Distance Spectra and Distance Polynomials of Fullerenes

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Distance matrices of fullerenes which contain important topological information on fullerenes are obtained. By use of the distance matrices, the distance level patterns are constructed for fullerenes. It is shown that the distance level patterns uniquely characterize fullerenes and thus appear to be topological invariants of fullerenes. The distance spectra and characteristic polynomials of the distance matrices of $C_{20}-C_{90}$ fullerenes are computed. The Wiener topological indices are computed for these fullerenes. The sums of powers of the distance spectra are computed and considered as structural invariants of fullerenes.

1. Introduction

Fullerene research has led to a new vista for several mathematical studies dealing with the structure, stability, spectroscopy, and other topological aspects of structures. The applications of group-theoretical, graph-theoretical, combinatorial, and related techniques to fullerenes are on the increase due to the importance of such techniques in both enumeration and characterization of fullerenes. Such studies have included the characterization of the structures, enumeration of fullerene cage isomers, enumeration of conjugated circuits, enumeration of the isomers arising from the substitution of the various centers with hydrogens, halogens, etc., construction of NMR and ESR spectral patterns, nuclear spin statistics of rovibronic levels, and so on.[1–12]

Topological indices and other structural invariants are quite important not only for structural characterizations but also in the prediction of physicochemical properties since such properties are closely related to the topological and structural features.[13] The characteristic polynomials, spectra of the adjacency matrices, Wiener index, matching polynomials, etc., have been shown to be useful structural invariants although these invariants may not be unique. While the characteristic polynomials, spectra, and matching polynomials of fullerenes have been obtained,[6–9] the structural invariants derived from the distance matrices have received much less attention.

Fullerenes are actively investigated both experimentally and theoretically by several investigators.[14–30] Such studies are in part fueled by the isolation of gram quantities of several fullerenes and subsequent reactivity and spectroscopic studies on the derivatives of fullerenes. Fullerenes are closed carbon cages that contain 12 pentagons and any number of hexagons. Fullerenes containing isolated pentagons are likely to be more stable compared to other fullerenes.

Distance matrices play an important role in the topological analysis of structures.[31–32] As discussed in one of the previous papers of the author,[31] distance matrices have numerous applications in many different disciplines ranging from music theory to archeology. In the topological analysis of molecular structures, distance matrices play a very important role since they yield fundamental structural invariants and indices such as the Wiener number.[32] The Wiener number finds wide applications in the prediction of the physicochemical properties of molecules.

Although the structural invariants based on the adjacency matrices have been investigated before,[5–9] such invariants based on the distance matrices for the analysis of the fullerene structures have not been explored to the same extent. Ori and D'Mello[4] have studied the distance matrix of the C_{76} fullerene. They have also computed the Wiener numbers for the C_{60} and C_{70} fullerenes. The distance polynomials and the distance spectra of the C_{60} and C_{70} fullerenes have been computed by the author in a recent communication.[11] In that study the author showed that the distance matrices could serve as very useful structural invariants. In the current study, we compute the distance matrices, distance spectra, and distance polynomials of the $C_{20}-C_{90}$ fullerenes. The distance level patterns, which are shown to be structural invariants for fullerenes, are computed as signatures of fullerenes. The distance level patterns could also be used for the computation of the self-avoiding walk generating functions, which are in turn useful in the computation of properties. The Wiener numbers of the $C_{20}-C_{90}$ fullerenes are computed. The Riemann zeta functions[33] of the distance spectra of fullerenes are considered.

2. Distance Matrices, Distance Level Patterns, and Distance Polynomials

The adjacency matrix **A** of a graph can be defined as

$$A_{ij} = \begin{cases} 1 & \text{if } i \neq j \text{ and } i \text{ and } j \text{ are connected,} \\ 0 & \text{otherwise.} \end{cases}$$

The distance matrix contains information on the shortest "distance" from a vertex i to any other vertex j such that the movement from the vertex i to j is restricted through the edges or bonds of the graph. A walk is defined as a continuous sequence of edges from the vertices i to j. The ijth distance matrix entry is given by the shortest walk from i to j. The distance matrix can be defined more rigorously as follows.

$$D_{ij} = \begin{cases} 0 & \text{if } i = j, \\ d_{ij} & \text{if } i \neq j \text{ and } d_{ij} \text{ is the length of the} \\ & \quad \text{shortest walk from } i \text{ to } j. \end{cases}$$

The elements of the distance matrix have to be constructed from the walks of various lengths, and the shortest walk is chosen. Thus, the construction of the distance matrix can be a computing intensive problem for a general graph. However, since fullerenes are closed cage structures, some simplification can be accomplished.

Although several techniques have been developed for the generation of distance matrices, we found the matrix power method to be most suitable for fullerenes. The matrix power technique derives its origin from the fact that kth powers of the

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adjacency matrix of a graph enumerate walks of length k. Equivalently, the ijth matrix element of the $\mathbf{A}^k$ matrix enumerates all walks of length k from the vertex i to the vertex j. The construction of the distance matrix involves finding the shortest walk, and thus, one has to seek the smallest value of k for which the matrix element ij becomes nonzero in the $\mathbf{A}^k$ matrix. This is a consequence of the fact that the first time the ijth element in $\mathbf{A}^k$ becomes nonzero for some k suggests that the shortest walk between the vertices i and j would be of length k, and consequently,

$$d_{ij} = \begin{cases} k & \text{if } A_{ij}^k \neq 0, \text{ and} \\ & A_{ij}^l = 0 \text{ for all } l = 1,2,3, ..., k-1 \end{cases}$$

The computation of powers of the adjacency matrix can be stopped when the distance matrix generated up to the kth power of the adjacency matrix is the same as the $(k + 1)$th power of the adjacency matrix. Until this is accomplished, convergence is not reached and the computations of the powers of the adjacency matrix are iterated. In the worst case the maximum number of iterations would be n, if n is the number of vertices. Fortunately, since fullerenes are closed structures, convergence is reached most of the time within 10-14 iterations for the fullerenes C_{60}-C_{90} and a smaller number of iterations for smaller fullerenes.

Topological indices and structural invariants can be obtained from the distance matrices. A commonly used topological index known as the Wiener index is defined as

$$W = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} D_{ij}$$

where n is the number of vertices. The Wiener index finds numerous applications in the topological prediction of the properties of molecules.[32] There are several other indices that can be defined from the distance matrices such as the Balaban J-index.[32] In this investigation we restrict ourselves to the computation of the Wiener indices for all fullerenes from C_{20} to C_{90}.

The distance polynomial of a fullerene structure can be defined as

$$P_L(G) = |\lambda I - D|$$

where D is the distance matrix of the fullerene cage. The roots of the distance polynomial constitute the distance spectrum of the graph. A few general characteristics of the distance spectrum and distance polynomial may be discussed prior to discussing the results for fullerenes. In general, the distance spectrum exhibits a higher degree of degeneracy compared to the ordinary graph spectrum derived from the adjacency matrix.

An important structural invariant associated with the distance spectrum is the largest and positive eigenvalue, also known as the principal eigenvalue, and the corresponding eigenvector called the principal eigenvector. The other interesting feature pertaining to the distance spectrum is that it often contains several zero eigenvalues. If there are l zero eigenvalues in the distance spectrum, then the coefficients of the distance polynomial denoted as C_k's (the coefficient of λ^k in the distance polynomial) are zero for all $k \leq l - 1$.

Another interesting structural signature of a fullerene can be constructed from the distance matrix. We call this the distance level pattern. It is possible to construct such a pattern that was found to be unique for each fullerene, since fullerenes are regular graphs. If the rows of the distance matrices are arranged so that the entries in each row are in an ascending order, then all rows would become identical. This is a consequence of the fact that fullerenes are regular graphs. Therefore, a row containing n entries constitutes a unique signature for a fullerene and is thus a unique structural descriptor. The entries in a row could be repeated in which case we collect the frequencies of all entries with the same value. This could be referred to as the degeneracy of this entry. This leads to a signature of reduced length. We shall call the irreducible vector thus generated, which consists of the unique distances from a given vertex and the number of times that entry appears, a distance level pattern. Such distance level patterns are constructed for all fullerenes C_{20}-C_{90}.

3. Results and Discussion

The distance matrices, spectra, distance polynomials, and the distance level patterns of all fullerenes were computed in quadruple precision arithmetic. In addition a scaling technique may have to be invoked for larger fullerenes. The coefficients of the distance polynomials grow rapidly out of bound for larger fullerenes, and thus, the scaling technique may be desirable for that purpose. In any case, quadruple precision ensures 31-digit accuracy, and thus, if coefficients have more than 31 digits, then they are omitted in this study.

Table 1 shows the distance level patterns of all fullerenes considered here. The smallest fullerene that consists of only pentagons is the dodecahedral C_{20} fullerene. As evidenced from Table 1, this structure exhibits 0(1), 1(3), 2(6), 3(6), 4(3), 5(1) as the distance level pattern. This means that there is only 1 vertex at zero distance from any given vertex, 3 vertices with unit distances from any given vertex, 6 vertices with distances 3, ..., and one vertex with distance 5. This pattern, we believe, is a unique structural signature for a fullerene. That is, no two fullerenes were found to have the same distance level patterns. Moreover, the distance level pattern is invariant to labeling. Since fullerenes are regular graphs, all vertices have the same distance level patterns for a given fullerene. The fact that fullerenes are regular graphs with vertex degrees 3 is reflected in the 3-fold degeneracy of the distance 1 for all fullerenes (see Table 1). The distance level patterns may also be useful in the characterization of the symmetry of fullerene as well as complete connectivity since it contains all of the distances from any vertex to any other vertex.

