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Resistance Distances in Fullerene Graphs*

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Resistance distances are computed for all 1812 C_{60} fullerenes and found to correlate with the number of pentagon adjacencies and hence with relative energy. Within the set, the unique isolated-pentagon isomer has the lowest resistance distance (R_T = 479482/209), the lowest Wiener index (W = 8340) and the highest Balaban index (J = 2025/2224). The most stable C_{40} fullerene isomer, one of two with the lowest achievable number of pentagon adjacencies, also has the lowest resistance distance in the set.

Key words: Balaban index, C_{40} fullerenes, C_{60} fullerenes, resistance distance, Wiener index.

INTRODUCTION

Within the potentially vast class of the fullerenes, thermodynamic stability and isomer selectivity are determined by a delicate balance of steric and electronic factors.[1] Graph theory gives a tool for dealing with π-electronic structure, in the shape of Hückel theory,[2] but it is also useful in the modelling of the competing steric effects. One approach to quantification of steric strain in polyhedral cage molecules is through distance-based invariants. The Wiener index, for example, is an established measure of molecular compactness,[3] and shows selectivity in picking fullerenes from general cubic polyhedra, isolated-pentagon fullerenes from general fullerenes and, in combination with other invariants, it can in some cases identify the low-energy cages in the sub-set of isolated-pentagon fullerenes.[4] Several other indices

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* Dedicated to Professor Milan Randić on the occasion of his 70th birthday.

have similar characteristics, and there are many distance-related invariants in the literature of chemical graph theory.

Recently, resistance distances[5] have been calculated for Platonic polyhedra[6,7] in an algebraic treatment that was described as presenting some difficulty for the dodecahedron.[7] Numerical solution of the problem is straightforward, and is applied here to a representative sample set of fullerenes, the 1812 isomers of C_{60}, to compare the extremal properties of resistance distance with those of other distance-related indices. It is found that the unique truncated icosahedral isomer, the experimental C_{60} molecule, is extremal in this property, as it is in the Wiener and Balaban indices, and is in fact the isomer with the lowest resistance distance of all the cages that can be assembled from 12 pentagonal and 20 hexagonal faces. A previous study concentrated on the relative abilities of these and other indices to *characterise* C_{60} fullerenes.[8] The focus here is on the ability of the resistance distance to reflect the physically and chemically important energetics of the fullerenes. In this context, the multiplicity of an index value is less important than its extremal properties.

METHOD

The concept of resistance distance of a graph is based on an electrical analogy.[5] Each edge of the graph is taken to be a wire of unit resistance, and pairs of vertices are treated as terminals across which there is an applied potential drop. Unit current is assumed to flow in at one terminal and out at the other. For each choice of a pair of terminal vertices, bond currents are calculated over the whole graph by application of Kirchhoff's laws,[9] and the resistance between the terminals follows from the sum of bond currents taken along any route from one to the other. Summation of the calculated resistance over all distinct choices of the terminal pair gives the total resistance distance $R_T(G)$ of the graph G.[5,7]

If resistance is regarded as a metric defining a separation Ω_{ij} for each pair of vertices i and j of G, then $R_T(G)$ is the half sum of all the entries, related to the matrix Ω in the same way that W, the Wiener Index, derives from the ordinary distance matrix $\boldsymbol{D}$. To emphasise this similarity, $R_T(G)$ is sometimes called the Kirchhoff Index, Kf.[9] In an acyclic graph Wiener and Kirchhoff indices are equal; in a general graph Kf is equal to the quasi-Wiener index.[10,11]

If the vertices are labelled 1 to n, each edge vector is given a positive sense in the direction from lower to higher vertex label. Bond currents are then scalar multiples (positive or negative) of the bond vectors $<ij>$, described by coefficients c_{ij}. Kirchhoff's first and second laws give the current sums at the vertices:

$$\begin{aligned}\sum_{j=1}^{n} A'_{ij}\, c_{ij} &= +1 \quad (i = \text{input terminal})\\ &= -1 \quad (i = \text{output terminal}) \qquad (1)\\ &= \;\;0 \quad (\text{otherwise})\end{aligned}$$

where $\boldsymbol{A}'$ is a signed adjacency matrix with elements $A'_{ij} = +1$ for neighbours $j > i$, $A'_{ij} = -1$ for neighbours $j < i$, and $A'_{ij} = 0$ otherwise. Similarly, for the cycles $i_1\, i_2\, i_3 \,...\, i_r$,

$$A'_{i_1 i_2}\, c_{i_1 i_2} + A'_{i_2 i_3}\, c_{i_2 i_3} + \,...\, + A'_{i_r i_1}\, c_{i_r i_1} = 0\ . \qquad (2)$$

