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Matching Polynomial-Based Similarity Matrices and Descriptors for Isomers of Fullerenes

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Abstract: I have computed the matching polynomials of a number of isomers of fullerenes of various sizes with the objective of developing molecular descriptors and similarity measures for isomers of fullerenes on the basis of their matching polynomials. Two novel matching polynomial-based topological descriptors are developed, and they are demonstrated to have the discriminating power to contrast a number of closely related isomers of fullerenes. The number of ways to place up to seven disjoint dimers on fullerene isomers are shown to be identical, as they are not structure-dependent. Moreover, similarity matrices that provide quantitative similarity measures among a given set of isomers of fullerenes are developed from their matching polynomials and are shown to provide robust quantitative measures of similarity.

Keywords: fullerene isomers; matching polynomials; similarity matrices; topological descriptors; quantitative matching similarity measures

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1. Introduction

Fullerene cages, their isomers, stabilities, structures, aromaticities, electronic and magnetic properties, and spectra have been the subject of intense scrutiny over the years [1–7] ever since the pioneering work of Smalley and coworkers [1] that resulted in the discovery of another state of carbon with a dome-shaped icosahedral structure of C_{60}, named buckminsterfullerene. Subsequent discovery of carbon nanotubes [8] further fueled a plethora of research papers related to fullerenes and carbon nanomaterials. Fullerenes are cage-like closed structures that contain 12 pentagons and a varied number of hexagons. Numerous isomers are possible for a fullerene with a given molecular formula; for example, there are 1812 isomers for C_{60} while there are 8149 isomers for the C_{70} fullerene.

Fullerenes and related polycyclic aromatic compounds of various kinds have attracted several theoretical and mathematical studies due to the subject matter of aromaticity, local aromaticity, global aromaticity, ring currents, electronic and magnetic properties, and so forth [9–23]. Due to a large number of isomers for larger fullerenes, it is quite challenging to carry out ab initio computations on each one of them to gain insights into their structures, properties, similarities, and stabilities. Consequently, mathematical techniques primarily derived from combinatorics and graph theory such as the conjugated circuits, enumeration of Kekulé structures, sextet polynomials, matching polynomials, etc., of fullerenes and related polycyclic aromatic compounds have been studied over the decades [9–23]. Furthermore, giant fullerenes pose even more computational challenges for ab initio quantum chemical studies. The existence of multiple low-lying isomers and minima in their potential energy surfaces has caused further complexity in such high-level quantum chemical studies which can be computationally quite intensive. Quantum chemical studies have been made on some of the fullerenes including their vibrational spectra [24–27]. Although fullerenes that exhibit isolated pentagon structures have been generally attributed to be more stable, recent studies have revealed the existence of stable non-isolated pentagon structures, for example, the $C_{72}(C_{2v})$-11188 isomer [28]. Consequently, there is a clear and compelling need for the topological or graph theoretical characterization of fullerene cages, as such studies cumulatively can provide viable alternatives for gaining insights into their structures, properties, stabilities, and spectra. Although there is no direct correlation between the number of Kekulé structures and the stabilities of fullerene isomers, there appears to be a very good correlation between the overall topological resonance energies, conjugated circuits, and sextet polynomials with stabilities. Another application of graph theory is the enumeration of isomerization or rearrangement pathways that convert one isomer to the other as demonstrated in Stone–Wales rearrangement graphs [27] and the internal rotation isomerization graphs of isomers of alkanes [29] as well as water clusters and other fluxional molecules.

Topological characterization of fullerenes through the development of topological indices of various kinds has been the topic of several studies [30–37]. A number of structural invariants such as the Wiener indices, Mostar indices, and several other vertex-degree and distance-based indices have been developed to characterize the isomers of fullerenes so that they can be employed in QSPR/QSAR relations. Several graph theoretical polynomials and their spectra such as characteristic polynomials, graph spectra, matching polynomials, distance polynomials, enumeration of walks, spanning trees, Laplacians, graph automorphisms, and combinatorial enumerations of isomers of polysubstituted fullerenes, etc., have been considered over the years [38–52]. Among these matching polynomials of fullerenes, lattices and various other graphs and related graph polynomials have been the subject matter of several studies [40,44–64]. Various graph polynomials, Laplacians, and the enumeration of spanning trees have been considered for the isomers of fullerenes [65–67] and holey nanographenes [68]. Furthermore, such graph theoretical techniques including the enumeration of matchings have been stimulated by applications to phase-transition phenomena and statistical mechanics [69–73].

The present study is stimulated by several applications of combinatorial and graph theoretical techniques for the characterization of fullerene cages. In the present study, I propose topological invariants based on matching polynomials inspired by the pioneering studies of Hosoya and coworkers [55–61]. In the current study, while analyzing the coefficients of matching polynomials of fullerene isomers that contain only pentagons and hexagons, it was discovered that the first several coefficients were identical for the isomers and, hence, a reduced Z-index was developed to compare the isomers. A new similarity matrix was developed to provide quantitative similarity measures among a given set of isomers of fullerenes.

2. Preliminaries and Computational Methods

The adjacency matrix of a graph is defined as:

$$A_{ij} = \begin{cases} 1\ if\ vertices\ i\ and\ j\ are\ connected \\ 0\ otherwise \end{cases} \tag{1}$$

The characteristic polynomial of the graph, P_G, is given by the secular determinant of the adjacency matrix A:

$$P_G(x) = |A - xI| = C_n x^n + C_{n-1} x^{n-1} + \ldots + C_1 x + C_0 \tag{2}$$

where the coefficient C_k in the characteristic polynomial of a graph yields several combinatorial quantities pertinent to the structure as per Sach's theorem:

$$C_k = \sum_{g \in G_i} (-1)^{c(g)} 2^{r(g)} \tag{3}$$

where G_is are Sach's subgraphs of G containing k vertices, c(g) is the disjoint components in g, and r(g) is the number of cycles in the subgraph. For example, for a fullerene, the coefficient of x^{10} term would be comprised of 5 disjoint dimers, 1 6-membered ring and 2 disjoint dimers not contained in the ring, 2 isolated pentagons, a 10-membered ring arising from 2 fused hexagons, and so forth. The matching polynomial, which is also referred to as the acyclic polynomial of a graph G, is defined as

