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# Analysis of Electronic Delocalization in Buckminsterfullerene (C<sub>60</sub>)

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J. POATER, M. DURAN, M. SOLÀ

*Institut de Química Computacional and Departament de Química, Universitat de Girona, 17071 Girona, Catalonia, Spain*

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**ABSTRACT:** Buckminsterfullerene (C<sub>60</sub>) presents an extensive conjugation that, in principle, should lead to a high delocalization of its electrons, together with a notorious aromaticity. However, previous studies have shown that C<sub>60</sub> behaves chemically and physically as an electron-deficient alkene rather than an electron-rich aromatic system. In the current work, we try to better elucidate the extension of electron delocalization in C<sub>60</sub> by computing the delocalization index for a given carbon atom of C<sub>60</sub>. We show that, in C<sub>60</sub>, local electron delocalization per carbon atom is lower than that in benzene and naphthalene. However, C<sub>60</sub> presents a global electron delocalization per carbon atom that is almost the same as that of clearly aromatic systems such as benzene or naphthalene. This is attributed to the fact that the electron charge of each atom in C<sub>60</sub> can be shared with a larger number of atoms. © 2004 Wiley Periodicals, Inc. *Int J Quantum Chem* 98: 361–366, 2004

**Key words:** aromaticity; atoms in molecules (AIM); buckminsterfullerene (C<sub>60</sub>); electron delocalization index

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## Introduction

At the initial stages after the discovery of fullerenes [1], researchers worldwide focused their efforts on determining the physical properties and reactivity of this new family of carbon clusters. It was initially assumed that fullerenes exhibited extremely stable aromatic character [2, 3]. However,

such an initial hypothesis was soon rejected in the light of the numerous chemical reactions undergone by fullerenes [3–6]. Nowadays, it is generally assumed that fullerenes have an ambiguous aromatic character [7–11], with some properties that support the aromatic view of these systems and others that do not. For instance, there is broad evidence that fullerenes experience substantial ring currents [12–18]. This fact, together with their rather considerable stability, seems to stress their aromatic character [9]. However, evidence from chemical reactivity is against the aromaticity of these systems, because fullerenes are very reactive

*Correspondence to:* M. Solà; e-mail: miquel.sola@udg.es  
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molecules that easily undergo a large variety of chemical transformations [4–6, 19–21], which, unlike with most aromatic compounds, are in most cases addition reactions to the conjugated  $\pi$ -system [3, 22, 23]. The enthalpy of formation of fullerenes [24] does not support an aromatic character either [25]. In addition, the existence of two types of bonds in  $C_{60}$  ([6,6]- and [5,6]-bonds) [26, 27] and eight different types of bonds in  $C_{70}$  [28, 29] indicates that  $\pi$ -orbitals of fullerenes are partially localized.

Studies based on principal component analyses stressed the multidimensional character of aromaticity. In general, it was found that aromatic compounds cannot be characterized by a single property [30–33]. To deal with this multidimensional character, it is recommended that one analyze the different features of aromaticity in a given compound, the most relevant being their energetic, structural, magnetic, and electronic properties. Indeed, the aromatic character of  $C_{60}$  and  $C_{70}$  was analyzed using structure-based measures for aromaticity such as the harmonic oscillator model of aromaticity (HOMA) values [11], from magnetic-based properties [34] by means of the nucleus independent chemical shift (NICS) indices defined by Schleyer and coworkers [35], and from the para delocalization index [36], which is an electronic-based criterion of aromaticity defined recently [37]. The studies show that in most cases six-membered rings (6-MR) are partially aromatic, whereas 5-MRs are clearly antiaromatic. The fact that  $C_{60}$  is found to be slightly less aromatic than  $C_{70}$  is attributed to the smaller fraction of 5-MRs in  $C_{70}$  as compared with  $C_{60}$  [7, 10, 11]. The aromaticities of higher fullerenes and nanotubes were also recently studied by Bühl [34] and by van Lier and coworkers [38], respectively, using magnetic criteria. Finally, it is worth noting the existence of a  $2(N + 1)^2$  rule [39, 40] for spherical fullerenes, which is equivalent to the  $4N + 2$  Hückel rule for planar polycyclic aromatic hydrocarbons. According to this rule, charged  $C_{60}$  systems with completely filled shells, such as  $C_{60}^{+10}$ , are much more aromatic than  $C_{60}$  and exhibit a less pronounced bond-length alternation.