As seen from Table 1, different structural isomers of fullerenes have different distance level patterns. For example, the C_{40} fullerene with the T_d symmetry, has the distance level pattern of 0(1), 1(3), 2(6), 3(6), 4(9), 5(9), 6(6), while the C_{40} structural isomer with the D_5 symmetry, has 0(1), 1(3), 2(6), 3(8), 4(10), 5(8), 6(3), 7(1). Notably, the largest distance is 7 for the C_{40} fullerene with the D_5 symmetry, while it is 6 for the C_{40} fullerene with T_d symmetry. The 6-fold degeneracy of the largest distance in the case of C_{40} (T_d) is quite interesting.

C_{78} is quite interesting in that isomers of this fullerene have been isolated experimentally.[22] There are five C_{78} fullerenes containing isolated pentagons. The distance level patterns of all these isomers are different, as evidenced from Table 1. It is also interesting that the last two fullerenes with D_{3h} symmetries have similar, but not identical, distance level patterns. Perhaps the distance level patterns could be used as measures of structural similarities. The difference in the two structures is mainly in the distance levels 4 and 5.

Table 2 shows the Wiener indices of all fullerenes considered here. Although the Wiener indices of the fullerene cages were constructed from the entire distance matrices, we note that the

TABLE 1: Distance Level Patterns for Fullerenes

Dodecahedral C_{20} Fullerene (I_h Symmetry)
O(1) 1(3) 2(6) 3(6) 4(3) 5(1)

C_{24} Fullerene with D_{6d} Symmetry
O(1) 1(3) 2(6) 3(7) 4(5) 5(2)

C_{26} Fullerene with D_{3h} Symmetry
O(1) 1(3) 2(6) 3(6) 4(6) 5(3) 6(1)

C_{28} Fullerene with T_d Symmetry
O(1) 1(3) 2(6) 3(6) 4(6) 5(6)

C_{30} Fullerene with D_{5h} Symmetry
O(1) 1(3) 2(6) 3(6) 4(6) 5(6) 6(2)

C_{32} Fullerene with D_3 Symmetry
O(1) 1(3) 2(6) 3(6) 4(6) 5(6) 6(3) 7(1)

C_{36} Fullerene with D_{6h} Symmetry
O(1) 1(3) 2(6) 3(7) 4(8) 5(7) 6(3) 7(1)

C_{38} Fullerene with D_{3h} Symmetry
O(1) 1(3) 2(6) 3(6) 4(6) 5(6) 6(6) 7(3) 8(1)

C_{40} Fullerene with T_d Symmetry
O(1) 1(3) 2(6) 3(6) 4(9) 5(9) 6(6)

C_{40} Fullerene with D_5 Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(8) 6(3) 7(1)

C_{42} Fullerene with D_3 Symmetry
O(1) 1(3) 2(6) 3(8) 4(9) 5(8) 6(5) 7(2)

C_{44} Fullerene with D_{3h} Symmetry
O(1) 1(3) 2(6) 3(6) 4(9) 5(9) 6(6) 7(3) 8(1)

C_{44} Fullerene with T Symmetry
O(1) 1(3) 2(6) 3(6) 4(9) 5(9) 6(6) 7(3) 8(1)

C_{46} Fullerene with C_3 Symmetry
O(1) 1(3) 2(6) 3(8) 4(9) 5(9) 6(6) 7(4)

C_{48} Fullerene with D_3 Symmetry
O(1) 1(3) 2(6) 3(8) 4(9) 5(9) 6(7) 7(4) 8(1)

C_{50} Fullerene with D_{5h} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(9) 6(7) 7(4) 8(2)

C_{52} Fullerene with T Symmetry
O(1) 1(3) 2(6) 3(8) 4(9) 5(9) 6(8) 7(6) 8(2)

Buckminsterfullerene C_{60}
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(10) 7(8) 8(3) 9(1)

C_{70} Fullerene with D_{5h} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(10) 7(9) 8(7) 9(4) 10(2)

C_{76} Cage ($p = q = 0$)
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(11) 7(10) 8(8) 9(7) 10(2)

C_{78} Fullerene with C_{2v} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(12) 6(12) 7(12) 8(10) 9(4)

Second C_{78} Fullerene with C_{2v} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(12) 6(12) 7(10) 8(9) 9(6) 10(1)

Third C_{78} Fullerene with D_3 Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(11) 7(10) 8(8) 9(8) 10(3)

Fourth C_{78} Fullerene with D_{3h} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(11) 7(10) 8(8) 9(7) 10(3) 11(1)

Fifth C_{78} Fullerene with D_{3h} Symmetry
O(1) 1(3) 2(6) 3(8) 4(10) 5(11) 6(11) 7(10) 8(8) 9(6) 10(3) 11(1)

C_{80} Fullerene with I_h Symmetry
O(1) 1(3) 2(6) 3(8) 4(11) 5(11) 6(11) 7(11) 8(8) 9(6) 10(3) 11(1)

C_{84} Coroninic Cages ($p = q = 0$)
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(11) 7(10) 8(9) 9(8) 10(5) 11(3)

C_{84} Second Cage Count = 105
O(1) 1(3) 2(6) 3(8) 4(10) 5(11) 6(12) 7(12) 8(10) 9(7) 10(3) 11(1)

C_{90} Coroninic Cage ($p = q = 0$)
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(10) 7(10) 8(10) 9(9) 10(7) 11(4) 12(2)

C_{90} Second Fullerene Cage Count = 6
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(11) 7(11) 8(10) 9(9) 10(6) 11(4) 12(1)

C_{90} Third Fullerene Count = 60
O(1) 1(3) 2(6) 3(8) 4(10) 5(10) 6(12) 7(12) 8(11) 9(10) 10(5) 11(2)

Wiener indices of fullerenes can be readily obtained from the distance level pattern vectors. Let the distance level pattern be denoted by p of length m. Let the degeneracy of the ith component of the distance pattern vector be g_i. Then it is easily seen that the Wiener index of the fullerene with the distance level pattern, p, is given by

$$W = \frac{n}{2}\sum_{i=1}^{m} p_i g_i$$

where the sum is over all the components of the distance pattern vector and n is the number of vertices in the fullerene under consideration.

TABLE 2: Wiener Numbers for Fullerenes (C_{20}–C_{90})

fullerene	Wiener number	fullerene	Wiener number
C_{20} (I_h)	500	C_{50} (D_{5h})	5275
C_{24} (D_{6d})	804	C_{52} (T)	5850
C_{26} (D_{3h})	987	C_{60} (I_h)	8340
C_{28} (T_d)	1194	C_{70} (D_{5h})	12375
C_{30} (D_{5h})	1435	C_{76} coroninic	15248
C_{32} (D_3)	1696	C_{78} (C_{2v};I)	16305
C_{36} (D_{6h})	2292	C_{78} (C_{2v})	16329
C_{38} (D_{3h})	2651	C_{78} (D_3)	16284
C_{40} (T_d)	3000	leapfrog C_{78} (D_{3h})	16293
C_{40} (D_5)	2990	C_{78} (D_{3h}; II)	16365
C_{42} (D_3)	3390	C_{80} (I_h)	17600
C_{44} (D_{3h})	3818	Coroninic C_{84}	19646
C_{44} (T)	3830	Coroninic C_{90}	24315
C_{46} (C_3)	4281	C_{90} (second)	23401
C_{48} (D_3)	4764	C_{90} (third)	23423

The spectra of the distance matrices of all fullerenes considered here were computed using the Givens–Householder method. The corresponding distance polynomials were computed using the author's code described before.[34,35] Quadruple precision was used for computing both the spectra and the distance polynomials. Tables 3 and 4 show our computed distance spectra and distance polynomials of fullerenes, respectively.

As seen from Table 3, the distance spectra exhibit considerable degeneracy especially for high-symmetry fullerene cages such as C_{20}, C_{28}, C_{60}, C_{80}, etc. For such high-symmetry cages, it is feasible to express the distance polynomials shown in Table 3 in more compact forms by identifying the eigenvalues in the distance spectra in surd forms. For example, consider the dodecahedral C_{20} fullerene shown in Table 3. The distance spectrum of C_{20} contains several integral eigenvalues. The nonintegral eigenvalues can be simplified into surd forms as follows. The eigenvalues $-13.708\,203\,932$ and $-0.291\,796\,068$ can be expressed as $-(7 + 3(5^{1/2}))$ and $-7 + 3(5^{1/2})$, respectively. Consequently, the distance polynomial of C_{20} shown in Table 3 can be expressed in a factored form as

$$P_D(C_{20}) = \lambda^9\{\lambda^2 + 14\lambda + 4\}^3 (\lambda + 2)^4 (\lambda - 50)$$

From the above form of the distance polynomial of C_{20}, one could obtain the factored form of the coefficient of the λ^9 term as

$$-4^3 \times 2^4 \times 50 = -2^{11} \times 5^2 = -51\,200$$

The value obtained above agrees with the value reported in Table 4 for the dodecahedral C_{20} fullerene, thus independently confirming the computed results in Table 4.