$$M_G(x) = \sum_{k=0}^{[\frac{n}{2}]} (-1)^k p(G,k) x^{n-2k} \tag{4}$$

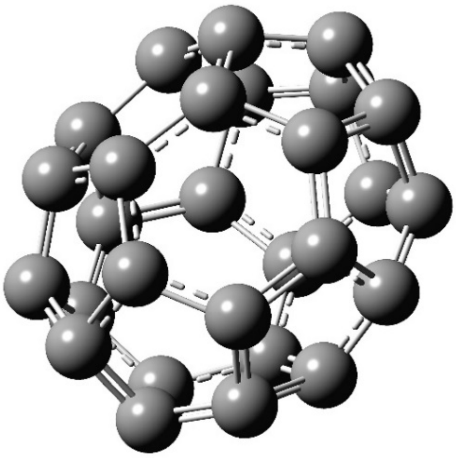
where p(G, k) enumerates the number of ways to place k disjoint dimers on the graph, and n is the number of vertices while [n/2] is the greatest integer contained in n/2. For fullerenes, as n is even, it can be readily seen that the upper limit is n/2 for any fullerene C_n. The characteristic and matching polynomials of trees are completely equivalent. Likewise, the matching polynomials of monocyclic rings as well as rings with pending bonds are all readily obtained. The constant coefficient or $C_{n/2}$ of the matching polynomials enumerates the number of perfect matchings. Consequently, the constant coefficient in the matching polynomial enumerates the number of Kekulé structures for a fullerene. We note that the number of Kekulé structures alone does not provide a direct measure of the relative stability of a fullerene, although it could be used as a preliminary indicator for further perusal.

While it is well known that the computation of the matching polynomial of a highly clustered graph is both CPU and disk intensive, several techniques have been developed specific to computing the matching polynomials and perfect matchings of fullerenes over the years [74,75]. One of the important outcomes is that the labeling of the graph or alternatively the order in which the edges of the graph are to be deleted in recursive reduction is critical to the intensity of the required computations. Although the matching polynomials are invariant to the labeling of the vertices, the order in which the edges are to be chosen for recursive pruning influences the evolution and dynamics of the recursive process and, hence, the overall computational time. In another investigation, Salvador et al. [50] made use of computer linguistic tools comprising theses, lines, and grammar to compute the matching polynomials of fullerenes, although their coefficients are limited to double precision or less than 15 digits. In the present study, I employ a combination of optimal vertex labeling and recursive reduction in conjunction with quadruple precision arithmetic. Furthermore, the characteristic polynomials of all line graphs up to the needed orders, monocyclic graphs, and other recurring fragments are computed upfront and stored in a data file so that they need not be repeatedly computed to generate the polynomials. The characteristic polynomials are computed using the author's previously developed codes enhanced further for efficiency and quadruple precision arithmetic. Hence, all the polynomial coefficients are accurate to 33–35 digits.

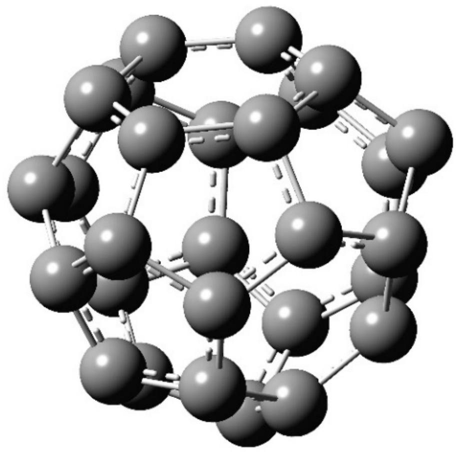
3. Results and Discussion

3.1. Matching Polynomials of Fullerenes

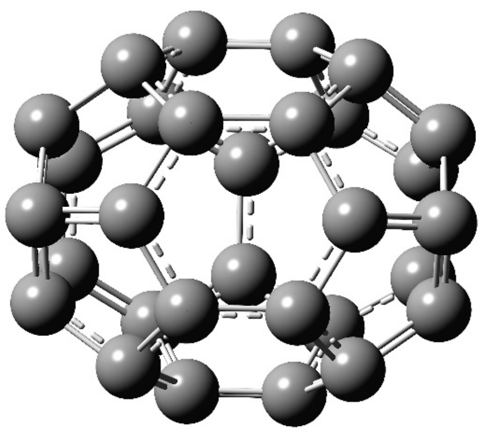
I have chosen a variety of isomers of fullerenes of varied sizes. In order to consider a contrasting case, I also included a relatively stable fullerene isomer of C_{58} with C_s symmetry that contains 1 heptagon and 13 pentagons. This isomer, denoted as $C_{58}(C_s)$-hept, is although strictly not a fullerene, several workers [74,75] have considered this as an energetically viable low-lying isomer compared to the $C_{58}(C_{3v})$-1 fullerene. Consequently, I have included this isomer also for the derivation of our matching polynomial-based similarity matrices. The fullerene isomers that are included in the present study are shown in Figure 1. I designate each fullerene by the number of carbon atoms, its symmetry, and a standard label as per fullerene library designations. Although there are several more isomers for each fullerene compared to the ones shown in Figure 1, I chose the isomers on the basis of their stabilities, differing symmetries, or shapes so that the similarity analysis would be meaningful and provide contrasting comparisons in order to assess the efficacy of the matching-based similarity analysis of these isomers of fullerenes. I have computed the matching polynomials of all of the fullerenes shown in Figure 1. As mentioned in the previous section, I employed a combination of recursive techniques and a binary database of previously computed and stored polynomials of the common fragments generated during the pruning process.



