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On the Aromatic Stability of a Conjugated C_{60} Cluster*

Milan Randić

*Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311 and Ames Laboratory-DOE**, Ames, Iowa State University, Ames, Iowa 50011, USA*

Sonja Nikolić and Nenad Trinajstić

The Rugjer Bošković Institute, P.O.B. 1016, 41001 Zagreb, Croatia, Yugoslavia

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The aromatic stability of recently reported conjugated sixty-carbon system of spherical shape (representing a truncated icosahedron and named buckminsterfullerene) is discussed. Buckminsterfullerene is predicted by a majority of theoretical methods to be aromatic compound with the degree of aromaticity smaller than that of benzene.

INTRODUCTION

The recent formation[1] of the sixty-carbon cluster C_{60}, which has the geometry of truncated icosahedron and exhibits unusual stability[2-3] that has yet to be properly understood, has opened up a new perspective in the chemistry of aromatic structures. The spherically shaped molecular skeleton of this sixty-carbon atom cage (see Figure 1) represents one of the thirteen polyhedra built from regular polygons,[4] already described by Archimedes, and known as the Archimedean semi-regular polyhedra.[5,6]

The Archimedean polyhedra were rediscovered during the Renaissance, because Archimedes work on the subject appears to have been forgotten,[7] and for the first shown in 1619 in Kepler's *Harmonice Mundi.*[8] It was Kepler also who gave the Archimedean polyhedra their now generally accepted names

The graphs (diagrams) which are used to depict polyhedra are called Schlegel graphs (diagrams).[9] These are planar graphs which are 3-connected.[10] The Schlegel graphs representing Archimedean polyhedra are vertex transitive, *i. e.* all vertices are equivalent. The Schlegel diagram depicting a sixty-carbon cluster is given in Figure 2.

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The truncated icosahedron has 60 vertices, 90 edges, and 32 faces, 12 of which are pentagonal and 20 hexagonal. This geometrical structure is of considerable interest in the design of geodesic polyhedra, *i. e.* polyhedra constructed on the surface of a sphere by a network of intersecting geodesic lines (*e. g.* line segments on great circles). R. Buckminster Fuller[11-13] developed the art of construction of geodesic (dome-like) polyhedra and the name buckminsterfullerene was suggested by Kroto *et al.*[1] for the sixty-carbon cluster with the geometry of a truncated icosahedron. This connection between structures in chemistry and architecture has been recognized for some time.[14]

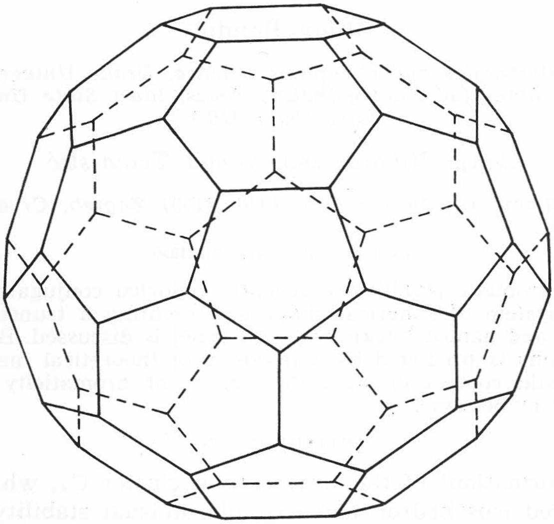

Figure 1. The assumed soccerball-like structure of buckminsterfullerene

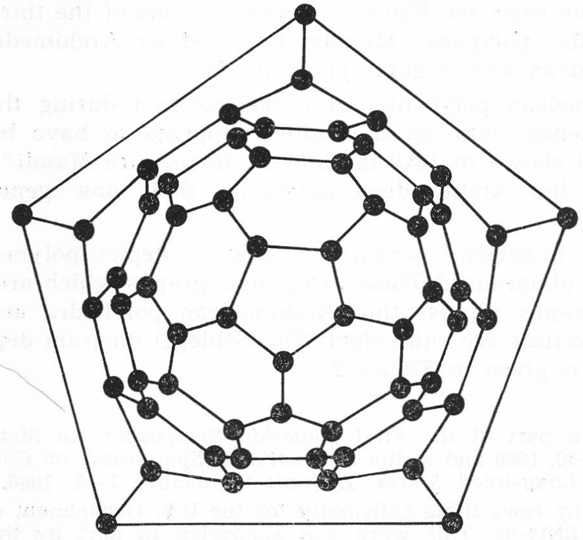

Figure 2. The Schlegel graph representing buckminsterfullerene

Another name which could be used for a sixty-carbon cage is soccerballene, because of its structural similarity with the surface structure of the modern soccerball. Other trivial names have been put forward,[15] but we will refer to the molecule as buckminsterfullerene or soccerballene.[16]