The distance polynomial of the tetrahedral C_{28} fullerene can be factored using a similar technique. In this case, the distance spectrum reported in Table 3 can be brought into surd forms for most of the eigenvalues. The eigenpairs exhibiting 2-fold degeneracy namely, $-1.618\,033\,989$ and $0.618\,033\,989$, can be brought into the form $-\,^1/_2 \pm (5^{1/2}/2)$, respectively. Likewise, the eigenpairs $-2.618\,033\,989$ and $-0.381\,966\,011$ can be

TABLE 3: Distance Spectra of Fullerenes C_{20}−C_{90}

Icosahedral C_{20} Fullerene

−13.708203932(3) −2.000000000(4) −0.291796068(3) 0.000000000(9) 50.000000000(1)

C_{24} Fullerene with D_{6d} Symmetry

−18.829968584(2) −15.615773106(1) −2.562336262(2) −2.000000000(2) −1.000000000(4) −0.887829303(2) −0.384226894(1) 0.000000000(6) 0.280134149(2) 0.984851962(1) 67.015148038(1)

C_{26} Fullerene with D_{3h} Symmetry

−22.000000000(1) −18.761355821(2) −3.000000000(1) −2.238644179(2) −2.000000000(3) −1.000000000(2) −0.948016854(1) 0.000000000(13) 75.948016854(1)

C_{28} Fullerene with T_d Symmetry

−22.201440469(3) −2.618033989(3) −2.515159615(1) −1.618033989(2) −1.518436059(3) −0.752906950(3) −0.381966011(3) 0.000000000(3) 0.223753797(1) 0.472783467(3) 0.618033989(2) 85.291405818(1)

C_{30} Fullerene with D_{5h} Symmetry

−28.972356907(1) −22.471976918(2) −4.192305057(1) −2.618033989(4) −2.473336729(2) −2.061495041(1) −1.803142804(2) −0.668870312(1) −0.381966011(4) 0.000000000(4) 0.093466380(2) 0.164661964(1) 1.094779835(2) 1.560210237(2) 95.730365353(1)

C_{32} Fullerene with D_3 Symmetry

−32.763245187(1) −24.379464730(2) −4.000000000(3) −3.236067977(2) −2.551734316(1) −2.434304474(1) −1.215626867(2) −0.802450339(1) −0.404908403(2) 0.000000000(13) 0.413533643(1) 1.236067977(2) 106.138200672(1)

C_{36} Fullerene with D_{6h} Symmetry

−34.607770936(1) −32.264910945(2) −5.121410769(1) −4.000000000(1) −3.414213562(2) −3.281771634(2) −2.000000000(4) −0.585786438(2) −0.453317421(2) −0.270818295(1) 0.000000000(14) 0.659649512(1) 2.000000000(2) 127.340350488(1)

C_{38} Fullerene with D_{3h} Symmetry

−45.861251951(1) −29.126322019(2) −5.741916524(1) −5.236067977(2) −5.000000000(1) −4.727654272(2) −2.831765063(1) −1.556187494(1) −1.296672637(2) −1.000000000(2) −0.763932023(2) −0.146715468(1) 0.000000000(15) 0.306981308(1) 0.839732483(1) 2.150648928(2) 139.991122710(1)

C_{40} Fullerene with T_d Symmetry

−38.553477442(3) −5.236067977(3) −3.905858668(3) −1.540663891(3) −0.763932023(3) 0.000000000(24) 150.000000000(1)

C_{40} Fullerene with D_5 Symmetry

−39.898256984(2) −33.677698923(1) −4.698705562(2) −4.205378615(2) −3.696370176(2) −3.656384955(1) −3.624636598(2) −1.670460872(2) −0.665916121(1) −0.582315121(1) −0.464349417(2) −0.447601232(2) −0.357065779(2) −0.322906084(2) 0.000000000(6) 0.232810020(2) 0.517518325(2) 0.910250710(2) 0.987240788(1) 1.725152261(2) 149.595074333(1)

C_{42} Fullerene with D_3 Symmetry

−42.145630198(2) −39.060920454(1) −4.940108419(1) −4.701940864(2) −4.476126117(1) −3.569177425(2) −3.558634651(1) −2.378492151(2) −1.965302529(2) −1.686491420(1) −1.485462900(1) −0.797807161(2) −0.542280946(2) −0.531109098(1) −0.293409312(2) −0.222735957(1) −0.197481971(1) 0.000000000(7) 0.262712799(2) 0.292289298(1) 0.666099218(1) 0.960807110(2) 1.170520676(2) 1.744351495(1) 161.456330977(1)

C_{44} Fullerene with D_{3h} Symmetry

−46.548551581(1) −42.824377646(2) −5.000000000(1) −4.837825428(2) −4.693962528(1) −4.618033989(2) −3.371950574(1) −2.967754643(1) −2.381966011(2) −1.193755854(2) −1.000000000(2) −0.545430138(1) −0.524353119(1) −0.480545943(2) −0.080817368(1) 0.000000000(15) 0.424301335(2) 0.912203536(2) 1.061736361(1) 1.099466204(1) 173.571617385(1)

C_{44} Fullerene with T Symmetry

−44.462676005(3) −5.961293139(3) −4.444021998(1) −4.029192812(3) −2.000000000(2) −0.661729723(1) −0.546838044(3) 0.000000000(27) 174.105751721(1)

C_{46} Fullerene with C_3 Symmetry

−47.967281177(2) −45.797001315(1) −6.285934678(1) −5.599090716(2) −4.218893890(2) −4.170007297(1) −3.477593497(2) −2.890944925(1) −2.440667421(1) −2.007686846(2) −1.438246836(2) −0.794412881(1) −0.516433478(2) −0.495435516(1) −0.225913130(1) −0.170301200(2) −0.081603355(1) 0.000000000(11) 0.230314171(2) 0.340627442(1) 0.853247097(2) 1.002769297(1) 1.311966372(2) 1.670394715(1) 186.168129064(1)

C_{48} Fullerene with D_3 Symmetry

−50.085558347(2) −49.961044504(1) −6.041572691(1) −5.724645250(2) −5.050183749(2) −4.419294715(1) −3.571522668(1) −3.301706253(2) −2.565736761(2) −2.496258083(1) −1.839268659(2) −1.250717686(1) −0.800749802(1) −0.673870754(2) −0.600469790(2) −0.544567657(2) −0.458478847(1) −0.422762225(1) −0.157842753(2) −0.073697324(1) 0.046312325(2) 0.060515206(1) 0.361845530(1) 0.403282617(2) 0.587529988(2) 0.646931349(2) 0.700499504(1) 0.788729801(1) 1.039935486(1) 1.165406745(2) 1.694386950(2) 198.544573020(1)

C_{50} Fullerene with D_{5h} Symmetry

−53.719248953(2) −51.922962794(1) −6.242887545(2) −5.000000000(1) −4.840566048(2) −4.427029742(2) −4.370477984(2) −1.969758577(2) −1.664388649(2) −1.371716357(2) −1.000000000(2) −0.692307258(2) −0.632530306(2) −0.289200979(2) −0.178556837(2) −0.077037206(1) 0.000000000(9) 0.280099823(2) 0.473842556(1) 0.590300242(2) 0.673206804(2) 0.855062365(2) 1.000000000(1) 2.520415870(1) 211.005741574(1)

C_{52} Fullerene with T Symmetry

−57.000881503(3) −5.833515693(3) −4.862296965(3) −4.730967191(1) −3.866198263(2) −2.892264396(3) −2.156709207(3) −0.789244119(2) −0.557978917(3) −0.517784531(1) −0.188511127(3) −0.045629275(3) 0.000000000(8) 0.080755496(1) 0.182338820(3) 0.655442382(2) 1.012182367(3) 1.145706924(1) 1.343265896(3) 225.022289302(1)

Buckminsterfullerene (C_{60})

−69.060712632(3) −5.828427125(4) −5.455618900(3) −4.236067977(4) −2.957586986(5) −2.618033989(5) −1.862273042(3) −0.621395426(3) −0.618033989(3) −0.381966011(5) −0.171572875(4) 0.236067977(4) 0.878468121(5) 1.618033989(3) 3.079118865(5) 278.000000000(1)

TABLE 3: (Continued)

C_{70} Fullerene with D_{5h} Symmetry

−94366395116(1) −84.401081825(2) −8.362818330(2) −7.451348006(2) −6.765945013(1) −6.347134260(2) −5.845883479(2) −4.886540027(2) −4.847621203(2) −4.261610868(2) −3.935432332(1) −2.851782559(1) −2.544630586(2) −1.768352211(2) −0.673693120(1) −0.618033989(1) −0.537401577(1) −0.498316193(2) −0.477058105(2) −0.451848561(2) −0.388626719(2) −0.247593858(2) −0.247441131(1) −0.196617729(2) −0.078961081(1) 0.000000000(4) 0.056359060(2) 0.111622813(2) 0.214471453(2) 0.323552428(2) 0.343800771(2) 0.379781259(1) 0.472833909(1) 0.643718990(2) 1.277095627(2) 1.618033989(1) 1.790095775(2) 1.938422337(1) 1.963067252(2) 2.253297791(2) 353.666014423(1)

C_{76} Cages ($p = q = 0$)

−106.590849781(1) −98.166036048(1) −93.002193911(1) −9.693548237(1) −9.301935852(1) −9.034365031(1) −8.468159565(1) −8.277912481(1) −7.838724102(1) −7.606770014(1) −6.994998470(1) −6.377080061(1) −5.149102765(1) −5.135741478(1) −4.896592955(1) −4.886304357(1) −4.587233975(1) −4.496525147(1) −4.079710222(1) −3.568221033(1) −2.762929719(1) −2.756063307(1) −2.657543232(1) −1.944860415(1) −1.463273351(1) −1.443709842(1) −1.440125168(1) −1.100656931(1) −0.911202712(1) −0.839500397(1) −0.816113992(1) −0.753859805(1)

C_{76} Cages ($p = q = 0$)

−0.695023242(1) −0.679353593(1) −0.527223366(1) −0.452633453(1) −0.409421938(1) −0.265065283(1) −0.242097617(1) −0.232315800(1) −0.225680856(1) −0.156358899(1) −0.086244875(1) −0.015553285(1) −0.003436871(1) 0.000000000(4) 0.018350318(1) 0.075916832(1) 0.108761559(1) 0.204337941(1) 0.247270565(1) 0.273114925(1) 0.320627661(1) 0.362214587(1) 0.565305917(1) 0.699427967(1) 0.718028720(1) 0.801669570(1) 0.843012175(1) 0.996016918(1) 1.044201004(1) 1.157280207(1) 1.332925128(1) 1.452107669(1) 1.516520350(1) 1.580854078(1) 1.813285566(1) 2.054895601(1) 2.353554674(1) 2.456838250(1) 2.869244963(1) 3.765372543(1) 401.401117745(1)