A cubic polyhedron such as a fullerene has n vertex conditions of type (1) and $(n/2+2)$ face-cycle conditions of type (2), of which $(n–1)$ and $(n/2+1)$, respectively, can be taken as independent in the absence of symmetry. Again in the absence of symmetry considerations, there are $n(n–1)/2$ distinct choices of terminal pairs, and the patterns of current are determined by the linear matrix equation

$$\underset{[(n-1) + (n/2+1)] \times 3n/2}{\boldsymbol{B}} \quad \times \quad \underset{3n/2 \times n(n-1)/2}{\boldsymbol{C}} \quad = \quad \underset{3n/2 \times n(n-1)/2}{\boldsymbol{D}} \qquad (3)$$

where $\boldsymbol{B}$ contains the various $\boldsymbol{A}'$ entries of the LHS of (1) and (2), $\boldsymbol{C}$ is the matrix of $n(n–1)/2$ column vectors $\boldsymbol{c}$ of scalar current coefficients, and $\boldsymbol{D}$ is a rectangular array of the RHS of (1) and (2), with one column for each choice of terminal pair. Symmetry can be used to reduce both the dimensions of $\boldsymbol{c}$ and the number of columns in $\boldsymbol{D}$, but as most fullerenes have no symmetry, and the dimensions of the equations are in any case easily manageable for C_{60}, no further manipulation of (3) is used here. The inversion of $\boldsymbol{B}$ is conveniently performed for these small cases using Gauss-Jordan elimination, for which standard subroutines are available.[12] The program was tested for the dodecahedron, and reproduced the results of Ref. 7.

RESULTS

All quantities needed for the solution of (3) follow from the face-spiral encoding of the adjacency information for fullerene isomers.[1,13] The 1812 isomer datasets were constructed and processed to produce patterns of currents for each of the 1770 pairings of terminals, the corresponding pair resistances, and hence the total resistance distances for each isomer. Full lists of other distance invariants are also available.[4]

The truncated icosahedral isomer 60:1812 has 23 distinct terminal pairings, equivalent to the number of derivatives $C_{60}X_2$, and these lead to 23 different contributions to R_T(60:1812). Conversion of the high precision numerical results to fractional form gives the total resistance distance for this isomer as R_T(60:1812) = 479482/209 (*i.e.* 2294.1722). The separate resistances are shown in Table I, using the standard vertex-spiral numbering scheme[14] for the atoms of C_{60}, and the pattern of currents for the 1,2 pairing across one of the formal double bonds of the structure is illustrated in Figure 1.

TABLE I

Contributing resistances for the distinct pairings of terminal vertices in icosahedral C_{60} fullerene. Each distinct pair 1,*m* in the IUPAC vertex-spiral numbering scheme[14] has a resistance *R(m)*, which can be expressed as a fraction *i(m)*/25080 where *i(m)* is an integer, contributing with multiplicity *g* to the total resistance distance, R_T(60:1812).

m	*g*	*R(m)* = *i(m)*/(120 × 209)
6	60	16273/25080 ≈ 0.648844
2	30	16778/25080 ≈ 0.668978
7	60	23234/25080 ≈ 0.926396
3	120	24749/25080 ≈ 0.986802
4	60	27274/25080 ≈ 1.087480
13	120	29359/25080 ≈ 1.170614
19	60	29864/25080 ≈ 1.190750
17	120	31488/25080 ≈ 1.255502
18	120	32519/25080 ≈ 1.296611
15	60	33133/25080 ≈ 1.321093
16	60	33835/25080 ≈ 1.349083
38	60	34405/25080 ≈ 1.371810
39	60	34843/25080 ≈ 1.389274
31	120	35369/25080 ≈ 1.410248
34	120	36048/25080 ≈ 1.437321
35	60	36704/25080 ≈ 1.463477
33	120	36769/25080 ≈ 1.466069
53	60	37534/25080 ≈ 1.496571
52	120	37859/25080 ≈ 1.509530
49	60	38054/25080 ≈ 1.517305
55	30	38438/25080 ≈ 1.532616
51	120	38503/25080 ≈ 1.535207
60	30	38760/25080 ≈ 1.545455