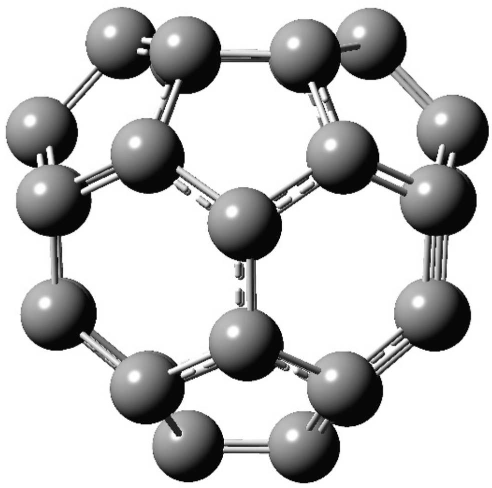
C_{28}-D_2



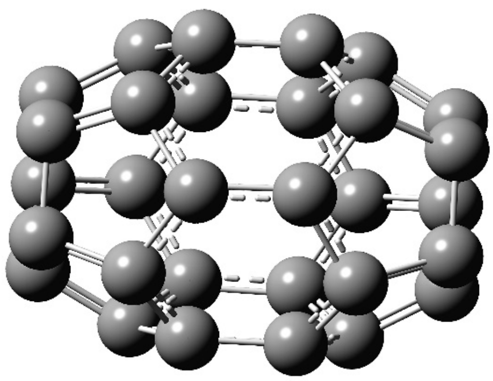
C_{28}-T_d



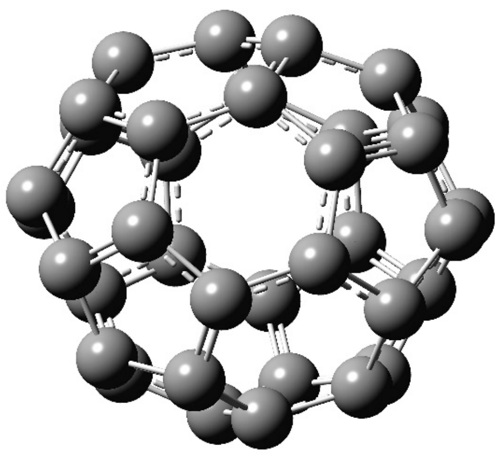
C_{30}-C_{2v}-2



C_{30}-C_{2v}-3

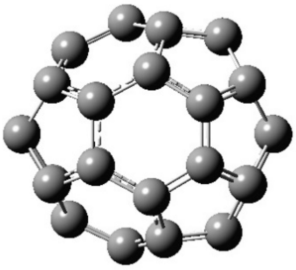


C_{30}-D_{5h}-1

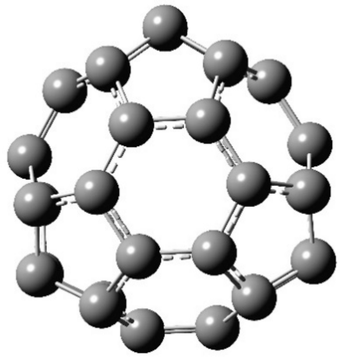


C_{36}-C_2-12

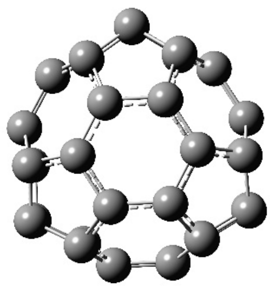
Figure 1. *Cont.*



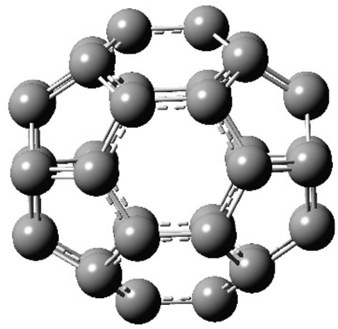
C_{36}-C_{2v}-9



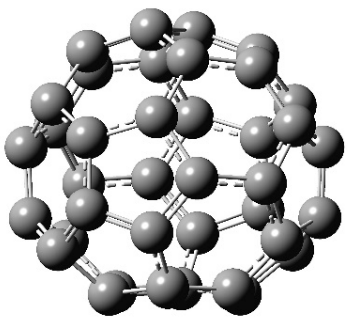
C_{36}-D_{2d}-14



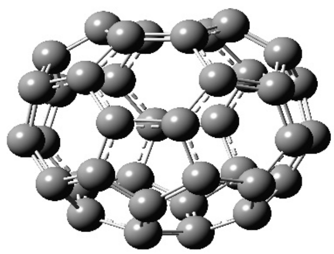
C_{36}-D_{3h}-13



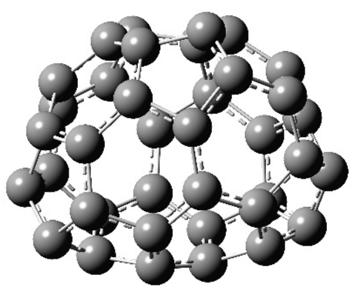
C_{36}-D_{5h}-15



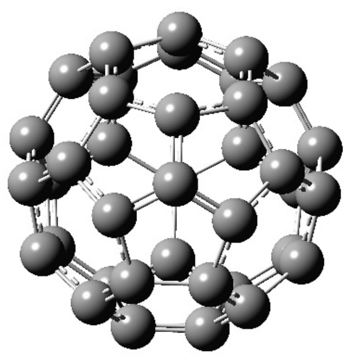
C_{38}-C_{2}-13



C_{38}-C_{2}-17

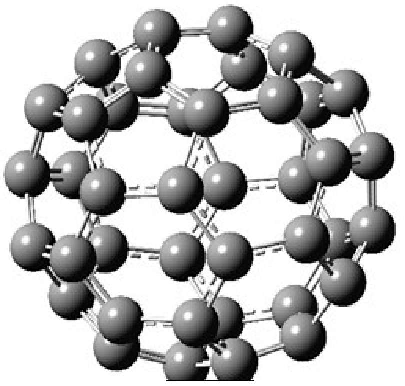


C_{38}-C_{2}-6

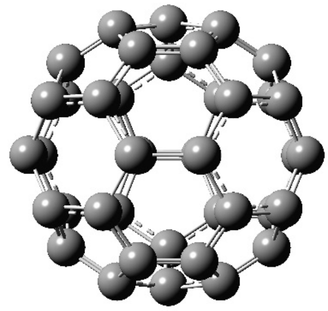


C_{38}-C_{3v}-16

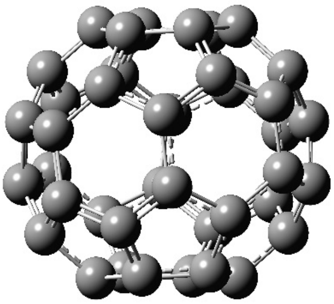
Figure 1. *Cont*.