C_{78} Fullerene with C_{2v} Symmetry

−111.785878648(1) −100.668759685(1) −98.788905139(1) −10.401118849(1) −9.630631221(1) −9.539726482(1) −9.192899417(1) −9.029265021(1) −8.225620529(1) −7.929354268(1) −6.085162387(1) −5.594581765(1) −5.577630704(1) −5.536216557(1) −5.216968472(1) −5.207055753(1) −4.696548117(1) −4.608776319(1) −4.446402431(1) −3.190286306(1) −2.838597617(1) −2.244618148(1) −1.943469860(1) −1.729650850(1) −1.701654599(1) −1.276099221(1) −1.210193721(1) −1.023453066(1) −1.005958107(1) −0.935257431(1) −0.754494706(1) −0.680951857(1) −0.600301627(1) −0.509607292(1) −0.469295267(1) −0.462895259(1) −0.426066895(1) −0.317141605(1) −0.288255655(1) −0.267568125(1) −0.260938101(1) −0.222773026(1) −0.151034913(1) −0.133985704(1) −0.131892369(1) −0.015673692(1) 0.000000000(8) 0.130560203(1) 0.24912106791) 0.256605490(1) 0.329390794(1) 0.457103541(1) 0.491300673(1) 0.535420525(1) 0.629383676(1) 0.845823480(1) 0.986124687(1) 0.998934256(1) 1.056281407(1) 1.164353642(1) 1.338791786(1) 1.368261817(1) 1.495836549(1) 1.566406647(1) 1.657862451(1) 1.756475983(1) 1.934166456(1) 2.100686739(1) 3.322313650(1) 4.064331218(1) 418.218080051(1)

Second C_{78} Fullerene with C_{2v} Symmetry

−110.332481234(1) −101.885422519(1) −100.747525688(1) −9.727219917(1) −9.586070917(1) −9.401199720(1) −9.356586228(1) −8.977474039(1) −8.944765685(1) −8.404846430(1) −6.741478363(1) −6.588036125(1) −6.378325859(1) −5.400661911(1) −4.940209367(1) −4.781854699(1) −3.975564878(1) −3.264464485(1) −3.027197715(1) −2.461110238(1) −2.344791553(1) −2.175416399(1) −1.818078537(1) −1.630451002(1) −1.283848602(1) −1.142980871(1) −1.127480119(1) −0.731017027(1) −0.614348922(1) −0.549963172(1) −0.544080807(1) −0.521129634(1) −0.515844255(1) −0.408283370(1) −0.384407806(1) −0.377724265(1) −0.297482097(1) −0.246028653(1) −0.223563949(1) −0.134157354(1) −0.060907251(1) 0.000000000(16) 0.142826174(1) 0.202451219(1) 0.220755140(1) 0.300713912(1) 0.479307744(1) 0.534199247(1) 0.584576664(1) 0.781567585(1) 0.865296339(1) 0.994492570(1) 1.135986168(1) 1.329537198(1) 1.394778664(1) 1.429808246(1) 1.459031326(1) 1.484216010(1) 1.748938672(1) 2.132394998(1) 2.878200369(1) 3.175273992(1) 418.780129424(1)

Third C_{78} Fullerene with D_3 Symmetry

−112.478063097(1) −98.403189745(2) −11.478703110(1) −9.455680423(2) −9.220338337(1) −8.973467506(1) −7.664401529(1) −6.702581272(2) −5.867335010(1) −5.571229660(1) −5.437564164(2) −4.755985941(2) −4.612682770(2) −3.532826001(1) −3.075441573(1) −2.779207726(2) −2.089554347(2) −1.479042480(2) −1.364377592(2) −1.134245115(1) −1.115795318(1) −0.785563956(1) −0.486147851(2) −0.352616954(2) −0.299618385(1) −0.275058951(1) −0.273736655(2) −0.151221874(1) −0.054529689(1) −0.047542705(2) 0.000000000(8) 0.012106001(1) 0.060796093(1) 0.089560649(2) 0.13985725991) 0.328344807(2) 0.431371634(2) 0.534748059(2) 0.542274627(1) 1.209549137(2) 1.352060809(2) 1.613980674(1) 1.614429397(1) 1.990661462(1) 2.099535503(2) 2.403533649(2) 3.791206376(2) 417.703733598(1)

Fourth C_{78} Fullerene with D_{3h} Symmetry

−113.262434760(1) −98.459532860(2) −12.165037093(1) −10.080743956(1) −9.689290384(2) −8.184126924(1) −7.472301289(2) −6.545074530(1) −5.785221579(1) −5.556064993(2) −5.027909510(2) −4.917285993(1) −4.242021586(1) −3.872964406(2) −2.465156367(2) −2.172709429(1) −1.819976063(2) −1.595526860(2) −1.120223676(1) −0.990187299(1) −0.859397765(2) −0.680449195(1) −0.524268181(1) −0.497154394(2) −0.384402996(1) −0.351407612(1) −0.262209206(2) −0.211589747(2) −0.152671627(1) −0.049037172(1) 0.000000000(13) 0.027300551(2) 0.289925041(1) 0.348569027(2) 0.597735188(1) 0.838022918(2) 0.984490276(2) 1.124641217(2) 1.154252632(1) 1.637756250(1) 1.719697256(2) 1.963223133(1) 2.139008418(2) 4.607344182(2) 417.964411366(1)

Fifth C_{78} Fullerene with D_{3h} Symmetry

−108.897492401(1) −103.196800322(2) −10.190903596(2) −9.973962712(1) −9.026669465(2) −8.757786935(1) −6.921336693(2) −6.761654794(1) −6.637893500(1) −5.885152211(2) −2.864882987(1) −2.796496727(2) −2.629808135(2) −2.436070169(2) −1.955311950(1) −1.000000000(1) −0.683556505(2) −0.609678490(1) −0.523670403(1) −0.515752653(1) −0.503166840(2) −0.207968358(1) −0.121113489(2) 0.000000000(31) 0.444016248(1) 1.029964636(2) 1.171031989(1) 1.225186315(2) 1.429503060(1) 1.957167045(2) 2.000000000(1) 2.178756155(2) 419.661503886(1)

C_{80} Fullerene with I_h Symmetry

−112.144797050(3) −13.418629947(3) −9.520834410(3) −8.000000000(4) −0.915738593(3) 0.000000000(63) 440.000000000(1)

TABLE 3: (Continued)

C_{84} Coroninic Cages ($p = q = 0$)

−127.485626939(1) −113.425987579(1) −103.512064586(1) −11.920366656(1) −11.695666243(1) −11.279560638(1) −10.708932793(1)
−10.132093835(1) −9.619274680(1) −9.511739460(1) −8.931557280(1) −6.849322169(1) −6.534956780(1) −5.856483964(1)
−5.616261752(1) −5.486436099(1) −5.137622498(1) −5.029340350(1) −4.683525723(1) −4.076256809(1) −3.316936689(1)
−2.578237101(1) −2.275373473(1) −2.129524171(1) −2.035531038(1) −1.681187653(1) −1.555173663(1) −1.542844590(1)
−1.253601048(1) −1.150061060(1) −0.974121809(1) −0.901771415(1) −0.897009698(1) −0.881473468(1) −0.688637629(1)
−0.635842691(1) −0.632585767(1) −0.632373536(1) −0.485549597(1) −0.461220894(1) −0.429601554(1) −0.413364691(1)
−0.348810663(1) −0.321742218(1) −0.273897701(1) −0.249088611(1) −0.218990915(1) −0.116720034(1) −0.107889378(1)
−0.017219483(1) 0.013459735(1) 0.032978119(1) 0.069868101(1) 0.104263172(1) 0.122822138(1) 0.184700563(1) 0.201878119(1)
0.234801295(1) 0.286505426(1) 0.301402254(1) 0.377816430(1) 0.424858706(1) 0.431970164(1) 0.481342190(1) 0.572556012(1)
0.672109496(1) 0.931329914(1) 0.948091795(1) 1.083708617(1) 1.217350575(1) 1.249905143(1) 1.334782224(1) 1.413474785(1)
1.420347092(1) 1.479014089(1) 1.498856694(1) 1.522182615(1) 2.243933079(1) 2.376505099(1) 2.541188835(1) 3.041945298(1)
4.824268431(1) 4.919695609(1) 468.139547254(1)

C_{84} Second Cage

−116.801837552(3) −12.314871881(3) −9.844006191(3) −7.906302529(1) −6.274682309(3) −5.877863556(2) −4.366476436(3)
−3.846661161(2) −3.414213562(1) −2.342846056(3) −1.150106210(3) −0.726509899(3) −0.634998583(3) −0.585786438(1)
−0.249641593(1) −0.099918576(3) 0.000000000(31) 0.376767443(2) 0.742292318(3) 1.557964426(3) 2.347757274(2) 3.255996949(3)
4.396841981(1) 468.759102141(1)

C_{90} Coroninic Cages ($p = q = 0$)

−151.870957203(1) −113.465280160(2) −13.625980515(2) −13.232962419(1) −12.246873137(2) −11.615783352(2) −8.420306506(1)
−8.053583266(2) −6.862367503(2) −6.243376446(1) −6.237877640(2) −4.540132214(2) −4.005285772(2) −1.904342201(2)
−1.900953409(1) −1.596985032(2) −1.472364186(2) −1.135230023(2) 1.058292349(2) −0.950083230(2) −0.918242647(1)
−0.747463150(2) −0.651447353(2) −0.618033989(1) −0.582099566(1) −0.467160890(2) −0.279004170(1) −0.266292618(2)
−0.239883651(1) 0.000000000(10) 0.091134210(2) 0.102664302(2) 0.161028202(2) 0.335519857(2) 0.432578522(2) 0.825476012(1)
1.033468413(1) 1.051867990(1) 1.104212984(2) 1.123143486(2) 1.123665340(2) 1.186074869(2) 1.618033989(1) 1.758463486(2)
2.380350820(2) 2.479279370(1) 2.985234984(2) 6.118753532(2) 521.297694232(1)