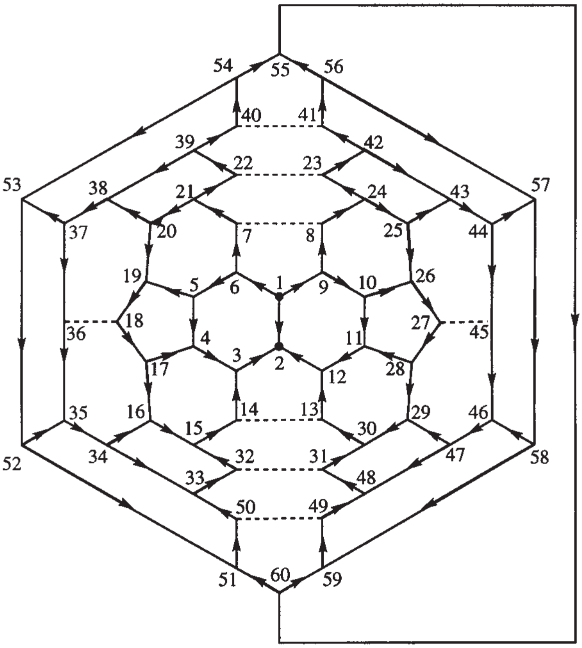

Figure 1. Bond currents in truncated-icosahedral C_{60} for a pair of terminals spanning the hexagon-hexagon edge of the polyhedron. The standard IUPAC numbering scheme is used.[14] Arrows on the diagram show the direction of current flow; dotted lines are graph edges with zero current. The non-zero currents are (in units of 501610^{-1}): 33556 (1→2); 8302 (1→6, 1→9, 3→2, 12→2); 5951 (4→3, 6→5, 9→10, 11→12); 5050 (5→4, 10→11); 2351 (6→7, 9→8, 14→3, 7→21, 8→24, 13→12, 15→14, 30→13); 1624 (18→17, 19→18, 26→27, 27→28); 1427 (16→15, 21→20, 24→25, 29→30); 987 (35→34, 38→37, 43→44, 46→47); 924 (21→22, 22→39, 23→42, 24→23, 31→30, 32→15, 33→32, 48→31); 901 (17→4, 5→19, 10→26, 28→11); 723 (17→16, 20→19, 25→26, 28→29); 704 (20→38, 25→43, 34→16, 47→29); 656 (36→35, 37→36, 44→45, 45→46); 650 (53→52, 57→58); 644 (55→60); 641 (39→40, 40→54, 41→56, 42→41, 49→48, 50→33, 51→50, 59→49); 331 (37→53, 44→57, 52→35, 58→46); 322 (54→55, 56→55, 60→51, 60→59); 319 (52→51, 54→53, 56→57, 58→59); 283 (34→33, 39→38, 42→43, 47→48).

Several patterns emerge when all 1812 values of R_T are considered. The whole set of isomers spans a range of 264.94 and the average over the distribution is 2320.08. As shown in Figure 2(a), R_T correlates smoothly with N_p, the number of pentagon adjacencies in the fullerene polyhedron, which is known to be a useful qualitative measure of relative energy in lower fullerenes.[15] The isolated-pentagon isomer has, of course, $N_p = 0$, and minimum R_T; the isomer next in R_T is also the C_{60} fullerene with the smallest non-zero N_p (isomer 60:1809), which is related to the truncated icosahedron by a sin-

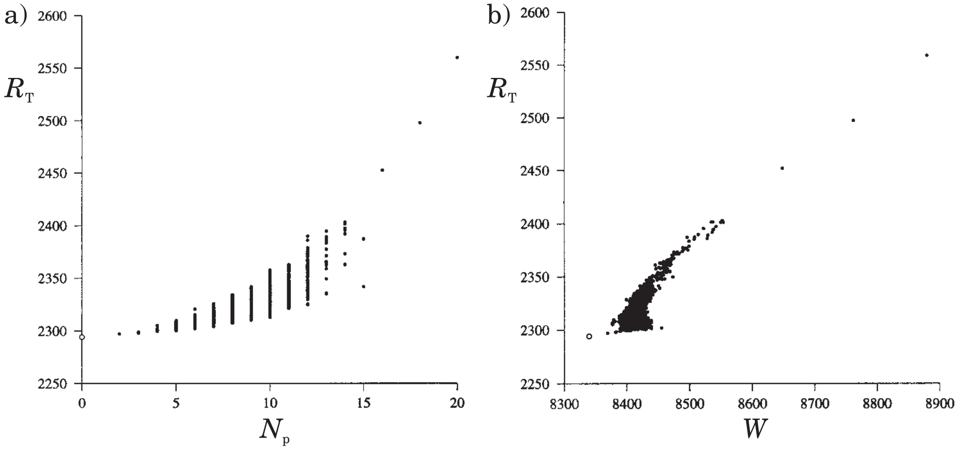

Figure 2. Correlations between resistance distances and other graph theoretical invariants for the set of 1812 fullerene isomers of C_{60}. (a) Scatter plot of R_T against N_p, the number of pentagon adjacencies. (b) Scatter plot of R_T against W, the Wiener index. The isolated-pentagon isomer is denoted by the empty circle, other isomers by the filled circles.