It appears that the first time that buckminsterfullerene was mentioned in the literature was in 1973 by Bochvar and Gal'pern as a hypothetical systems.[17]* They named this molecule carbo-s-icosahedron. Buckminsterfullerene was also predicted by Davidson[18] to be a stable carbon cluster and he also suggested a way of preparing the molecule by pyrolytic routes from carbon polymers.

Buckminsterfullerene is an important molecule for many reasons.[1–3,19] Below we give some of them. Since buckminsterfullerene appears to be remarkably stable under the most violent reaction conditions, it is conjectured[1] that it may be widely distributed in the Universe. This molecule may also appear to be valuable for understanding surface-catalyzed chemical processes which lead to the formation of interstellar molecules.[20,21] The diameter of the inner cavity of buckminsterfullerene is approximately 7 Å, so it may be possible to put other atoms or even small molecules inside, provided a mechanism allows the formation of such cage species. Heath *et al.*[22] have obtained convincing evidence for a uniquely stable metal binding site on some of the carbon cages in the range C_{44}—C_{80} which is plausibly explained on the basis of a central caged position.

Buckminsterfullerene, with a foreign atom in the cavity, may exhibit unusual properties, such as, for example, an extraordinary chemical shift in the NMR of the central atom because of the ring currents. It may be possible to change the »outside« surface of buckminsterfullerene by saturating some or all of the CC double bonds, producing structures that will retain spherical shape, such as for instance $C_{60}F_{60}$ which might be a superlubricant. Finally, it is of interest to consider whether the molecular ions are stable,[3] and in particular, determine the difference in the relative stabilities of anions and cations, if significant. All this indicates that buckminsterfullerene is a molecule worthy of further experimental studies. A synthetic route to buckminsterfullerene woud be an especially atractive achievement.[23]* In addition, this molecule is certainly also attractive for theoretical studies.

In the present note we wish to report some theoretical results on the aromatic stability of buckminsterfullerene. We will try to calculate its resonance energy and compare it with benzene, the paradigm of 2-dimensional aromatic structures.[24,25] Resonance energy (*RE*) is a parameter that represents a measure of the intrinsic stability of a conjugated molecule. *RE* is defined as that part of the molecular binding energy which is not accounted for by bond additivity. This extra stability, present in some conjugated systems, is associated with the aromatic character of such compounds, and one speaks of aromatic stability in polycyclic conjugated systems.

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* However, Professor D. J. Klein (Galveston) informed us in the letter of August 13, 1986 that he has found an article, written in the Japanese and published in 1971, which might be an earlier discussion of C_{60}.

* An attempt to synthesize buckminsterfullerene is under way (H. W. Kroto, private communication, September 3, 1986; R. Taylor, private communication, October 17, 1986).

ON THE RESONANCE ENERGY ESTIMATES FOR BUCKMINSTERFULLERENE

This molecule introduces an important novelty to the chemistry of *conjugated* systems: it is a molecule without a periphery. The only other case, in the ideal infinite limit, is graphite. It is therefore of considerable interest to study the topological and combinatorial as well as the electronic properties of such a system. The novelty of the structure is also reflected in the difficulties of extending present schemes and algorithms. In part, of course, this is due to the relatively large size, but in addition it is also due to its novel topology. Such difficulties include the derivation of a systematic name within existing schemes, which involve labelling vertices, counting valence structures, and enumerating various graph-theoretical as well as structural invariants for the molecule.

The molecule is the first example (if we exclude infinite graphite) of a fully conjugated carbon structure. Hence, the usual classification of conjugated compounds such as conjugated hydrocarbons and heteroconjugated systems is no longer valid! We have, in buckminsterfullerene, the first case of a truly conjugated carbon compound.

The σ-skeleton of buckminsterfullerene may be approximately described by the overlap of sp^2 hybrid orbitals with $\sim 120^\circ$ angles. Strictly speaking, we should not talk of σ and π electrons (or orbitals), which implies the presence of a plane of symmetry. Instead we should use symmetry labels for the icosahedral group to which structure belongs, but because *locally* the carbon atom environment does not deviate too much from planarity it is satisfactory to continue to use the symbols σ and π as electron labels. The π orbitals are highly delocalized over the spherically shaped structure. The deviation from planarity at each carbon center is indicated by the dihedral angles known to be:[26] 138°11′ between hexagon faces and 142°37′ for pentagon-hexagon faces.