C_{90} Second Fullerene Cage

−142.640197274(1) −123.328321750(1) −116.626236157(1) −13.307438109(1) −12.523455216(1) −12.277922119(1) −11.916891324(1)
−11.012624322(1) −10.580925749(1) −9.276105176(1) −9.145092527(1) −9.086672716(1) −7.455462083(1) −6.758733339(1)
−6.670787679(1) −6.237637070(1) −5.620281603(1) −5.618046221(1) −5.013641718(1) −4.446675132(1) −3.556276346(1)
−2.517015640(1) −2.469994076(1) −2.284135486(1) −1.878781408(1) −1.824958605(1) −1.700230559(1) −1.614350767(1)
−1.452950748(1) −1.309105568(1) −1.209546260(1) −1.021757805(1) −0.983942174(1) −0.982682216(1) −0.854711322(1)
−0.766759241(1) −0.691473010(1) −0.675891956(1) −0.633372233(1) −0.598948208(1) −0.467483078(1) −0.451658149(1)
−0.432511720(1) −0.371408620(1) −0.368530495(1) −0.339175441(1) −0.274225119(1) −0.245087841(1) −0.204299000(1)
−0.141102140(1) −0.113624620(1) −0.091102695(1) −0.066535877(1) 0.000000000(2) 0.002754366(1) 0.097287150(1)
0.138509602(1) 0.173696926(1) 0.250398908(1) 0.266761216(1) 0.306668118(1) 0.336956656(1) 0.357280916(1) 0.409106260(1)
0.464857310(1) 0.513473417(1) 0.551022038(1) 0.579800667(1) 0.596155581(1) 0.656420241(1) 0.671908038(1) 0.691847443(1)
0.910090252(1) 1.032388043(1) 1.046490662(1) 1.150151582(1) 1.256454366(1) 1.407751547(1) 1.453346779(1) 1.571920242(1)
1.817216341(1) 2.192245630(1) 2.280257394(1) 2.397512287(1) 2.466842753(1) 3.734770796(1) 4.914657242(1) 4.982174661(1)
520.457600279(1)

C_{90} Third Fullerene Count = 60

−133.363951845(1) −132.796934464(1) −119.915864559(1) −13.575726891(1) −12.981692486(1) −12.686563222(1) −11.955554509(1)
−11.341681501(1) −9.954307440(1) −8.762082778(1) −8.685421156(1) −6.473046070(1) −6.403717708(1) −6.365212473(1)
−5.958935942(1) −5.768636995(1) −5.544223065(1) −5.206797758(1) −5.064375789(1) −4.951566465(1) −4.082808782(1)
−3.272984337(1) −3.093901050(1) −2.789603753(1) −2.170674200(1) −2.052722178(1) −1.809312147(1) −1.548552181(1)
−1.143789926(1) −0.951252525(1) −0.933159796(1) −0.876139879(1) −0.816439990(1) −0.784154137(1) −0.780446415(1)
−0.741140969(1) −0.739523242(1) −0.660155899(1) −0.625805247(1) −0.495511425(1) −0.460838344(1) −0.421344475(1)
−0.413792360(1) −0.349187054(1) −0.340850612(1) −0.309520707(1) −0.236765822(1) −0.231055087(1) −0.208463732(1)
−0.192894618(1) −0.129016158(1) −0.081151383(1) −0.035597286(1) 0.000000000(4) 0.020889006(1) 0.067902197(1)
0.123943388(1) 0.168106380(1) 0.223365959(1) 0.253547435(1) 0.269215805(1) 0.350954143(1) 0.388867045(1) 0.390480257(1)
0.424658630(1) 0.443855986(1) 0.452151686(1) 0.602704821(1) 0.667478920(1) 0.698939808(1) 0.700230201(1) 0.829569741(1)
1.095334244(1) 1.203483599(1) 1.338291769(1) 1.607432947(1) 1.816230452(1) 1.905456508(1) 1.931800579(1) 1.940589027(1)
2.253426371(1) 3.084142395(1) 3.245065180(1) 3.558767708(1) 4.061320650(1) 4.707140639(1) 520.709505358(1)

expressed as $-\,{}^{3}/_{2} \pm (5^{1/2}/2)$, respectively. The eigenvalues $\lambda_1 = -2.515\,159\,615$, $\lambda_2 = 0.223\,753\,797$, and $\lambda_3 = 85.291\,405\,818$ satisfy the following symmetric equations:

$$\lambda_1 + \lambda_2 + \lambda_3 = 83$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = -196$$

$$\lambda_1\lambda_2\lambda_3 = -48$$

This leaves us with four nonintegral eigenvalues exhibiting 3-fold degeneracies namely, −22.201 440 469, −1.518 436 049, −0.752 906 950, and 0.472 783 467. The eigenvalues satisfy the following symmetric equations:

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = -24$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4 = 40$$

$$\lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4 = -10$$

$$\lambda_1\lambda_2\lambda_3\lambda_4 = -12$$

If one combines all of these results, it can be seen that the distance polynomial of the C_{28} tetrahedral fullerene is given by

$$P_D(C_{28}) = \lambda^3\{\lambda^4 + 24\lambda^3 + 40\lambda^2 + 10\lambda - 12\}^3 \times \{\lambda^2 + 3\lambda + 1\}^3 \times \{\lambda^3 - 83\lambda^2 - 196\lambda - 48\}\{\lambda^2 + \lambda - 1\}^2$$

The above form of the distance polynomial of the C_{28} fullerene yields the coefficient of λ^3 of the distance polynomial as

$$-12^3 \times 48 = -2^{10} \times 3^4 = -829\,44$$

The result thus obtained is in accord with the value reported in Table 4 for the λ^3 coefficient of the C_{28} fullerene.

TABLE 4: Distance Polynomials of Fullerenes

Dodecahedral C_{20} Fullerene (I_h)

power	coefficient	power	coefficient
20	1	18	−1540
17	−39080	16	−403200
15	−2026336	14	−5512000
13	−8417280	12	−7074560
11	−3059200	10	−638976
9	−51200		

C_{24} Fullerene (D_{6d})

power	coefficient	power	coefficient
24	1	22	−2736
21	−94584	20	−1377246
19	−10415904	18	−45969404
17	−124556256	16	−204044439
15	−169447920	14	22374228
13	213132120	12	221006524
11	92149776	10	−3634224
9	−16630272	8	−3842496
7	601344	6	228096

C_{26} Fullerene with D_{3h} Symmetry

power	coefficient	power	coefficient
26	1	24	−3495
23	−138048	22	−2330793
21	−20934816	20	−113258029
19	−395667456	18	−924405204
17	−1458741024	16	−1533918960
15	−1028401920	14	−397027008
13	−67060224		

C_{28} Fullerene with T_d Symmetry

power	coefficient	power	coefficient
28	1	26	−4398
25	−195848	24	−3741105
23	−38150880	22	−234681512
21	−927001032	20	−2391196479
19	−3863773080	18	−3134603922
17	855509256	16	4737775233
15	3842885040	14	−577254636
13	−2733304064	12	−1123207845
11	617302368	10	563300334
9	163680	8	−108630111
7	−19392664	6	8925744
5	2490048	4	−221184
3	−82944		

C_{30} Fullerene with D_{5h} Symmetry

power	coefficient	power	coefficient
30	1	28	−5545
27	−276700	26	−5926410
25	−67295460	24	−443843850
23	−1707943480	22	−3201702685
21	1492906860	20	21943181737
19	42249156800	18	2760646090
17	−109451825940	16	−149259541150
15	12897248060	14	201634053805
13	157123930160	12	−27183067685
11	−98802589480	10	−50710612096
9	−6598147520	8	2079637200
7	534610560	6	−31909120
5	−9684992	4	675840

C_{32} Fullerene with D_3 Symmetry

power	coefficient	power	coefficient
32	1	30	−6808
29	−377080	28	−9017376
27	−115787552	26	−885480688
25	−4205964864	24	−12172328384
23	−18228278528	22	937230336
21	55109633024	20	86917673984
19	26159812608	18	−71177007104
17	−84960280576	16	−27872329728
15	7324303360	14	6414139392
13	1056964608		

C_{36} Fullerene with D_{6h} Symmetry

power	coefficient	power	coefficient
36	1	34	−9804
33	−651968	32	−18577800
31	−280879104	30	−2511927168
29	−13827345408	28	−44820285168
27	−59594127872	26	136312855488
25	788023090176	24	1434829469184
23	417852954624	22	−3110784043008
21	−6371375341568	20	−5505943449600
19	−1437769629696	18	1407594315776
17	1492163100672	16	611196862464
15	121060196352	14	9512681472

C_{38} Fullerene with D_{3h} Symmetry

power	coefficient	power	coefficient
38	1	36	−11791
35	−865592	34	−27968649
33	−497910640	32	−5371295557
31	−36301365240	30	−148532181284
29	−289586987232	28	305935536768
27	3317248716672	26	7714913727104
25	3839637216768	24	−18209227675136
23	−43382135498752	22	−37515237249024
21	40575705088	20	26871241289728
19	21161692102656	18	5161317023744
17	−1117499424768	16	−714357080064
15	−72477573120		

C_{40} Fullerene with T_d Symmetry

power	coefficient	power	coefficient
40	1	38	−13548
37	−1067488	36	−36446064
35	−674064000	34	−7638698624
33	−56995855872	32	−291888314880
31	−1049125705728	30	−2669826877440
29	−4799359229952	28	−6012404035584
27	−5101989101568	26	−2779917631488
25	−873474818048	24	−119876812800