gle Stone-Wales transformation.[16] The isomer of highest resistance distance is the high-energy 1812:1, the cylinder with hemi-dodecahedral caps, for which $N_p = 20$. This isomer has $R_T = 2559.1089$ (to machine accuracy, 47105517/18407). The extreme values of *Kf* and *W* for 60:1 and 60:1812 have been reported,[8] though in the case of the Kirchhoff index, multiplied by an unconventional extra factor of two.

Other distance invariants have been calculated for this set of fullerenes.[4,8] Isomer 60:1812 has the lowest Wiener index, *W*, and the highest Balaban index,[17] *J*, in the set. Figure 2(b) shows that there is a strong correlation, isomer-by-isomer, between *W* and R_T. The correlation between *J* and R_T (not shown) is of similar quality, as *W* and *J* are strongly (inversely) correlated.[4]

For C_{60}, all three invariants pick out the icosahedral isomer, tracking both the total energy and the number of pentagon adjacencies. For other numbers of vertices, there are some indications that R_T will in fact have a better performance than the other distance invariants as a predictor of energy. Table II shows *W* and R_T for the 40 fullerene isomers of C_{40}, all of which necessarily have some adjacent pentagons. Isomer 40:38 is one of two with the minimal 10 pentagon adjacencies, and is predicted to be the C_{40} fullerene of lowest energy by many methods;[15] it turns out also to have the smallest resistance distance, by a margin of 1 part in 1000, whereas its Wie-

TABLE II

Comparison of Wiener index (W), resistance distance (R_T) and pentagon adjacency count (N_p) for fullerene isomers of C_{40}

Isomer	N_p	W	R_T	Isomer	N_p	W	R_T
1	20	3035	955.1508	21	12	2992	925.6598
2	16	3008	936.8771	22	12	2995	924.5173
3	18	3018	944.0339	23	13	2993	926.3707
4	15	3001	931.9751	24	11	2994	922.7119
5	14	2997	931.1004	25	12	2996	924.0879
6	14	2999	929.6359	26	11	2996	922.1277
7	15	2998	930.1360	27	12	2996	923.2515
8	15	3002	932.5192	28	12	2993	924.0695
9	13	2995	926.8919	29	11	2993	921.8688
10	13	2995	926.8944	30	12	2994	923.0316
11	15	2997	929.3356	31	11	2995	921.3638
12	13	2997	925.8184	32	14	3004	927.2869
13	13	2998	926.7625	33	14	3004	927.9411
14	12	2995	924.1053	34	12	2997	923.1334
15	12	3001	923.7521	35	11	2999	922.0602
16	13	3001	924.6078	36	11	2997	921.3521
17	13	3000	924.1504	37	11	2995	921.4915
18	14	2999	926.3455	38	10	2994	920.2679
19	13	2998	924.3389	39	10	2990	921.3031
20	12	3000	925.7556	40	12	3000	921.4659

ner index of 2994 is shared by 2 isomers and beaten by 6 others. The C_{40} isomer of lowest Wiener Index is actually the other fullerene with 10 adjacencies, 40:39, which quantum mechanical methods predict to be marginally less stable than 40:38. In this case, R_T is performing better than both the very robust pentagon-adjacency index, which would not decide between 40:38 and 40:39 and the Wiener index which would plump for the wrong isomer. Further investigation of the resistance distance for large sets of fullerenes may be worthwhile.

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SAŽETAK

Otporne udaljenosti u fullerenskim grafovima

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Za svih 1812 C_{60} fulerena izračunane su otporne udaljenosti i nađeno je da koreliraju s brojem susjednih peterokuta i stoga s relativnom energijom. Unutar toga skupa, izomer s potpuno izoliranim peterokutima ima najmanju otpornu udaljenost (R_T = 479482/209), najmanji Wienerov indeks (W = 8340) i najveći Balabanov indeks (J = 2025/2224). Najstabilniji izomer C_{40} fulerena, jedan od dva s najmanjim mogućim brojem susjednih peterokuta, također ima najmanju otpornu udaljenost u pripadnom skupu izomera.