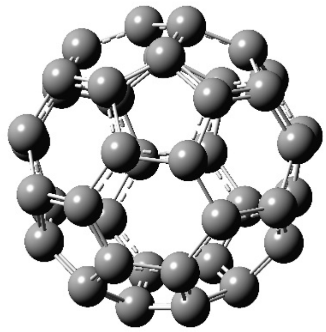
C_{40}-C_2-35



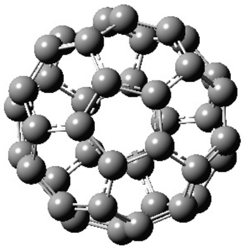
C_{40}-C_2-36



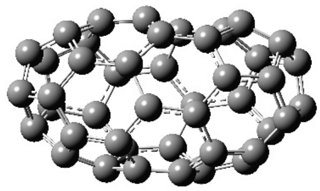
C_{40}-C_{2v}-37



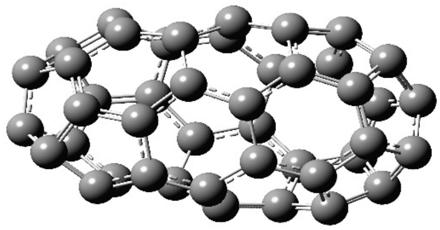
C_{40}-D_2-38



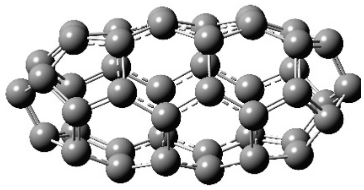
C_{40}-D_{5d}-39



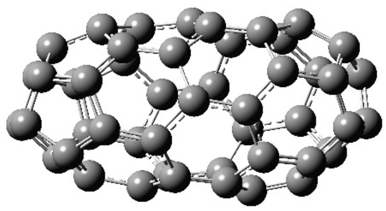
C_{44}-C_2-1



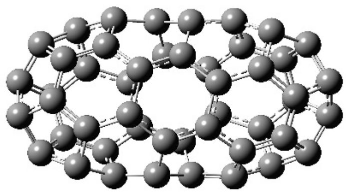
C_{44}-D_2-2



C_{44}-D_{3d}-3

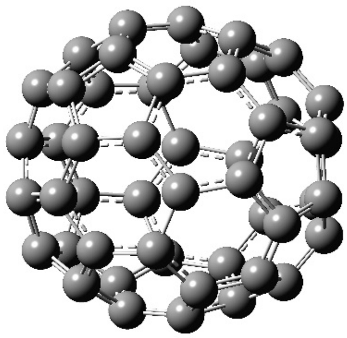


C_{48}-C_2-1

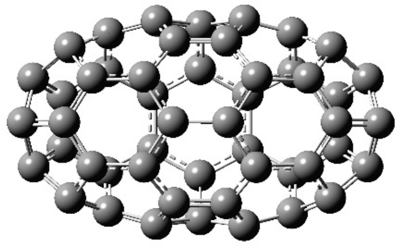


C_{48}-C_2-2

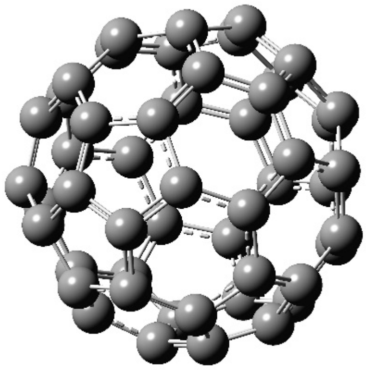
Figure 1. *Cont.*



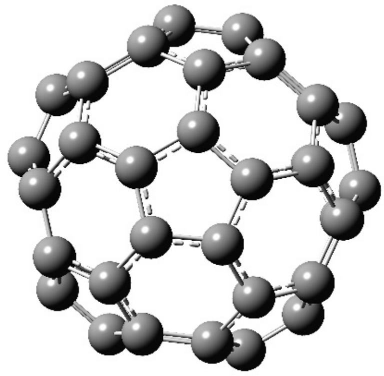
C_{50}-C_2-269



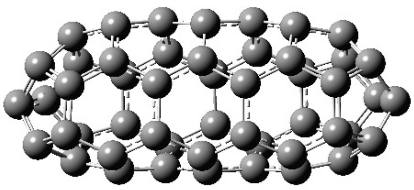
C_{50}-C_{2v}-13



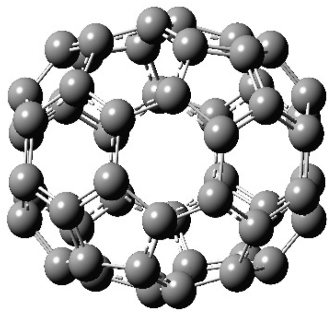
C_{50}-D_3-270



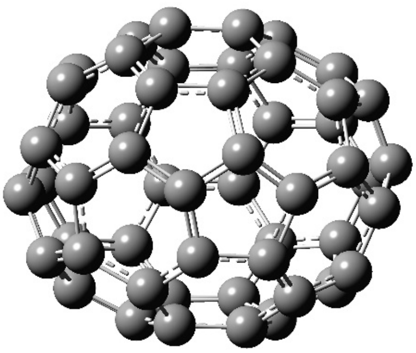
C_{50}-D_{5h}-271



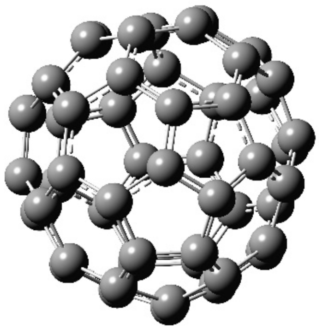
C_{50}-D_{3h}-3



C_{52}-D_2-433

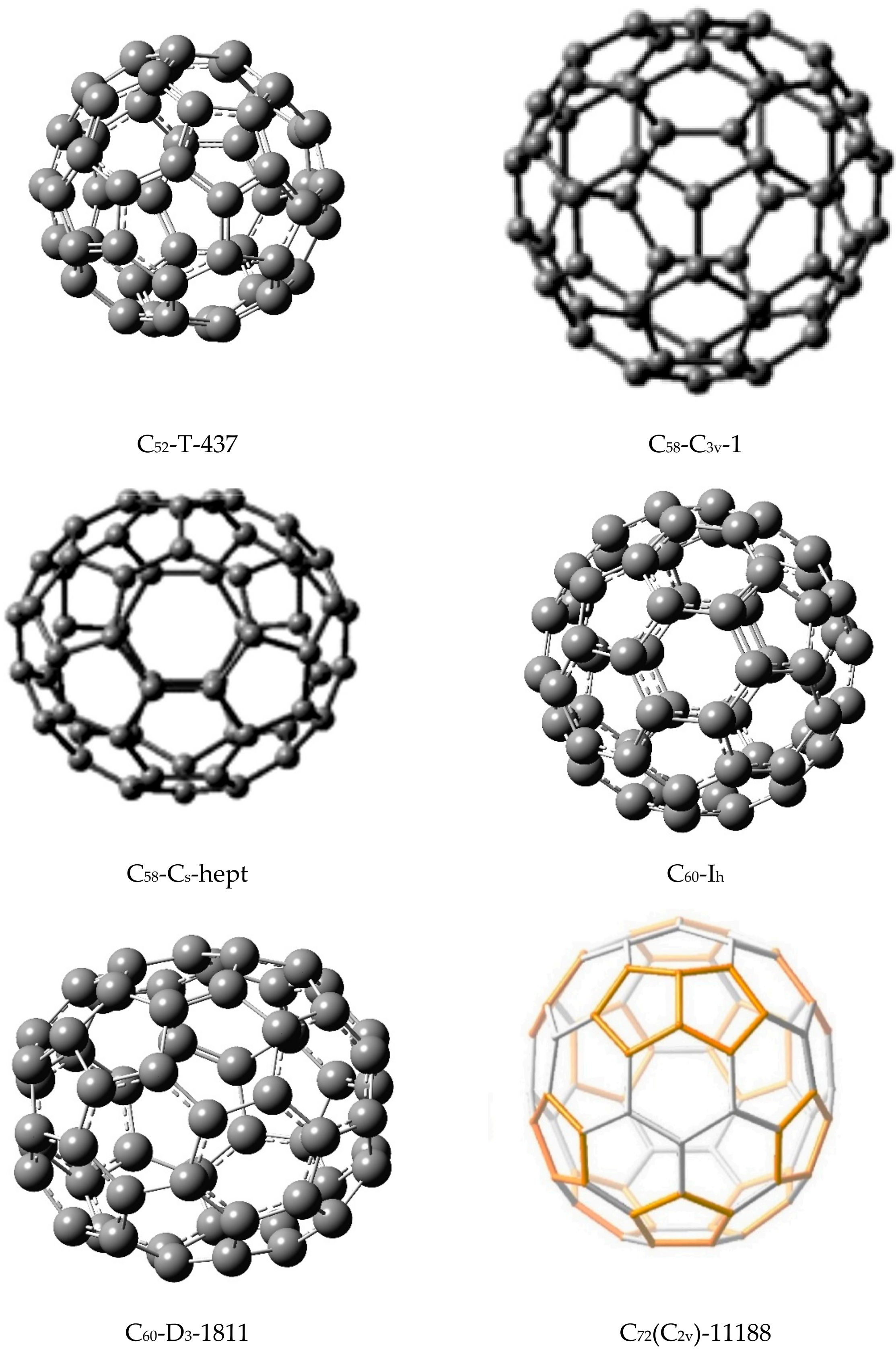


C_{52}-C_2-434



C_{52}-C_1-436

Figure 1. *Cont.*



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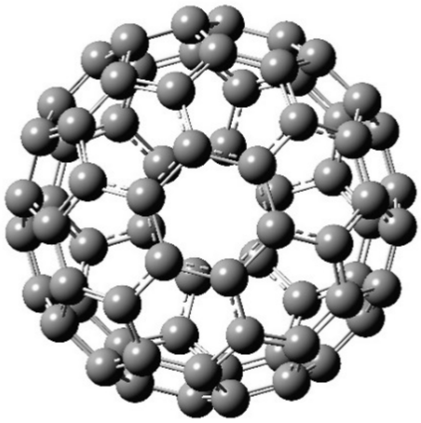

$C_{72}(D_{6d})$-11190

Figure 1. Structures of fullerene isomers C_{28}-C_{72} considered in this study for similarity matrices.

Tables 1–12 show the matching polynomials of the various isomers of fullerenes organized according to their formula. In each table, the various columns provide the matching polynomials of the isomers of a given constitution. The tables are constructed in the same order as the structures appear in Figure 1. All the results shown in Tables 1–12 were computed with quadruple precision accuracy and, hence, every digit in these tables is valid. Consider Table 1, which shows the matching polynomials of two isomers of C_{28}, namely $C_{28}(D_2)$ and $C_{28}(T_d)$. They have different symmetries but their shapes are somewhat similar (see, Figure 1). The T_d structure has less strain compared to the D_2 structure. As a result of the close similarity between the T_d and D_2 isomers of $C_{28,}$ their matching polynomials are also quite similar, as can be seen in Table 1. The identical nature of the first eight coefficients of the matching polynomials of the isomers of fullerenes has nothing to do with the symmetry of the structure of C_{28}. This arises from the fact that the first 8 coefficients of all fullerenes, that is, for the cage