C_{40} Fullerene with D_5 Symmetry

power	coefficient	power	coefficient
40	1	38	−13430
37	−1060640	36	−36608205
35	−690106672	34	−7922698150
33	−58160244660	32	−271433532115
31	−719500754620	30	−407460613532
29	4046596359100	28	13457006956140
27	10887412407160	26	−30682857825560
25	−79353465153472	24	−27465458540640
23	119974951795520	22	145878012780560
21	−33243413522880	20	−158003119968992
19	−63901990358080	18	61677483189440
17	57666862185280	16	347971761600
15	−16808947519872	14	−5609398754880
13	1369248419840	12	1146007632640
11	127655462400	10	−62000507648
9	−17480965120	8	27028480
7	474009600	6	45132800

C_{42} Fullerene with D_3 Symmetry

power	coefficient	power	coefficient
42	1	40	−15654
39	−1332984	38	−49523379
37	−1005565224	36	−12566309172
35	−102815240016	34	−561587919534
33	−1981903464556	32	−3773236388274
31	784282180152	30	24968402150434
29	59660950634976	28	28920701872980
27	−139429594354892	26	−287074888375515
25	−67464367476276	24	438995890400490
23	517245656471700	22	−103435837819806
21	−584458712674272	20	−285737052163926
19	217833329720664	18	254267546744135
17	23070458033868	16	−70955223930474
15	−29681556241360	14	3951621167895
13	4831935734412	12	563180682654
11	−260952705216	10	−67002022887
9	1749399440	8	1885666512
7	151668864		

C_{44} Fullerene with D_{3h} Symmetry

power	coefficient	power	coefficient
44	1	42	−18070
41	−1656844	40	−66504399
39	−1467702128	38	−20123195790
37	−183550950924	36	−1152265986888
35	−5004137029888	34	−14536195987614
33	−24625402869176	32	−7533627861903
31	68410268173632	30	151680649963674
29	82018058115268	28	−174215797180791
27	−313617532424488	26	−78417730248756
25	242249793961836	24	222071331994980
23	−19031245843864	22	−113497969602924
21	−41782278122672	20	14583479964608
19	12371186037312	18	1177298693056
17	−887415608320	16	−235818992640
15	−13109043200		

TABLE 4 (Continued)

C_{44} Fullerene with T Symmetry

power	coefficient	power	coefficient
44	1	42	−18214
41	−1671000	40	−66774195
39	−1456130400	38	−19592542432
37	−174748737936	36	−1076840503184
35	−4686703078400	34	−14525532648192
33	−31966256531968	32	−49307101149440
31	−52078662193152	30	−36344371523584
29	−15851222896640	28	−3888169365504
27	−407913889792		

Fullerene C_{46} with C_3 Symmetry

power	coefficient	power	coefficient
46	1	44	−20787
43	−2044860	42	−88002417
41	−2077274214	40	−30291206465
39	−290776217280	38	−1882649686359
37	−8071919585870	36	−20460225013569
35	−13273014017010	34	99851621446213
33	350616668054592	32	331730582904414
31	−716951897306612	30	−2187539326804965
29	−1057182283553556	28	3474329795587396
27	5133723464801862	26	−809341931681892
25	−6423867278020520	24	−2980708726958067
23	3175286816224956	22	3054598026274912
21	−232192422311112	20	−1076371754247645
19	−257042659924738	18	117199757456619
17	52557392180976	16	−1453621699784
15	−3216156138720	14	−307463529492
13	53545030032	12	10209994992
11	434529792		

C_{48} Fullerene with D_3 Symmetry

power	coefficient	power	coefficient
48	1	46	−23592
45	−2483172	44	−114897348
43	−2933633436	42	−46481097532
41	−486104159676	40	−3428212502196
39	−15894808083332	38	−42006034075959
37	−12389433528732	36	342352167231524
35	1152092383756896	34	768644866775550
33	−4548705939947928	32	−11698347602591844
31	−204556490548560	30	38078588927473572
29	41429962328312136	28	−53438877772232307
27	−125049460581687512	26	13429966668327741
25	193899922261624068	24	70354469606089662
23	−185373941879740500	22	−125526024456039336
21	114360907882436804	20	112811336681492745
19	−44567403368203644	18	−64334920071536375
17	9405097744755804	16	24718183708260171
15	−35671999056372	14	−6479219377192521
13	−591256213660548	12	1141447241694376
11	175801679889948	10	−129273139473165
9	−25642928616796	8	8554729843089
7	1989844713432	6	−262138455882
5	−71094477780	4	1230786582
3	629380920	2	−10980381
1	−1714020	0	51425

C_{50} Fullerene with D_{5h} Symmetry

power	coefficient	power	coefficient
50	1	48	−26625
47	−2981160	46	−147120970
45	−4029009596	44	−69176883030
43	−797362510760	42	−6380349125365
41	−35547495607600	40	−132009560723779
39	−268434346622920	38	108596939827710
37	2611652254039860	36	8098068867341100
35	10238441910180268	34	−5852810450447645
33	−39584068684718600	32	−45517289674514635
31	20822529428768760	30	97750569657138654
29	58844410534534540	28	−71033980722985330
27	−105608153605118440	26	1652486721251310
25	77072132857616048	24	30665784684546800
23	−28802575097557940	22	−22077656199913975
21	4522694925327820	20	7668498395381071
19	450597371017560	18	−1461586197547900
17	−309794836839440	16	142594934661040
15	50251307687680	14	−4638974959680
13	−3412624894720	12	−190563726080
11	77030912000	10	11817827328
9	465776640		

C_{52} Fullerene with T Symmetry

power	coefficient	power	coefficient
52	1	50	−30330
49	−3612384	48	−188941221
47	−5462557968	46	−98870517726
45	−1201095848352	44	−10132123850253
43	−59551924048168	42	−234037134465888
41	−516185820498528	40	33154631543500
39	4098230414127504	38	11372815232636334
37	4314627119103696	36	−44506392069903711
35	−90701492165170488	34	24411719927314818
33	288484916040854184	32	220862682248076957
31	−415117913768668104	30	−665716024660429344
29	226982316131658336	28	918600497848538144
27	142868848116484992	26	−714231121603779072
25	−313935413932122592	24	310724639719077792
23	215632253409003456	22	−62711125430424256
21	−73331171606539776	20	−3050938652l9168
19	11958940346295424	18	1922261744664576
17	−733039015557120	16	−180649682648576
15	16601732296704	14	6264514762752
13	−14472884736	12	−85260190464
11	−3454368768	10	273811968
9	20404224	8	352512

Buckminsterfullerene (C60)

power	coefficient	power	coefficient
60	1	58	−46020
57	−6831720	56	−451346640
55	−16750287600	54	−393261842080
53	−6214157184360	52	−67404303867240
51	−484951936279520	50	−1896906855591648
49	1950349169327040	48	76105926453878020
47	451149959779416840	46	841450173070749000
45	−4881471170768184912	44	−3814767557520962832 0
43	−8613992940696305304 0	42	19235432863982278856 0
41	17304998148979855369 20	40	35676330529139242313 52
39	−57111538652416467971 20	38	−45555335686244193577 440
37	−73650075800401841117 280	36	12371498726547966842 6190
35	69070045240998921634 0680	34	75676001029103085048 0000
33	−16729189748344341367 08480	32	−58018764995670251618 67840
31	−33525554439369764067 33360	30	12638333412173510908 810240
29	25671679340527964972 088840	28	22270177908941329555 59240
27	−49403346508552611979 155680	26	−55304048033983845970 530720
25	22991839626968921917 109376	24	94327135661242682862 609620
23	50297134529254334138 149080	22	−57052143717896317488 473160
21	−83950900831419917902 763120	20	−11975087534330473929 016416
19	47093000559470243245 935600	18	33673249963051619234 234960
17	−41896423232366685474 03960	16	−15692701549650223559 385240
15	−60876000407315818124 76928	14	17005889644166675628 58080
13	21322057814225925000 18720	12	51066011970662488823 2665
11	−13502781567208408534 5960	10	−98698112318782286909 628
9	−12704440893170959013 720	8	46577404995844345687 20
7	17236388644900370260 80	6	76035605550036774400
5	−5648040547692654681 6	4	−1055738430756155904 0
3	−362698702532608 00	2	1821990995302809 60
1	2068999754219520 0	0	755012598759424

C_{70} Fullerene with D_{5h} Symmetry

power	coefficient	power	coefficient
70	1	68	−74445
67	−14063240	66	−1185404710
65	−56467467828	64	−1720698728700
63	−36007766595500	62	−537691364849655
61	−5805557684089980	60	−44600020360380489
59	−225643204283194860	58	−520059587216342725
57	196379311440236526 0	56	220267810969448173 05
55	731844190143679540 08	54	−326390678515968267 95
53	−112108240283092469 3180	52	−322421501239799367 6375
51	273071588781442263 5600	50	366412725182915504 79290
49	567538140354000069 30240	48	−156734684388083460 586680
47	−620224554689304710 246540	46	−244254114279291757 87345
45	301893968471720407 1090652	44	347160892310534808 8853385
43	−802107096438194890 5856580	42	−183288789473757518 40830640
41	928822795384491820 3536680	40	518488933317336304 38954998
39	101847002008772764 8766020	38	−910139545788472293 39262310
37	−581626929851359108 08405420	36	999159453820024352 49606590
35	105071468356372128 031999008	34	−628273789924679240 15052885
33	−108083760428723677 136138660	32	136801558874436808 66233005
31	693497570150298554 44836080	30	982350820508330113 2094748
29	−284960281597300239 42216120	28	−955941771632170109 1805530
27	747210741706011050 7332240	26	394801793264170772 0936690
25	−118311481968901458 1395928	24	−986382396315394654 864380
23	849035576891001507 91040	22	162125882332658075 427025
21	576832549894686907 8060	20	−180198151289118256 52753
19	−210245879906332178 0820	18	135706826623469684 5620
17	242660209864094296 000	16	−681228065649327019 20
15	−159636071338242090 88	14	220736212578351208 0
13	646475360583789440	12	−44513987031104320
11	−1602585680074880 0	10	572680097019648
9	231660957117440	8	−5978597505280
7	−1753489858560	6	53381447680
5	4919732224	4	−193290240