The degree of  $\pi$ -electron delocalization in an aromatic compound is generally considered to provide a measure of its aromaticity [41]. Although it is usually claimed that the delocalization of electrons in the cage of  $C_{60}$  is poor [3], magnetic and nuclear magnetic resonance (NMR) properties seem to indicate that extensive cyclic delocalization of  $\pi$ -electrons takes place in fullerenes as expected for aromatic molecules [9]. Thus, the degree of electronic localization/delocalization is an aspect of the aro-

maticity in fullerenes that should be clarified. For this purpose, we have undertaken a study of the electronic delocalization in  $C_{60}$  by means of the delocalization indices [42] in the framework of the atoms-in-molecules (AIM) theory [43]. Comparison with benzene and naphthalene, two archetypal molecules that exhibit aromaticity in all their manifestations, is carried out to provide a deeper understanding of electron delocalization in fullerenes. This kind of study can help to improve and deepen our understanding of the principles of aromaticity [41].

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## Computational Methods

We have used the Austin model 1 (AM1) semiempirical method [44] as implemented in Gaussian 98 [45] to perform geometry optimizations within the restricted formalism. We previously showed that the AM1 method yields reliable results for the geometries of  $C_{60}$  [46, 47] and  $C_{70}$  [47]. Calculations of delocalization indices have been carried out using the ab initio Hartree-Fock (HF) method with the 6-31G\* basis set [48–50] at the AM1-optimized geometries (HF/6-31G\*//AM1) by means of the AIMPACK collection of programs [51]. At the HF level of theory, delocalization indices are calculated as [42, 52]:

$$\delta(A, B) = 4 \sum_{i,j}^{N/2} S_{ij}(A)S_{ij}(B). \quad (1)$$

The summations in Eq. (1) run over all the occupied orbitals;  $S_{ij}(A)$  stands for the overlap between orbitals  $i$  and  $j$  within the basin of atom  $A$ ; the delocalization index (DI),  $\delta(A, B)$ , corresponds to the number of electrons delocalized or shared between atoms  $A$  and  $B$  [42, 52]. Furthermore, the localization index is defined as:

$$\lambda(A) = 2 \sum_{i,j}^{N/2} (S_{ij}(A))^2. \quad (2)$$

The localization index (LI),  $\lambda(A)$ , yields the number of electrons that are localized in atom  $A$ . The electrons associated with a given atomic basin, its atomic population,  $N(A)$ ,

$$N(A) = \int_A \rho(\vec{r})d\vec{r}, \quad (3)$$

are either localized into that basin or “shared with” or delocalized into the basins of other atoms in the molecule, with each  $\delta(A, B)$  having an equal contribution from  $A$  and  $B$ , hence, the factor of one half multiplying the sum of the DI values, that is,

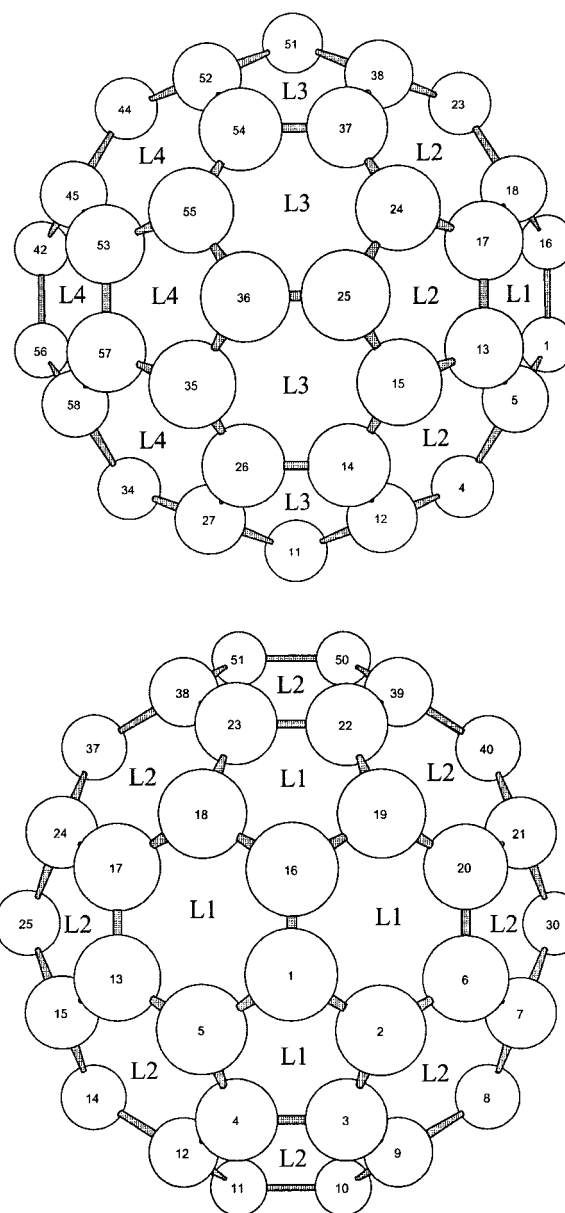
$$N(A) = \lambda(A) + \frac{1}{2} \sum_{B \neq A} \delta(A, B). \quad (4)$$

From the last term of the above Eq. (4), one can obtain the global delocalization term, which is defined as the total number of electrons of an atom that are delocalized into other atomic basins.