structures with 12 pentagons and any number of hexagons, do not depend on the structures but only on the number of carbon atoms. I shall discuss this in depth subsequently. However, it is noted that other coefficients for the $C_{28}(D_2)$ versus $C_{28}(T_d)$ structures also differ very little, consistent with the similarity of the shapes and other structural features, as seen from Figure 1.

Table 1. Matching polynomials of two isomers of C_{28} fullerene.

k	$C_{28}(D_2)$	$C_{28}(T_d)$
0	1	1
1	−42	−42
2	777	777
3	−8344	−8344
4	57,708	57,708
5	−269,628	−269,628
6	868,440	868,440
7	−1,932,444	−1,932,444
8	2,932,010	2,932,008
9	−2,944,736	−2,944,708
10	1,859,796	1,859,652
11	−678,656	−678,312
12	123,782	123,387
13	−8492	−8274
14	90	75

Table 2. Matching polynomials of isomers of C_{30} fullerene.

k	$C_{30}(D_{5h})$-1	$C_{30}(C_{2v})$-2	$C_{30}(C_{2v})$-3
0	1	1	1
1	−45	−45	−45
2	900	900	900
3	−10,560	−10,560	−10,560
4	80,820	80,820	80,820
5	−424,392	−424,392	−424,392
6	1,566,065	1,566,065	1,566,065
7	−4,091,265	−4,091,265	−4,091,265
8	7,524,770	7,524,768	7,524,767
9	−9,568,000	−9,567,966	−9,567,949
10	8,137,551	8,137,327	8,137,216
11	−4,388,255	−4,387,529	−4,387,172
12	1,377,420	1,376,198	1,375,602
13	−217,960	−216,930	−216,418
14	13,265	12,867	12,661
15	−151	−117	−107

Table 3. Matching polynomials of isomers of C_{36} fullerene.

k	$C_{36}(C_2)$-12	$C_{36}(C_{2v})$-9	$C_{36}(D_{2d})$-14	$C_{36}(D_{3h})$-13	$C_{36}(D_{6h})$-15
0	1	1	1	1	1
1	−54	−54	−54	−54	−54
2	1323	1323	1323	1323	1323
3	−19,476	−19,476	−19,476	−19,476	−19,476
4	192,321	192,321	192,321	192,321	192,321
5	−1,346,910	−1,346,910	−1,346,910	−1,346,910	−1,346,910
6	6,898,019	6,898,019	6,898,019	6,898,019	6,898,019
7	−26,255,052	−26,255,052	−26,255,052	−26,255,052	−26,255,052
8	74,743,468	74,743,468	74,743,467	74,743,470	74,743,467
9	−158,920,900	−158,920,900	−158,920,874	−158,920,952	−158,920,874
10	250,185,492	250,185,493	250,185,213	250,186,053	250,185,213
11	−286,863,270	−286,863,284	−286,861,644	−286,866,564	−286,861,644
12	233,454,871	233,454,925	233,449,143	233,466,479	233,449,135
13	−129,759,156	−129,759,130	−129,746,290	−129,784,686	−129,746,178
14	46,513,097	46,512,605	46,494,509	46,548,279	46,494,021
15	−9,838,170	−9,837,524	−9,822,212	−9,867,396	−9,821,428
16	1,057,103	1,057,253	1,050,796	1,070,007	1,050,468
17	−43,008	−43,278	−42,320	−45,186	−42,288
18	289	312	288	364	272