TABLE 4 (Continued)

C_{76} Cages ($p = q = 0$)

power	coefficient	power	coefficient
76	1	74	−95824
73	−20569184	72	−1973226882
71	−107132579696	70	−3720660150482
69	−88600191564958	68	−1500222687922303
67	−18232791935708256	66	−154992752724887428
65	−822269597258159184	64	−1241086234598202201
63	1947834648154465970 4	62	17439225069860347651 2
61	54413011966692656757 6	60	−1101305034690718128236
59	−1586425870418082452640 8	58	−4508703079000854357606 6
57	8117116232052710003496 0	56	8602919361886663044017 27
55	1422339717785582566237880	54	−5556441033893483004811234
53	−2532754184045702251428054 4	52	−2593592901308437424781937

C_{78} Fullerene with C_{2v} Symmetry

power	coefficient	power	coefficient
78	1	76	−104115
75	−23253700	74	−2316631213
73	−130345447180	72	−4686485352895
71	−115540214240800	70	−2028181293510050
69	−25645063322388444	68	−228814759193612146
67	−1310266443958581028	66	−2806375853714534485
65	25132852759289952268	64	27187155694457782427 1
63	104462399085653239895 2	62	−485585105244924973467
61	−2286624580691423323505 6	60	−8726813630722771365145 5
59	1902936070852064739211 6	58	11883710088997232033539 80
57	3128961946835315994995492	56	−4118559282898822323974096
55	−3656098965855833208166190 8	54	−3811466764827484988032173 8
53	1882792057306065428636799 92	52	5159931843220885945256996 18

Second C_{78} Fullerene with C_{2v} Symmetry

power	coefficient	power	coefficient
78	1	76	−104493
75	−23338056	74	−2319618880
73	−129880586096	72	−4644034709764
71	−114022969342820	70	−2002043796585520
69	−25573911779106260	68	−235952365749791098
67	−1495594222903104348	66	−5346063132746378636
65	3118118329351357340	64	155991590305254006308
63	82329615761593081951 2	62	1180688942266585248892
61	−801294209265333586645 2	60	−4588525814511307522347 8
59	−5313242977825824774221 6	58	3235440717297414768473 45
57	1273658977746131709649212	56	1983502085785986689089 65

Second C_{78} Fullerene with C_{2v} Symmetry

power	coefficient	power	coefficient
55	−8388660848967800235944600	54	−1505425158385559481619451
53	2260250215369163720465641 2	52	9887714475765751011792686 5
51	1847656856012118990343692 0	50	−3375160643145290908334025 21
49	−3538345864696142063487537 64	48	6646633905362589086708967 03
47	1323872052016327262549960216	46	−6125056535656159971216412 49

Third C_{78} Fullerene with D_3 Symmetry

power	coefficient	power	coefficient
78	1	76	−103728
75	−23181300	74	−2317666680
73	−131307632244	72	−4762109965935
71	−118467055603896	70	−2095818764845032
69	−26601901461823356	68	−235703924049692388
67	−1291214613386442744	66	−1735955398478189697
65	37643624328931966788	64	344317182281974465185
63	1132927224116177236836	62	−2410088037612705429888
61	−37772369081522238156276	60	−121637861735527698482111
59	170197232049835794354156	58	2449610300457421418561085
57	539543455711207212224771 2	56	−1402694358650396879611328 4
55	−918798819781681423259590 92	54	−7381576024298069767782809 6
53	6170440754312783511241607 88	52	1650637814240860519201192692

Fourth C_{78} Fullerene with D_{3h} Symmetry

power	coefficient	power	coefficient
78	1	76	−103947
75	−23215596	74	−2315179425
73	−130473524196	72	−4691459711505
71	−115235949455556	70	−2001126062343432
69	−24685414076206860	68	−207949419579065430
67	−1000763418213856716	66	4216140541518278 86
65	48223653881316513036	64	369486192952204938732
63	1072653590091201963688	62	−3208667441617409056974
61	−41599049863392106361580	60	−137723068722507823180132
59	987538028193833182157 88	58	2290192837052816507800581
57	6221215875982736502988200	56	−6486843716671880165339589
55	−74339808667238267384456136	54	−114291177610032559078998075
53	30751206897861149125793866 8	52	127608004989810532536247152 3
51	294915007475633944913086720	50	
25	−361213580647682420319266304	24	306279681228140468266558080
23	100613921233303199007952896	22	−60616133851191241745326 08
21	−7837290168325700993142784	20	−1056955021509795466887168
19	1357788337082513130455 04	18	5217460460611892880998 4
17	50910456224838140559 36	16	946137836110994472 96
15	−1025535828836745216 0	14	−21945292055956684 8

Fifth C_{78} Cage with D_{3h} Symmetry

power	coefficient	power	coefficient
78	1	76	−105081
75	−23470872	74	−2325062802
73	−129221449560	72	−4574672087040
71	−111091821759672	70	−1930700381008341
69	−24502856858545452	68	−226915785509741535
67	−1485573168255189996	66	−6141372164513101419
65	−8076965351371365408	64	75941992406913406893
63	525227354049261204740	62	1152022706720679857094
61	−2431299028846894009860	60	−20553173447372791767808
59	−33678216580792244672496	58	90104324294192393152134
57	431213922729763301180780	56	217168546163031586666320
55	−2005287509415961912860360	54	−379797757012473450556048 3
53	3614005850372368668850596	52	17296789914876505642941843
51	51589871829365406475969 08	50	−41262302697695415327393288
49	−42169796951272298684861484	48	51809010389474109816277508
47	100682546893942014846571392	46	−169989984830352733364046 60
45	−127853321694932584478600304	44	−44624315193872608893006576
43	86275402348213515335194944	42	69182923569964528466618784
41	−199703931675906072731253 12	40	−41124773053628012483667648
39	−93587549146196006663758 08	38	880005249721221558644275 2
37	577656166253485856365670 4	36	665992044461777955333120
35	−503096186177764588210176	34	−230431497061019962908672
33	−42090117128186687078400	32	−3650967717755581956096

C_{80} Fullerene with I_h Symmetry

power	coefficient	power	coefficient
80	1	78	−116200
77	−26980320	76	−2737680000
75	−152568382464	74	−5298478732800
73	−123471911700480	72	−2015374383759360
71	−23573977344409600	70	−199186750406885376
69	−1209532034052915200	68	−5179264730853539840
67	−15084069227908300800	66	−28155157475963699200
65	−30808423486455808000	64	−17661308040118272000
63	−4070184813854720000		

C_{84} Coroninic Cages ($p = q = 0$)

power	coefficient	power	coefficient
84	1	82	−130146
81	−32647928	80	−3674344167
79	−234967808104	78	−9614504498810
77	−268956917502648	76	−5313969228945946
75	−74347437365999376	74	−705027693014400866
73	−3723035364779879144	72	3823155681062145191
71	249215593699430229992	70	1990869286394699252448
69	4972943190652330821 20	68	−36371476635700933959528
67	−361742616204394859006992	66	−918063931966817472592092
65	397183240891467529639796 8	64	3388552772874944852332491 9
63	5154792446924438853067274 4	62	−3511131368811272112113101 34

C_{84} Second Cage Count = 105

power	coefficient	power	coefficient
84	1	82	−130926
81	−32737344	80	−3639688833
79	−227453772576	78	−9042091564940
77	−245396790138192	76	−4719926272353807
75	−65023712923021760	74	−626598149708286114
73	−3792428426237693664	72	−7123658073789006217
71	106807707604985423520	70	1133724869278852239672
69	4431424206068510273712	68	−4672897471204361061285
67	−13243404638468216363692 8	66	−5369512022524839691434 90
65	1062336943787405695867 20	64	8828983937717970077197173
63	2865078658853377556737059 2	62	−1681164103166414188575054 0
61	−3409497867111504000238278 24	60	−6968657851007531393058385 25
59	1076361558525013212371835072	58	6856859871797147508939496770

C_{90} Coroninic Cages ($p = q = 0$)

power	coefficient	power	coefficient
90	1	88	−161165
87	−45073960	86	−5691034550
85	−411411236804	84	−19104110553040
83	−606879344724920	82	−13583004790942515
81	−213702527318730440	80	−223234443832211192 1
79	−1179310070539367318 0	78	4794068369750088904 5
77	149649960246614292618 0	76	12222702612298334170165
75	260907780699689841335 44	74	−3740222940887588912536 55
73	−3629354489031556142447040	72	−9059635003810260393359945
71	5922359767494009073857008 0	70	5052195795153938102811944 52
69	7306084399834628599020246 80		

TABLE 4 (Continued)

C_{90} Second Fullerene Cage Count = 6

power	coefficient	power	coefficient
90	1	88	−160799
87	−44866980	86	−5622926975
85	−401200488960	84	−18373677808041
83	−577957322405924	82	−12935857448137095
81	−207763500329766024	80	−2329656907371519613
79	−16165749857353615120	78	−28027127856525715350
77	74580495545171838 1772	76	869472870807638999 0804
75	3715333755563940605 9040	74	−82757636073256403569053
73	−1836170546635192351812516	72	−786384898513265493228 7947
71	9333885184977151794488168	70	2229267942152239023983 73688