Buckminsterfullerene is a non-alternant molecule (*i. e.*, it has odd-membered rings), but as a result of the symmetry of the molecule (*i. e.*, icosahedral symmetry including inversion) the charge densities are all equal.

The size of buckminsterfullerene is such that it is difficult to guess the number of Kekulé structures, except to expect a large number.[1] Recently two independent studies indicated that K, the number of Kekulé valence structures, of C_{60} is 12,500. First to report K for the molecule were Klein and collaborators,[27] who used an elegant operator technique — the transfer matrix method, developed previously for counting the Kekulé structures of very large conjugated strips.[28,29] They viewed buckminsterfullerene as a periodic network and their result was confirmed by Müller *et al.*[30] who used a modification of the computer approach developed previously for the construction, enumeration, and determination of Kekulé valence structures in any conjugated molecule.[31] Buckminsterfullerene, with its 12,500 Kekulé structures is not however prohibitively large for the particular computer approach. Recently, it was applied to another Archimedean polyhedron, great rhombicosidodecahedron, which has 120 vertices, 30 square faces, 20 hexagonal faces, 12 decagonal faces, and 180 edges.[26] This 120-atom carbon cage structure, named archimedene,[32] was estimated to have K greater than an astronomical value of 2^{30} (approximately a billion). A computer search,[30] however, revealed that the number of Kekulé valence structures of archimedene is 21,956,126,976, *i. e.*, a value 200 times larger. The computer time needed for this calculation was about 4 seconds. The same value of K for archimedene has also been obtained by Klein, Schmalz and Seitz.[33,34]

We calculated the resonance energy of buckminsterfullerene using several theoretical models that are available for predicting the aromatic stabilities of conjugated systems. These models are based on the simple versions of MO and VB theories. The MO models used are as follows:

(1) Hückel's model[34]

$$RE\,(\mathrm{HMO}) = E_{\pi}\,(\mathrm{HMO}) - 2 \cdot n_{\mathrm{C=C}} \tag{1}$$

where E_{π} is the Hückel energy of a conjugated molecule and $n_{\mathrm{C=C}}$ is the number of double bonds in a molecule. $E_{\pi}\,(\mathrm{HMO}) = 93.162\beta$ for buckminsterfullerene.

(2) The Zagreb Group model (Milun's model)[35]

$$RE\,(\mathrm{Milun}) = E_{\pi}\,(\mathrm{HMO}) - (n_{\mathrm{C=C}} \cdot E_{\mathrm{C=C}} + n_{\mathrm{C-C}} \cdot E_{\mathrm{C-C}}) \tag{2}$$

where $E_{\mathrm{C=C}}$ (= 2.00 β) and $E_{\mathrm{C-C}}$ (= 0.52 β are bond parameters, and $n_{\mathrm{C=C}}$ and $n_{\mathrm{C-C}}$ are numbers of double and single bonds in an arbitrary Kekulé's structure of the conjugated molecule.

(3) Hess-Schaad's model[36]

$$RE\,(\mathrm{Hess\text{-}Schaad}) = E_{\pi}\,(\mathrm{HMO}) - \sum_{i} n_i E_i \tag{3}$$

where E_i are the parameters corresponding to the bond types that may occur in the conjugated molecule and n_i are their numbers.

For our work on buckminsterfullerene and benzene there are four types of bonds important. These are:

$$E_{\mathrm{C=C}} = 2.1716\,\beta$$

$$E_{\mathrm{C-C}} = 0.4358\,\beta$$

$$E_{\mathrm{HC-CH}} = 2.0699\,\beta$$

$$E_{\mathrm{HC=CH}} = 0.4660\,\beta$$

(4) Carter's model[37]

$$RE\,(\mathrm{Carter}) = 0.6\, n_{\mathrm{C=C}} + 1.5 \ln K - 1 \tag{4}$$

where K is the number of Kekulé valence structures of the conjugated molecule. We included Carter's model in the set of MO models because it has been derived to reproduce the *RE* (HMO) values.

The simple VB models used are as follows:

(5) Conjugated circuits CC model[38]

$$RE\,(\mathrm{CC}) = 1/K \sum_{n \geq 1} r_n R_n + q_n Q_n \tag{5}$$

where R_n and Q_n are the parametric values for 4n + 2 and 4n conjugated circuits, whilst r_n and q_n are their numbers in a conjugated molecule.