## Results and Discussion

The aim of the current work is to study the electron delocalization in  $C_{60}$ . In particular, we have focused our study on analyzing how the electron charge of a certain atom in  $C_{60}$  is spread out into the rest of the molecule. Thus, we have taken carbon atom  $C_1$  as reference (see Scheme 1) and calculated the delocalization indices between this carbon atom and the rest. Due to the symmetry of  $C_{60}$ , this involves the calculation of the 31 DIs between the reference atom and the rest of the carbon atoms located in a hemisphere of  $C_{60}$ .

Table I contains all DIs between carbon atom  $C_1$  and the rest of the symmetrically different atoms in a  $C_{60}$  hemisphere (see Scheme 1), together with the respective C–C distances. The largest DI corresponds to interactions between atoms in ortho position,  $\delta(1, 5) = 1.118$  and  $\delta(1, 16) = 1.415$  e (for comparison, benzene:  $\delta_{\text{ortho}} = 1.401$  e). At variance with benzene, each atom of  $C_{60}$  has two different ortho positions. The presence of pentagonal rings in  $C_{60}$  partially localizes the  $\pi$ -bonds (Mills–Nixon effect [53]) and leads to two different kind of bonds: shorter and electron-richer [6,6]-bonds in the ring junctions between two 6-MRs and longer [5,6]-bonds in the bridge connecting 6-MRs and 5-MRs. The electron-richer and shorter (1.385 Å) [6,6]-bond in  $C_{60}$  has a larger DI than the C–C bond in benzene, which in turn has a larger DI than the longer (1.464 Å) [5,6]-bond. This result reflects the loss of bond-length equalization in the 6-MRs of  $C_{60}$  as compared with benzene. Interestingly, 5-MRs having only the less delocalized [5,6]-bonds are anti-aromatic rings, whereas 6-MRs composed of equal numbers of [6,6]- and [5,6]-bonds have partial aro-



**SCHEME 1.**

matic character according to HOMA, NICS, and para delocalization index (PDI) values [36].

The atomic population of  $C_1$ , 6 electrons, is divided into 2.110 e that are delocalized all over the  $C_{60}$  molecule, and 3.890 e that are completely localized in the  $C_1$  atomic basin. This global delocalization value (2.110 e) is obtained by summing up all DIs in which atom  $C_1$  is involved and dividing it by 2, as each DI corresponds to two atoms [see Eq. (4)]. As can be seen in Table I, the DI decreases as the C–C distance increases, the DI being close to zero

**TABLE I**  
**The HF/6-31G\*\*/AM1 delocalization indices (in electrons) and C–C distances (in Å) between C<sub>1</sub> and the rest of atoms of C<sub>60</sub><sup>a</sup>**

| Atom A | Atom B | $\delta(A, B)$ | $r_{A,B}$          | Layer     |
|--------|--------|----------------|--------------------|-----------|
| 1      | 4      | 0.053          | 2.369              | 1         |
| 1      | 5      | 1.118          | 1.464 <sup>b</sup> | 1 (ortho) |
| 1      | 11     | 0.002          | 4.525              | 2         |
| 1      | 12     | 0.012          | 3.583              | 2         |
| 1      | 13     | 0.056          | 2.467              | 1 (meta)  |
| 1      | 14     | 0.003          | 4.124              | 2         |
| 1      | 15     | 0.007          | 3.705              | 2         |
| 1      | 16     | 1.415          | 1.385 <sup>c</sup> | 1 (ortho) |
| 1      | 17     | 0.046          | 2.849              | 1 (para)  |
| 1      | 18     | 0.056          | 2.467              | 1 (meta)  |
| 1      | 23     | 0.012          | 3.583              | 1         |
| 1      | 24     | 0.003          | 4.124              | 2         |
| 1      | 25     | 0.002          | 4.525              | 2         |
| 1      | 26     | 0.000          | 5.217              | 3         |
| 1      | 27     | 0.000          | 5.419              | 3         |
| 1      | 34     | 0.000          | 6.146              | 4         |
| 1      | 35     | 0.000          | 5.797              | 3         |
| 1      | 36     | 0.000          | 5.489              | 3         |
| 1      | 37     | 0.008          | 4.836              | 2         |
| 1      | 38     | 0.003          | 4.609              | 2         |
| 1      | 42     | 0.000          | 7.114              | 4         |
| 1      | 44     | 0.000          | 6.708              | 4         |
| 1      | 45     | 0.000          | 6.961              | 4         |
| 1      | 51     | 0.000          | 5.489              | 2         |
| 1      | 52     | 0.000          | 6.146              | 3         |
| 1      | 53     | 0.000          | 6.672              | 4         |
| 1      | 54     | 0.000          | 5.797              | 3         |
| 1      | 55     | 0.002          | 6.073              | 3         |
| 1      | 56     | 0.000          | 6.978              | 4         |
| 1      | 57     | 0.000          | 6.518              | 4         |
| 1      | 58     | 0.000          | 6.672              | 4         |

