} - 2\sqrt{(19+\sqrt{5})}]/4\sqrt{2}$	3
$(7 - \sqrt{17})/2$	4
2	9
$(7 - \sqrt{5})/2$	5
$[9\sqrt{2} - \sqrt{10} + 2\sqrt{(19 - \sqrt{5})}]/4\sqrt{2}$	3
$(9 - \sqrt{5})/2$	3
$(5 + \sqrt{13})/2$	5
$[9\sqrt{2} + \sqrt{10} + 2\sqrt{(19 + \sqrt{5})}]/4\sqrt{2}$	3
$(7 + \sqrt{5})/2$	5
5	4
$(7 + \sqrt{17})/2$	4
$(9 + \sqrt{5})/2$	3

cage, mathematical implications of this hypothesis might be of importance for a synthesis of fullerenes in less vigorous conditions. A recent study^{103,104} showed that buckminsterfullerene may be built up from carbon chains with 2, 3 or more atoms. It is in full accord with the finding that buckminsterfullerene possesses a Hamiltonian cycle (a cycle passing exactly once through all atoms). There are^{34(b)} 1090 different ways in which a Hamiltonian cycle may be realized in the buckminsterfullerene graph, but only 16 of them are so different that they cannot be interconnected by the symmetry operations. It was a bit surprising to find¹⁰⁴ that buckminsterfullerene cannot be assembled from star-shaped fragments composed of four carbon atoms, but that it is possible to construct it from isoprene-like monomers in many different ways (2420).¹⁰⁵

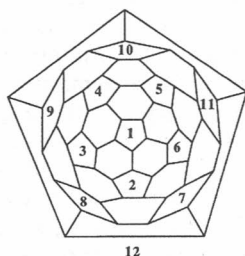
The results obtained by Diederich *et al.*¹⁰⁶ implied that two C_{30} rings may coalesce into buckminsterfullerene. There is also an older scheme by McKee and Herndon that describes how to make C_{60} out of two C_{30} .¹⁰⁷ The fact that it can be realized in only two different ways¹⁰⁴ means that the coalescence process is subject to stringent conditions.

Characterization of fullerenes

Characterization of fullerenes is an important subject since the numerous different but structurally similar isomers pose serious difficulties to chemical nomenclature. Chemists also need some practical tools to get orientation in the space of fullerene isomers. One can try, for example, to characterize the fullerene isomers by using topological indices, as it has been done in the case of the C_{60} isomers¹⁰¹ and C_{76} isomers.¹⁰²

One of the interesting proposals is the characterization of fullerenes by the distance matrix of pentagons.¹⁰³ The element of the matrix is the distance between the two pentagons determined by the corresponding row and column of the matrix, as

measured by the number of edges on the shortest path concerning two vertices of the pentagons. For buckminsterfullerene, this matrix is given in Figure 10, together with its spectrum.



$${}^5D = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 4 & 4 & 4 & 4 & 4 & 7 \\ 1 & 0 & 1 & 4 & 4 & 1 & 1 & 1 & 4 & 7 & 4 & 4 \\ 1 & 1 & 0 & 1 & 4 & 4 & 4 & 1 & 1 & 4 & 7 & 4 \\ 1 & 4 & 1 & 0 & 1 & 4 & 7 & 4 & 1 & 1 & 4 & 4 \\ 1 & 4 & 4 & 1 & 0 & 1 & 4 & 7 & 4 & 1 & 1 & 4 \\ 1 & 1 & 4 & 4 & 1 & 0 & 1 & 4 & 7 & 4 & 1 & 4 \\ 4 & 1 & 4 & 7 & 4 & 1 & 0 & 1 & 4 & 4 & 1 & 1 \\ 4 & 1 & 1 & 4 & 7 & 4 & 1 & 0 & 1 & 4 & 4 & 1 \\ 4 & 4 & 1 & 1 & 4 & 7 & 4 & 1 & 0 & 1 & 4 & 1 \\ 4 & 7 & 4 & 1 & 1 & 4 & 4 & 4 & 1 & 0 & 1 & 1 \\ 4 & 4 & 7 & 4 & 1 & 1 & 1 & 4 & 4 & 1 & 0 & 1 \\ 7 & 4 & 4 & 4 & 4 & 4 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

Spectrum of the 5D matrix: $\{2, 2, 2, 2, 2, -0.29, -0.29, -0.29, -13.71, -13.71, -13.71, 32\}$

Figure 10. The characterization of buckminsterfullerene by the distance matrix 5D of pentagons.