In using this model here we followed the suggestion by Klein *et al.*[27] and truncated the set of conjugated circuits at circuits of size ten. The numbers of R_1 (= r_1), R_2 (= r_2), and Q_1 (= q_1) circuits are obtained by the Galveston group.[27] These numbers are as follows:

$$r_1 = 83{,}160$$
$$r_2 = 59{,}760$$
$$q_1 = 0$$

We also used two sets of parameters.

(5.1) Randić's parameters[38]

$$R_1 = 0.869 \text{ eV}$$
$$R_2 = 0.246 \text{ eV}$$
$$Q_1 = -1.60 \text{ eV}$$

(5.2) Herndon's parameters[39]

$$R_1 = 0.841 \text{ eV}$$
$$R_2 = 0.336 \text{ eV}$$
$$Q_1 = -0.65 \text{ eV}$$

(6) Herndon's model[39]

$$RE\,(\text{Herndon}) = A \cdot \ln \mathrm{K} \tag{6}$$
$$A = 1.185$$

Since buckminsterfullerene is a spherical molecule, the values of the *RE*s are also corrected for non-planarity according to formula:

$$(RE)_{\text{corr}} = (RE)_{\text{uncor}} \cdot \mathrm{C} \tag{7}$$

where C is the correction for nonplanarity. The following values for the correction C are used:

$$(\mathrm{C})_{\text{MO model}} = 0.92 \tag{8}$$

$$(\mathrm{C})_{\text{VB model}} = 0.84 \tag{9}$$

In this we also followed the work by Klein *et al.*[27] and Haddon *et al.*[39a]

Calculation of *RE*s for buckminsterfullerene and benzene are reported in the Table.

All models agree with one another that the C_{60} structure is highly aromatic, even taking into account the nonplanarity. However, they differ when the aromatic stability of buckminsterfullerene is compared to that of benzene.

The HMO model and Carter's model predict buckminsterfullerene to be more aromatic than benzene. However, this prediction is not reliable. It has been shown by Hess and Schaad,[36] and by Milun *et al.*[35] that HMO model (and any approximation to this model) works well only for benzenoid systems. Therefore, it is not surprising that Hückel's model produces results which are at variance with other models (except Herndon's logarithmic formula). A possible reason for the tendency of Herndon's formula to overestimate the aromatic stability of buckminsterfullerene lies in the nature of the Kekulé structures of C_{60}.[27] Many of Kekulé structures of buckminsterfullerene differ from one another only in a simple local manner so that they interact among one another rather less strongly than is typical in non-closed networks.

TABLE

Various Resonance Energies for Buckminsterfullerene and Benzene

Theoretical method		Resonance energy				
		Buckminsterfullerene			Benzene	
		RE	*RE*/e		*RE*	*RE*/e
			uncor-rected	corrected[a]		
HMO model		33.16 β	0.553 β	0.508 β	2 β	0.333 β
Milun's model		1.96 β	0.033 β	0.030 β	0.44 β	0.073 β
Hess-Schaad's model		1.87 β	0.031 β	0.029 β	0.39 β	0.065 β
Carter's model		31.15 β	0.519 β	0.477 β	1.840 β	0.307 β
Conjugated circuits model	Randić's parameters	6.96 eV	0.116 eV	0.097 eV	0.869 eV	0.145 eV
	Herndon's parameters[b]	7.20 eV	0.120 eV	0.101 eV	0.841 eV	0.140 eV
Herndon's model		11.18 eV	0.186 eV	0.157 eV	0.821 eV	0.137 eV

[a] Corrected *RE*s for nonplanarity

[b] D. J. Klein, T. G. Schmalz, G. E. Hite, and W. A. Seitz, *J. Amer. Chem. Soc.* **108** (1986) 1301.

Milun's model, Hess-Schaad's model, and conjugated circuits model indicate that benzene is more aromatic than buckminsterfullerene. This may be so, but it could also mean that we do not possess a model to account for the aromatic stability of 3D or closed conjugated structures.

Other reports in the literature on the aromatic stability of buckminsterfullerene also point to its considerable aromaticity.[27,32,40-44] The majority of these reports state that the aromatic stability of buckminsterfullerene is smaller than that of benzene and thus the question arises as to why buckminsterfullerene is so stable and inert molecule as observed by Kroto *et al.*[1]?