<sup>a</sup> Only symmetrically different delocalization indices are included. The layer to which atom B belongs is also given.

<sup>b</sup> Exp. value is 1.458 Å [27].

<sup>c</sup> Exp. value is 1.401 Å [27].

for carbon atoms with C–C distances larger than 4.5 Å.

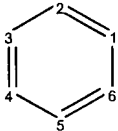
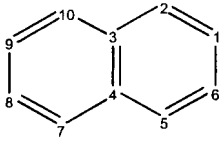
To better understand the electron delocalization in this molecule, let us now compare the DIs in a 6-MR of C<sub>60</sub> with those of benzene (see Table II). For benzene, the global DI of a carbon atom is obtained as half the sum of all possible DIs between the carbon atom of reference and the rest of the carbon atoms. The DIs between the reference carbon atom and the hydrogen atoms are not included in the global DI, to allow a better comparison between benzene and C<sub>60</sub>. Thus, the global DI for

benzene is 1.524 e, 0.179 e larger than that obtained for a 6-MR of C<sub>60</sub>. Therefore, there is a lower delocalization in a 6-MR of C<sub>60</sub> as compared with the 6-MR of benzene, which in turn translates into a less local aromatic character of the 6-MR of C<sub>60</sub>. It is also worth comparing the DI<sub>meta</sub> and DI<sub>para</sub> values in C<sub>60</sub> with respect to those of benzene. For a given 6-MR in buckminsterfullerene, DI<sub>meta</sub> = 0.056 e and DI<sub>para</sub> = 0.046 e, whereas for benzene, DI<sub>meta</sub> = 0.073 e and DI<sub>para</sub> = 0.101 e. A larger delocalization in the para than the meta position was found to be characteristic of highly aromatic systems [37, 54]. The DI<sub>para</sub> > DI<sub>meta</sub> relation found in benzene does not apply for a 6-MR in C<sub>60</sub>, indicating a lower local aromaticity of its 6-MRs because of its higher  $\pi$ -bond localization.

The same procedure can be applied for a carbon atom located in the ring junction between two adjacent 6-MRs of C<sub>60</sub>, and the result obtained can be compared to that of a carbon atom in the ring junction of naphthalene (see Table II). Again we found that the global DI of one of the bridge carbon atoms (2.052 e) is larger than the global DI for two adjacent 6-MRs of C<sub>60</sub>, 1.983 e.

The LIs of a carbon atom in C<sub>60</sub> and a carbon atom of naphthalene located in the ring junction are 3.890 and 3.888 e, respectively. Thus, electron localization in the two systems is almost the same. The overall delocalization of the electron charge of a certain carbon in both structures is also almost identical [2.110 and 2.108 e for C<sub>60</sub> and naphthalene

**TABLE II**  
**The HF/6-31G\*\*/AM1 delocalization indices (in electrons) of benzene and naphthalene, together with the global delocalization index of the reference atom.<sup>a</sup>**

| Molecule   | Atom A | Atom B | $\delta(A, B)$ | Global $\delta$ |
|--|--------|--------|----------------|-----------------|
|   | 1      | 2      | 1.401          | 1.524           |
|  | 1      | 3      | 0.073          |                 |
|  | 1      | 4      | 0.101          |                 |
|  | 3      | 1      | 0.667          | 2.052           |
|  | 3      | 2      | 1.234          |                 |
|  | 3      | 4      | 1.264          |                 |
|  | 3      | 5      | 0.058          |                 |
|  | 3      | 6      | 0.062          |                 |
|  | 3      | 6      | 0.062          |                 |

<sup>a</sup> Only symmetrically different delocalization indices are included.