C_{90} Third Fullerene Count = 60

power	coefficient	power	coefficient
90	1	88	−161223
87	−44910752	86	−5591146593
85	−393795468080	84	−17725541213447
83	−546404842866612	82	−11958500412750362
81	−187453511420140060	80	−2047147119416998764
79	−13781759661085802740	78	−22312353459297671409
77	611428873175019788836	76	6793233144024500458455
75	26658309656391547630776	74	−79918686536244458646319
73	−1407399793744795429809784	72	−5308227018466643473900465
71	1126224342839831448133 5428	70	17204265071354284867774 1525

The author[11] considered in a previous study the factorization of the C_{60} buckminsterfullerene. This was based on expressing the eigenvalues −5.8284 and −0.17157 exhibiting 4-fold degeneracy as $-(3 \pm 8^{1/2})$. The eigenpairs −4.2360 ... and 0.2360... were brought into $-(2 \pm 5^{1/2})$. The eigenpairs 1.618 03 ... and −0.618 03 ... are represented by $(^1/_2 \pm (5/4)^{1/2})$. The eigenpairs −2.618 033 ... and −0.381 966 ... can be expressed as $-(^3/_2 \pm (5/4)^{1/2})$. The remaining four eigenvalues exhibiting 4-fold degeneracy in Table 3 for the C_{60} buckminsterfullerene were shown to satisfy the following symmetric equations:

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = -77$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4 = 563$$

$$\lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4 = -1022$$

$$\lambda_1\lambda_2\lambda_3\lambda_4 = 436$$

The remaining three eigenvalues (−2.9575 ..., 0.878 46 ..., 3.079 11 ...) satisfy the three symmetric equations shown below:

$$\lambda_1 + \lambda_2 + \lambda_3 = 1$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = -9$$

$$\lambda_1\lambda_2\lambda_3 = -8$$

All of these results were combined to factor the distance polynomial of C_{60}[11] as

$$P_D = (\lambda - 278)(\lambda^2 + 1)^9 (\lambda^2 - 1)^7 \{\lambda^4 + 77\lambda^3 + 563\lambda^2 + 1022\lambda + 436\}^3 \times \{\lambda^3 - \lambda^2 - 9\lambda + 8\}^5$$

The distance polynomial of the C_{80} fullerene with the I_h point group can be factored also. The four nonintegral eigenvalues namely, −112.144 797 050, −13.418 629 947, −9.520 834 410, and −0.915 738 593 satisfy the following symmetric equations:

$$\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = -136$$

$$\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4 = 2824$$

$$\lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4 = -16\,800$$

$$\lambda_1\lambda_2\lambda_3\lambda_4 = 1312$$

From these equations and the integral distance eigenvalues of the C_{80} fullerene, it is immediately seen that the factored form of the distance polynomial of the C_{80} fullerene with the I_h point group is

$$P_D = \lambda^{63}(\lambda + 8)^4 (\lambda - 440)\{\lambda^4 + 136\lambda^3 + 2824\lambda^2 + 168\,00\lambda + 1312\}^3$$

The prime factors contained in the coefficient of the λ^{63} term of the distance polynomial can thus be inferred from the factored form as

$$-2^{30} \times 5 \times 11 \times 41^3 = -4\,070\,184\,813\,854\,720\,000$$

The number obtained this way agrees with the computed result in Table 4.

As seen from Table 3, the distance spectra satisfy a few general trends. The highest eigenvalue in the distance spectrum of all fullerenes is always singly degenerate. This result appears to be true for all graphs and may thus have nothing to do with fullerenes. The other interesting point is the distance between the highest eigenvalue and the next higher eigenvalue. As seen from Table 3, this distance is large for all fullerenes. This finding again may have nothing to do with fullerenes as this appears to hold for several other structures that we have studied before.[31] The largest eigenvalue of the distance spectrum, also known as the principal eigenvalue of the distance spectrum, seems to uniquely characterize all fullerenes, and thus, it appears to be a structural invariant in so far as fullerenes are concerned. For example, let us consider the five structural isomers of the C_{78} fullerene. The principal eigenvalues for all these fullerenes are different, as seen from Table 3.

The Riemann zeta functions are useful not only in the distribution of prime numbers[33] but also in the characterization of structures. The Riemann zeta functions can be defined for the distance spectra analogous to the definition for the ordinary graph spectra. The ordinary Riemann zeta function for the prime number distribution is defined as

$$\zeta(x) = 1 + 1^{-x} + 2^{-x} + 3^{-x} + \ldots$$

That is, the distribution of the primes is well known to be given by the Riemann Zeta function as

$$\zeta(x) = \prod_p \left(1 - \frac{1}{p^x}\right)^{-1}$$

where the product is over all primes.

The Riemann zeta function for the distance spectra can be defined, following the definition for the Laplacian spectra, as

$$\zeta(2x) = d_0 + \sum_{\lambda_i \neq 0}^{n} \lambda_i^{-x}$$

where x is any complex or real variable and d_0 is the degeneracy of the zeroth eigenvalue. Note that in the above definition we have omitted all zero distance eigenvalues since inclusion of the zero eigenvalues would lead to infinity or indetermination for certain values of x. Alternatively, one could redefine the distance spectra such that the lowest eigenvalue becomes zero. This is tantamount to adding the absolute value of the lowest eigenvalue to the entire distance spectrum in which case the

TABLE 5: Riemann Zeta Function Values for the Distance Spectra of Fullerenes

fullerene	$\Sigma_i\lambda_i^2$	$\Sigma_i\lambda_i^3$	$\Sigma_i\lambda_i^4$	$\Sigma_i\lambda_i^5$
C_{20}	3080	117240	6356000	311047680
C_{24}	5472	283752	20480376	1345988640
C_{26}	6990	414144	33753222	2517062880
C_{28}	8796	587544	53649228	4497451920
C_{30}	11090	830100	85199690	8007984800
C_{32}	13616	1131240	128767232	13414740960
C_{36}	19608	1955904	266548032	33363866880
C_{38}	23582	2596776	389929958	53520529560
C_{40} (1)	27096	3202464	512880864	75681957120
C_{40} (2)	26860	3181920	507162620	74672509360
C_{42}	31308	3998952	688188948	109360483800
C_{44} (1)	36140	4970532	919067396	157034366040
C_{44} (2)	36428	5013000	930596372	159458622000
C_{46}	41574	6134580	1216208406	222918895170
C_{48}	47184	7449516	1572754320	307583136300
C_{50}	53250	8943480	2006265130	417011972980
C_{52}	60660	10837152	2595582684	575130823440
C_{60}	92040	20495160	6041067360	1655730210000
C_{70}	148890	42189720	15825734890	5517026848140
C_{76}	191648	61707552	26257385480	10390770336560
C_{78} (1)	208230	69761100	30946391302	12757022113400
C_{78} (2)	208986	70014168	31116049618	12842720358520
C_{78} (3)	207456	69543900	30789662688	12679287593220
C_{78} (4)	207894	69646788	30870675318	12718325408040
C_{78} (5)	210162	70412616	31384284330	12977820750960
C_{80}	232400	80940960	37955600000	16438407832320
C_{84} (1)	260292	97943784	48573339300	22419825227960
C_{84} (2)	261852	98212032	48841990284	22568116365600
C_{90} (1)	322330	135221880	74712452650	38378780001020
C_{90} (2)	321598	134600940	74204344702	38078830029900
C_{90} (3)	322446	134732256	74350297830	38172208188880

definition below holds for such a modified distance spectrum:

$$\zeta(2x) = d_0 + \sum_{i=2}^{n} \lambda_i^{-x}$$

where it is assumed that the distance spectrum takes the form

$$0 = \lambda_1(d_0) < \lambda_2 \le \lambda_3 \le \dots \lambda_{n-1} \le \lambda_n$$

and d_0 is the degeneracy of the zero eigenvalue in the transformed distance spectrum.

The Riemann zeta functions for the distance spectra of fullerenes are likely to be important structural invariants. We shall now explore particular values of the Riemann zeta functions for the distance spectra of fullerenes. It can be seen that the Riemann zeta functions for all fullerenes with $x = 0$, -1, -2, -3, ..., -5 are given by

$$\zeta(0) = 1$$

$$\zeta(-2) = d_0 + \sum_{\lambda_i \neq 0} \lambda_i = d_0$$

$$\zeta(-4) = d_0 + \sum_{\lambda_i \neq 0} \lambda_i^2$$

$$\zeta(-6) = d_0 + \sum_{\lambda_i \neq 0} \lambda_i^3$$

$$\zeta(-8) = d_0 + \sum_{\lambda_i \neq 0} \lambda_i^4$$

$$\zeta(-10) = d_0 + \sum_{\lambda_i \neq 0} \lambda_i^5$$

It thus seems that the sums of the positive powers of the distance spectra could be useful structural invariants. Table 5 shows our computed results up to the sum of fifth powers of the distance spectra of all fullerenes. As seen from Table 5, the sums of powers of all distance eigenvalues are integers. All of these characterize fullerenes uniquely. For example, the sums of the squares of the distance spectra are all different for five isomers of C_{78}, as well as isomers of C_{84}, and C_{90}. It thus seems that the sums of the powers of the distance spectra could be useful structural invariants.

In conclusion, it should be stated that the distance spectra and the distance polynomials depend on the structures of fullerenes. Since they depend on the distance level patterns of fullerenes, the coefficients of the distance polynomial are considerably more complex than the coefficients of the ordinary characteristic polynomials. Evidently, the coefficients contain structural information and thus simple analytical expressions may not exist for the coefficients of the distance polynomials. This is easily illustrated in Table 4 for the structural isomers of fullerenes. For example, with the exception of the leading coefficient of unity, all coefficients in the distance polynomials of the isomers of C_{40} are quite different. The same comment applies to the isomers of C_{44}, C_{78}, C_{84}, and C_{90}. Consequently, the coefficient of λ^{n-2} in the distance polynomial can be used as a structural invariant, where n is the number of vertices.

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