Theoretical work indicates that buckminsterfullerene is a molecule without unusual aromatic features and abnormalities. It is unusually inert, but this, in part may be due to a lack of hydrogens on its surface, as pointed out by Dias,[45] consequently makes it impossible for the molecule to undergo substitution reactions without cage rupture.

Other C_n ($n = 44, \ldots, 100$; $n =$ even) carbon-clusters have also been generated.[46] It appears that all clusters from C_{44} to C_{100} are closed and that C_{60} is the most stable structure.[46] It also has, perhaps, the least strain as all carbon atoms in C_{60} are equivalent and the strain will be evenly distributed. For instance, the C_{72} structure is flat like a thick pancake.[46]

Using Pauling's bond order[47] and in particular Pauling-Brockway-Beach's bond order — bond length relationship,[48] we obtained (see also Ref. 27) a bond order of 0.28 for a bond separating pentagonal and hexagonal faces and a bond order of 0.44 for a bond separating two hexagonal faces. The associated CC bond lengths are 1.433 Å and 1.403 Å, respectively. Thus, buckminsterfullerene possesses 30 bonds of length 1.403 Å and 60 bonds of length 1.433 Å. Kekulé structure of buckminsterfullerene corresponding to this geometry is shown in Figure 3.

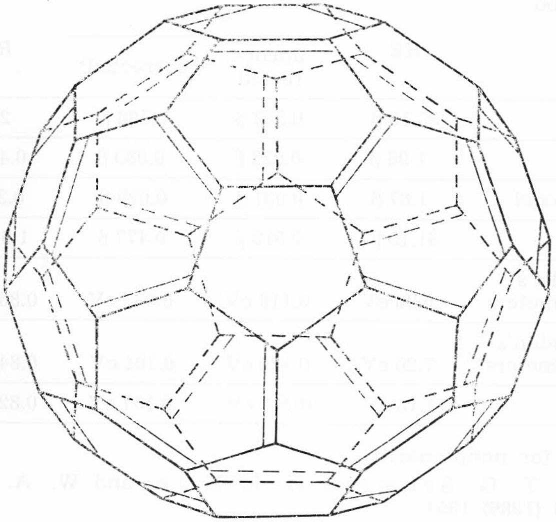

Figure 3. The principal Kekulé structure of buckminsterfullerene

In this Kekulé structure of buckminsterfullerene *every* hexagonal face is represented by a Kekulé valence structure of benzene. This valence structure has the maximum number (20) of Kekulé benzene rings. It will be the most important Kekulé structure of buckminsterfullerene according to the empirical Fries rule,[49] which preceded the early VB method. This is an empirical rule which states that the Kekulé valence structures with the largest number Kekulé benzene rings are the most dominant. The principal Kekulé structure of buckminsterfullerene possesses the full symmetry of the molecule, therefore, it contains both threefold and fivefold rotational symmetry axes.

CONCLUDING REMARKS

Several theoretical methods have been used for calculating the *RE* of buckminsterfullerene. It is found that Hückel theory-based methods and methods based on counting Kekulé structures are not reliable for estimating the *RE* of buckminsterfullerene or in comparing it with that of benzene. Hückel theory-based methods probably fail because of the non-alternant structure of the molecule.

It appears that the conjugated circuits model may be a more suitable theoretical model for assessing the aromatic stability of buckminsterfullerene and predicting the stabilization consistent with experimental observation. However, the chemistry of buckminsterfullerene and other carbon cages perhaps points to need for a more detailed and possibly novel theoretical model for studying aromaticity of 3D conjugated systems. Mere extension of the theoretical models otherwise suitable for 2 D systems by introducing the correction for nonplanarity may not be good enough for 3D or closed conjugated structures.

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SAŽETAK

O aromatičkoj stabilnosti kavezaste konjugirane ugljikove molekule C_{60}

Milan Randić, Sonja Nikolić i Nenad Trinajstić

Raspravlja se o aromatičkoj stabilnosti nedavno priređene kavezaste konjugirane ugljikove molekule C_{60}, koja posjeduje oblik krnjeg ikozaedra. Ta je molekula nazvana *buckminsterfulleren* u čast američkom arhitektu R. Buckminster Fulleru, koji se istakao projektiranjem vrlo stabilnih kupola poliedarskih oblika. Različite teorijske metode koje se upotrebljavaju za predviđanje aromatičnosti konjugiranih sustava upućuju na to da je ugljikova molekula C_{60} aromatička molekula, ali u manjoj mjeri nego benzen.