(C<sub>3</sub>), respectively]. The values show that both structures present a similar delocalization per carbon atom. However, this does not mean that they have a similar aromatic character, because the patterns in delocalization are clearly different. The larger number of carbon atoms in C<sub>60</sub> allows for a larger global delocalization despite the delocalization in two adjacent 6-MRs of C<sub>60</sub> being clearly smaller than that of naphthalene. To go deeper into the above observation, we have calculated the global DI between a certain carbon atom of reference and the three atoms to which it is bonded (C<sub>60</sub>: C<sub>5</sub> with C<sub>1</sub>, C<sub>4</sub>, and C<sub>13</sub>; naphthalene: C<sub>3</sub> with C<sub>2</sub>, C<sub>4</sub>, and C<sub>10</sub>). As before, in each case we have halved the sum of the three DIs. For C<sub>60</sub>, the DI is 1.825 e, and for naphthalene, 1.866 e. Thus, when only local delocalization is taken into account, it is seen again that C<sub>60</sub> is less delocalized with respect to a system as clearly aromatic as naphthalene. Therefore, we could say that C<sub>60</sub> presents a global electron delocalization per carbon atom similar to that of naphthalene because of the possibility of each carbon atom delocalizing its electron charge into the remaining 59 carbon atoms. However, the local electron delocalization is smaller, as expected for a less aromatic system. On the other hand, whereas delocalization in ortho position is larger for C<sub>60</sub> than for benzene or naphthalene, the delocalization in the para position is smaller, reflecting also the lower local aromatic character of C<sub>60</sub> and a different pattern of delocalization within the 6-MR.

Up to this point, we have focused on the electron delocalization of one or two rings in C<sub>60</sub>. Nevertheless, the ultimate aim of the current work is to measure the overall delocalization of C<sub>60</sub>, so we must consider the rest of the rings. As mentioned above, in general, as the C-C distance increases the delocalization decreases. Indeed, we can say that the atomic population of a certain atom, in this case the reference atom C<sub>1</sub>, is spread out into only half the sphere of C<sub>60</sub>, that is, into the closest 30 atoms. This can be seen from the values of the DIs given in Table I. To better monitor this effect, we have split C<sub>60</sub> into different layers, calculating the global DI in each layer, by following the same procedure as before for obtaining the DI in one or two 6-MRs. The first layer corresponds to the pyracyclene unit involving two 6-MRs in which C<sub>1</sub> is a bridge atom, together with the two closest 5-MRs. The second layer corresponds to the 6-MRs and two 5-MRs next to the first layer (see Scheme 1). The third layer contains the four 6-MRs and four 5-MRs closest to the second layer, forming the equatorial belt of the

buckminsterfullerene. Finally, the fourth layer corresponds to the rest of the molecule. Thus, the global DI of layer 1 is 2.049 e, the one for layer 2 is 0.040 e, the one for layer 3 is 0.003 e, and the one for layer 4 is 0.018 e. The values indicate that the electron delocalization of the atomic charge of a certain atom, for example, C<sub>1</sub>, is noticeable only until the second layer is reached. The sum of the global DI for the four layers gives 2.110 e, which is the total number of electrons of C<sub>1</sub> that are delocalized all over the molecule.

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## Conclusions

In the current study we have measured the whole electron delocalization in buckminsterfullerene, C<sub>60</sub>, with the aim of discussing whether the electron charge of each carbon is more or less localized into the corresponding atomic basin. To carry out the study, we have divided C<sub>60</sub> into four different layers according to the proximity of the carbon atoms to the reference atom, and the global electron DI has been calculated for each layer.

From the results obtained, as a whole, we see that the electron charge of an atom in C<sub>60</sub> is mostly delocalized into the first layer, that is, into the 13 closest atoms, enclosing two 6-MRs and two 5-MRs. When moving away from the first layer, the DIs rapidly tend to zero. In addition, mention must be made that the global electron delocalization of C<sub>60</sub> per carbon atom cannot be considered poor. Indeed, it is very similar to that of clearly aromatic systems, even though it does not behave in the same way. This is attributed to the fact that the electron charge of each carbon atom in C<sub>60</sub> can be delocalized into many more atoms than in smaller aromatic systems such as benzene or naphthalene, thus giving an unexpectedly large value for the global DI per carbon atom. However, when the electron delocalization is analyzed from a local point of view, it is seen that C<sub>60</sub> has a lower delocalization and aromaticity than typical aromatic molecules, because of its partial  $\pi$ -bond localization that unfavors particularly the delocalization between carbon atoms in para positions.

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