Table 4. Matching polynomials of isomers of C_{38} fullerene.

k	$C_{38}(C_2)$-13	$C_{38}(C_2)$-17	$C_{38}(C_2)$-6	$C_{38}(C_{3v})$-16
0	1	1	1	1
1	−57	−57	−57	−57
2	1482	1482	1482	1482
3	−23,294	−23,294	−23,294	−23,294
4	247,323	247,323	247,323	247,323
5	−1,877,511	−1,877,511	−1,877,511	−1,877,511
6	10,521,461	10,521,461	10,521,461	10,521,461
7	−44,311,485	−44,311,485	−44,311,485	−44,311,485
8	141,457,329	141,457,328	141,457,331	141,457,329
9	−342,789,923	−342,789,894	−342,789,983	−342,789,924
10	627,517,764	627,517,410	627,518,522	627,517,788
11	−858,202,534	−858,200,138	−858,207,810	−858,202,755
12	860,996,587	860,986,593	861,018,781	860,997,544
13	−616,691,139	−616,664,107	−616,749,327	−616,692,840
14	303,148,423	303,100,171	303,243,068	303,147,594
15	−96,506,463	−96,451,021	−96,598,748	−96,498,792
16	18,197,166	18,159,923	18,247,447	18,186,867
17	−1,750,486	−1,738,799	−1,763,805	−1,745,700
18	64,190	63,204	65,385	63,675
19	−386	−382	−385	−378

Table 5. Matching polynomials of isomers of C_{40} fullerene.

k	$C_{40}(C_2)$-35	$C_{40}(C_2)$-36	$C_{40}(C_{2v})$-37	$C_{40}(D_2)$-38	$C_{40}(D_{5d})$-39
0	1	1	1	1	1
1	−60	−60	−60	−60	−60
2	1650	1650	1650	1650	1650
3	−27,580	−27,580	−27,580	−27,580	−27,580
4	313,335	313,335	313,335	313,335	313,335
5	−2,563,260	−2,563,260	−2,563,260	−2,563,260	−2,563,260
6	15,606,390	15,606,390	15,606,390	15,606,390	15,606,390
7	−72,094,680	−72,094,680	−72,094,680	−72,094,680	−72,094,680
8	255,308,426	255,308,426	255,308,426	255,308,425	255,308,425
9	−695,619,674	−695,619,674	−695,619,674	−695,619,640	−695,619,640
10	1,455,391,494	1,455,391,494	1,455,391,494	1,455,391,002	1,455,391,002
11	−2,321,341,062	−2,321,341,062	−2,321,341,066	−2,321,337,096	−2,321,337,100
12	2,786,393,230	2,786,393,242	2,786,393,329	2,786,373,686	2,786,373,750
13	−2,468,240,914	−2,468,241,118	−2,468,241,896	−2,468,180,232	−2,468,180,640
14	1,568,689,230	1,568,690,574	1,568,694,249	1,568,571,626	1,568,572,975
15	−687,082,056	−687,086,328	−687,096,074	−686,946,860	−686,949,378
16	195,552,995	195,559,583	195,573,824	195,471,357	195,473,975
17	−33,038,938	−33,043,186	−33,053,906	−33,020,784	−33,022,120
18	2,846,500	2,847,204	2,851,269	2,848,766	2,849,295
19	−93,008	−92,940	−93,740	−94,080	−94,470
20	493	473	513	518	562

Table 6. Matching polynomials of isomers of C_{44} fullerene.

k	$C_{44}(C_2)$-1	$C_{44}(D_2)$-2	$C_{44}(D_{3d})$-3
0	1	1	1
1	−66	−66	−66
2	2013	2013	2013
3	−37,664	−37,664	−37,664
4	483,978	483,978	483,978
5	−4,531,152	−4,531,152	−4,531,152
6	32,000,462	32,000,462	32,000,462
7	−174,145,908	−174,145,908	−174,145,908
8	739,662,349	739,662,351	739,662,351
9	−2,468,621,824	−2,468,621,902	−2,468,621,902
10	6,487,128,811	6,487,130,145	6,487,130,145
11	−13,393,750,298	−13,393,763,496	−13,393,763,496
12	21,594,289,606	21,594,373,489	21,594,373,484
13	−26,906,332,278	−26,906,691,854	−26,906,691,732
14	25,516,302,649	25,517,364,447	25,517,363,112
15	−18,028,774,350	−18,030,941,516	−18,030,933,108
16	9,216,119,461	9,219,142,472	9,219,110,019
17	−3,272,339,730	−3,275,146,364	−3,275,069,730
18	761,369,684	763,026,684	762,920,396
19	−106,313,844	−106,892,800	−106,813,188
20	7,699,388	7,807,279	7,780,449
21	−215,950	−225,134	−222,470
22	892	1091	1170

Table 7. Matching Polynomials of Isomers of C_{48} Fullerene.

k	$C_{48}(C_2)$-1	$C_{48}(D_2)$-2
0	1	1
1	−72	−72
2	2412	2412
3	−49,944	−49,944
4	716,238	716,238
5	−7,554,444	−7,554,444
6	60,745,322	60,745,322
7	−380,928,456	−380,928,456
8	1,890,083,485	1,890,083,487
9	−7,486,060,102	−7,486,060,192
10	23,775,570,460	23,775,572,268
11	−60,611,207,684	−60,611,229,132
12	123,760,350,554	123,760,518,011
13	−201,341,648,072	−201,342,555,836
14	258,764,778,060	258,768,290,312
15	−259,526,848,576	−259,536,667,008
16	199,760,333,462	199,780,185,175
17	−115,384,812,402	−115,413,591,260
18	48,529,535,471	48,558,888,146
19	−14,261,258,162	−14,281,668,112
20	2,761,839,268	2,771,056,042
21	−322,801,582	−325,317,240
22	19,673,191	20,047,888
23	−465,508	−491,272
24	1,532	2,024

Table 8. Matching polynomials of isomers of C_{50} fullerene.