CONCLUDING REMARKS

In this article we have discussed several mathematical properties of a »uniquely elegant« molecule, attractively called buckminsterfullerene, a parent of the whole family of carbon cages named fullerenes. IUPAC and CAS seem to have remained relatively quiet about these names (although Dr Alan L. Goodson from CAS in his discussion at 208th American Chemical Society National Meeting – Applications of Graph Theory to Chemical Structure Representation and Structure-Activity Studies: Skolnik Award Symposium in Honor of A. T. Balaban (August 23, 1994) mentioned that they are quietly investing a considerable efforts to come up with rational names for carbon cages). However, the cover page of the *Journal of Chemical Education*, August issue of 1993 (volume 70, number 8), had a Schlegel diagram of buckminsterfullerene with the invitation beneath the diagram: »Name This Compound«. In the same issue there is an article by David Eckroth¹¹¹ entitled: »The Correct von Baeyer Name for (Buckminster)-fullerane«, which, however, seems not to be quite correct, as pointed out by Balaban *et al.*^{34(b)}

We have considered the geometrical, topological, group-theoretical and graph-theoretical properties of buckminsterfullerene. The geometry of buckminsterfullerene is depicted by the truncated icosahedron because all available early experimental data,^{33,112} pointed to such a geometry for this hollow carbon cage. The discovery of buckminsterfullerene has also had an impact on mathematics by reviving the interest in Platonic and Archimedean solids. Topological studies on buckminsterfullerene reveal that its surface must have 12 pentagonal rings and 20 hexagonal rings. The relationship between these rings is determined by simple energy arguments based on chemical experience (but also on semi-quantitative arguments, such as Hückel's $4n + 2$ rule, Dewar's PMO theory and the loop rule)^{38,39,113} which teach us, first, that 5- and 6-membered rings are more stable than 3-, 4-, 7- and 8-membered rings and, second, that energetically more favourable situations are these when 5-membered rings are not adjacent but surrounded with 6-membered rings. It should also be noted that every time a 7-membered ring is introduced into a fullerene, a 5-membered ring also needs to be introduced and thereby fullerene loses two hexagons and gets destabilized. Fowler and Steer^{50(b)} proposed the $6n+60$ ($n = 0, 2, 4, 6, \dots$) rule analogous to $4n+2$ ($n=1, 2, \dots$) rule for predicting stable giant fullerenes.¹¹⁴ The $K(4n+2)$ rule (K =natural integer, $n=0, 1, 2, 3, \dots$),¹¹⁵ has also been proposed but it has been shown to be of limited validity.¹⁰³

Buckminsterfullerene belongs to the I_h point group which was not so long ago considered by many to be of no importance for chemistry, so lists of character tables have often omitted that for I_h . But, this belief was shattered by the appearance of buckminsterfullerene on the chemical stage and presumably the icosahedral group will find its way now in standard chemistry texts on symmetry. The symmetry arguments help to reduce labour in diagonalizing the adjacency matrix and the Laplacian matrix of buckminsterfullerene and in addition they provide quantum numbers. NMR, UV, IR, Raman spectra are easily deciphered using the selection rules based on the buckminsterfullerene symmetry characteristics. Finally, the graph-theoretical analysis of buckminsterfullerene has proved to be a fertile area for obtaining many results of practical significance, such as predicting qualitatively the aromaticity and reactivity of the molecule. Besides, the combinatorial graph theory has also helped to obtain, in a simple way, the number of Kekulé structures and the number of spanning trees of buckminsterfullerene. Similarly, the number of C_{60} -isomers was found, and it was proved, on the basis of the graph-theoretical arguments coupled with a rather simple chemical reasoning, that the most stable structures among 1812 isomers is precisely buckminsterfullerene, a single C_{60} -isomer in which all 5-membered rings are separated by 6-membered rings.

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SAŽETAK

O matematičkim svojstvima buckminsterfullerena

N. Trinajstić, M. Randić, D. J. Klein, D. Babić i Z. Mihalić

Razmatrana su neka matematička svojstva buckminsterfullerena (npr. geometrijska, topologijska, grupno-teorijska i graf-teorijska svojstva). Neka od tih matematičkih svojstava uspješno su uporabljena za predviđanje niza strukturnih i kemijskih svojstava buckminsterfullerena.