k	$C_{50}(C_2)$-269	$C_{50}(C_{2v})$-13	$C_{50}(D_3)$-270	$C_{50}(D_{5h})$-271	$C_{50}(D_{3h})$-3
0	1	1	1	1	1
1	−75	−75	−75	−75	−75
2	2625	2625	2625	2625	2625
3	−56,975	−56,975	−56,975	−56,975	−56,975
4	859,575	859,575	859,575	859,575	859,575
5	−9,576,453	−9,576,453	−9,576,453	−9,576,453	−9,576,453
6	81,704,030	81,704,030	81,704,030	81,704,030	81,704,030
7	−546,377,070	−546,377,070	−546,377,070	−546,377,070	−546,377,070
8	2,907,494,483	2,907,494,489	2,907,494,481	2,907,494,480	2,907,494,493
9	−12,430,405,477	−12,430,405,765	−12,430,405,379	−12,430,405,330	−12,430,405,959
10	42,930,480,510	42,930,486,724	42,930,478,356	42,930,477,279	42,930,490,950
11	−120,030,365,482	−120,030,445,280	−120,030,337,392	−120,030,323,355	−120,030,500,010
12	271,475,360,667	271,476,041,210	271,475,118,473	271,474,997,635	271,476,511,246
13	−494,947,493,439	−494,951,565,536	−494,946,037,473	−494,945,313,135	−494,954,392,290
14	722,829,954,436	722,847,560,835	722,823,685,011	722,820,579,630	722,859,812,505
15	−837,705,092,102	−837,760,905,963	−837,685,538,979	−837,675,911,840	−837,799,701,683
16	760,514,520,422	760,644,785,556	760,470,388,059	760,448,826,260	760,734,797,436
17	−531,573,181,792	−531,795,993,434	−531,501,952,881	−531,467,488,160	−531,948,041,766
18	279,547,624,962	279,823,262,630	279,467,433,844	279,429,116,630	280,007,334,171
19	−107,244,065,832	−107,485,053,846	−107,183,756,466	−107,155,471,120	−107,640,515,031
20	28,768,905,085	28,912,538,934	28,740,833,451	28,728,154,280	29,000,371,557
21	−5,080,606,155	−5,135,852,304	−5,073,704,083	−5,070,966,660	−5,166,984,589
22	539,267,259	551,856,582	538,762,086	538,792,490	558,135,165
23	−29,582,483	−31,053,612	−29,652,450	−29,762,020	−31,680,375
24	623,747	690,021	630,684	642,645	717,746
25	−2099	−2719	−2136	−2343	−3276

Table 9. Matching polynomials of isomers of C_{52} fullerene.

K	$C_{52}(D_2)$-433	$C_{52}(C_2)$-434	$C_{52}(C_1)$-436	$C_{52}(T)$-437
0	1	1	1	1
1	−78	−78	−78	−78
2	2847	2847	2847	2847
3	−64,636	−64,636	−64,636	−64,636
4	1,023,399	1,023,399	1,023,399	1,023,399
5	−12,009,570	−12,009,570	−12,009,570	−12,009,570
6	108,366,033	108,366,033	108,366,033	108,366,033
7	−769,906,260	−769,906,260	−769,906,260	−769,906,260
8	4,374,890,420	4,374,890,419	4,374,890,418	4,374,890,418
9	−20,087,482,056	−20,087,482,004	−20,087,481,952	−20,087,481,952
10	74,993,403,696	74,993,402,475	74,993,401,254	74,993,401,254

Table 9. *Cont.*

K	$C_{52}(D_2)$-433	$C_{52}(C_2)$-434	$C_{52}(C_1)$-436	$C_{52}(T)$-437
11	−228,347,209,688	−228,347,192,556	−228,347,175,414	−228,347,175,408
12	567,290,814,788	567,290,654,621	567,290,494,046	567,290,493,824
13	−1,147,459,180,912	−1,147,458,127,888	−1,147,457,067,510	−1,147,457,063,880
14	1,881,094,347,028	1,881,089,339,988	1,881,084,255,692	1,881,084,221,076
15	−2,481,558,198,016	−2,481,540,762,864	−2,481,522,802,116	−2,481,522,588,124
16	2,608,075,274,168	2,608,030,772,458	2,607,983,836,736	2,607,982,934,853
17	−2,154,508,107,056	−2,154,425,661,680	−2,154,335,363,811	−2,154,332,709,330
18	1,374,351,797,384	1,374,243,411,072	1,374,117,256,664	1,374,111,754,991
19	−661,324,154,776	−661,227,247,200	−661,102,300,879	−661,094,291,988
20	232,679,709,256	232,625,587,423	232,541,130,115	232,533,025,512
21	−57,362,136,248	−57,347,243,516	−57,310,508,266	−57,304,888,024
22	9,326,080,656	9,326,685,034	9,317,305,137	9,314,670,876
23	−912,517,384	−913,967,662	−912,732,486	−911,913,672
24	46,175,688	46,459,731	46,372,434	46,216,468
25	−900,864	−913,906	−906,964	−893,568
26	2904	2941	2814	2700

Table 10. Matching polynomials of $C_{58}(C_{3v})$-1 and heptagonal $C_{58}(C_s)$-hept with 1 heptagon and 13 pentagons.

k	$C_{58}(C_{3v})$-1	$C_{58}(C_s)$-hept
0	1	1
1	−87	−87
2	3567	3567
3	−91,669	−91,669
4	1,656,828	1,656,828
5	−22,400,052	−22,400,051
6	235,240,023	235,239,954
7	−1,967,080,257	−1,967,078,043
8	13,320,537,624	13,320,493,739
9	−73,905,469,014	−73,904,866,941
10	338,630,578,458	338,624,507,555
11	−1,287,860,109,036	−1,287,813,476,284
12	4,076,572,360,408	4,076,293,247,395
13	−10,748,037,091,998	−10,746,716,517,904
14	23,577,708,216,708	23,572,726,102,672
15	−42,911,701,168,180	−42,896,647,640,354
16	64,495,465,418,163	64,459,007,350,761
17	−79,522,974,846,489	−79,452,370,129,844
18	79,733,207,226,754	79,624,483,458,808
19	−64,270,421,735,034	−64,138,493,127,215
20	41,044,816,761,150	40,920,303,468,711

Table 10. *Cont.*

k	$C_{58}(C_{3v})$-1	$C_{58}(C_s)$-hept
21	−20,382,041,191,170	−20,292,270,811,849
22	7,681,900,580,205	7,633,661,167,869
23	−2,128,631,549,481	−2,109,955,392,032
24	415,408,342,364	410,442,814,122
25	−53,747,261,070	−52,902,565,843
26	4,212,821,433	4,130,671,443
27	−172,462,371	−168,752,079
28	2,762,970	2,717,607
29	−7308	−7525

Table 11. Matching polynomials of buckminsterfullerene ($C_{60}(I_h)$) and its isomer $C_{60}(D_3)$-1811.

k	$C_{60}(I_h)$	$C_{60}(D_3)$-1811
0	1	1
1	−90	−90
2	3825	3825
3	−102,120	−102,120
4	1,922,040	1,922,040
5	−27,130,596	−27,130,596
6	298,317,860	298,317,860
7	−2,619,980,460	−2,619,980,460
8	18,697,786,680	18,697,786,686
9	−109,742,831,260	−109,742,831,644
10	534,162,544,380	534,162,555,702
11	−2,168,137,517,940	−2,168,137,722,048
12	7,362,904,561,730	7,362,907,079,705
13	−20,949,286,202,160	−20,949,308,744,700
14	49,924,889,888,850	49,925,041,449,174
15	−99,463,457,244,844	−99,464,238,463,876
16	165,074,851,632,300	165,077,976,023,361
17	−227,043,126,274,260	−227,052,877,002,918
18	256,967,614,454,320	256,991,374,424,828
19	−237,135,867,688,980	−237,180,889,766,676
20	176,345,540,119,296	176,411,295,787,590
21	−104,113,567,937,140	−104,186,538,219,098
22	47,883,826,976,580	47,944,056,256,236
23	−16,742,486,291,340	−16,778,325,531,438
24	4,310,718,227,685	4,325,385,183,252
25	−783,047,312,406	−786,868,226,034
26	94,541,532,165	95,084,107,821
27	−6,946,574,300	−6,969,881,806
28	269,272,620	266,597,229
29	−4,202,760	−3,954,300
30	12,500	9622

Table 12. Matching polynomials of two isomers of C_{72}: $C_{72}(C_{2v})$-11188 fullerene with non-isolated pentagon structure and $C_{72}(D_{6d})$-11190 [a].

k	$C_{72}(C_{2v})$-11188 (Non-ISP)	$C_{72}(D_{6d})$-11190
0	1	1
1	−108	−108
2	5562	5562
3	−181,836	−181,836
4	4,238,379	4,238,379
5	−74,997,996	−74,997,996
6	1,047,459,326	1,047,459,326
7	−11,852,752,392	−11,852,752,392
8	110,690,579,974	110,690,579,973
9	−864,652,893,966	−864,652,893,884
10	5,705,866,144,122	5,705,866,140,966
11	−32,043,716,552,498	−32,043,716,476,716
12	153,971,991,502,747	153,971,990,229,848
13	−635,430,828,140,544	−635,430,812,245,836
14	2,257,883,027,813,575	2,257,882,874,735,690
15	−6,917,120,612,820,084	−6,917,119,448,538,120
16	18,275,900,215,535,848	18,275,893,112,174,600
17	−41,618,256,862,032,538	−41,618,221,745,909,600
18	81,556,423,951,149,669	81,556,282,447,653,600
19	−137,186,547,343,055,238	−137,186,081,385,089,000
20	197,391,632,599,522,833	197,390,379,486,861,000
21	−241,844,737,361,104,930	−241,841,995,535,982,000
22	250,872,705,868,808,807	250,867,862,188,707,000
23	−218,784,208,970,190,972	−218,777,389,029,217,000
24	159,029,898,793,311,758	159,022,409,077,892,000
25	−95,339,702,590,544,974	−95,333,534,217,776,900
26	46,538,823,097,489,228	46,535,333,778,130,000
27	−18,206,425,404,161,442	−18,205,449,520,239,600
28	5,596,680,643,711,950	5,596,999,388,641,250
29	−1,318,481,294,247,250	−1,318,986,435,090,070
30	230,452,534,808,904	230,726,853,211,188
31	−28,618,179,154,208	−28,704,598,608,024
32	2,376,922,675,783	2,393,469,043,524
33	−120,715,631,942	−122,558,197,024
34	3,237,686,991	3,345,162,432
35	−34,480,394	−37,159,200
36	63,487	77,400

[a] Results shown for $C_{72}(D_{6d})$ in the third column are from [50].

Tables 2–10 display the computed matching polynomials of a number of isomers of fullerenes, C_{30} through C_{58}. Among these, fullerenes C_{36}, $C_{40,}$ and C_{50} were considered for five isomers with contrasting symmetries and shapes in Tables 3 and 5, respectively (see Figure 1 for the corresponding structures of the isomers). Tables 11 and 12 display the matching polynomials of two isomers, C_{60} and C_{72}, where for each case, two isomers of contrasting shapes or symmetries were considered. In the case of C_{72}, the two isomers as well as C_{70} have been considered in quantum chemical studies [76,77]. A critical analysis of all matching polynomials displayed in the Tables reveals that for all fullerenes containing only pentagons and hexagons, the first eight coefficients are identical for the isomers in that these coefficients do not exhibit any structural dependence. That is, they vary as polynomials of n. As discussed earlier [52], the exact analytical expressions for the first few coefficients of fullerene cages can be derived through a combination of Sach's theorem and the coefficients of the corresponding terms in the characteristic polynomials. The resulting expressions are shown below:

$$\mathrm{p(C_n{:}Full,0) = 1} \tag{5}$$

$$\mathrm{p(C_n{:}Full,1)} = -3\mathrm{n}/2 \tag{6}$$

$$\mathrm{p(C_n{:}Full,2)} = 3\mathrm{n}(3\mathrm{n}-10)/8 \tag{7}$$

$$\mathrm{p(C_n : Full, 3)} = -\frac{1}{16}\left(9n^3 - 90n^2 + 232n\right) \tag{8}$$

$$\mathrm{p(C_n : Full, 4)} = c_8 - \frac{1}{4}(3n-24)(n-20) + 2n_5^{(2)} \tag{9}$$

$$\mathrm{p(C_n : Full, 5)} = c_{10} - n_5^{(2)}(3n-30) + 2n_6^{(2)} - 4n_5'^{(2)} \tag{10}$$

where c_n is the corresponding coefficient in the characteristic polynomial of the fullerene, $n_l^{(k)}$ is the number of ways of choosing k adjacent l-membered rings in the fullerene whereas $n_l'^{(k)}$ is the number of ways to choose k disjoint l-membered rings from the fullerene.

The coefficients of the first 8 terms in the matching polynomials of all cages containing 12 pentagons and varied number of hexagons are the same for the isomers, as can be inferred to be identical from Tables 1–12. The only exception to this is the $C_{58}(C_s)$-hept structure which is comprised of 13 pentagons and 1 heptagon and, thus, the ring structures are different compared to the $C_{58}(C_{3v})$-1 fullerene, which contains 12 pentagons and no heptagons. Even then, the first five coefficients of the matching polynomials of the two isomers of C_{58} are identical, with the sixth coefficient differing only by unity. Although the results for $C_{72}(D_{6d})$ in Table 12 were derived from [50] and hence they lack the accuracy of $C_{72}(C_{2v})$-11188 computed here, the similarity indices computed subsequently for C_{72} do not suffer from the accuracy issue, as the similarity measures are based on a natural logarithmic scale.

The constant coefficients of the matching polynomials yield the number of Kekulé structures of fullerene isomers, although there exists no direct correlation between the stability of the fullerene structure and the number of resonance structures. However, a number of related topological indices have been derived and used from the coefficients of the matching polynomials as well as their spectra. For example, the sum of the absolute values of the coefficients of the matching polynomials is the well-known Hosoya's topological index [78] while the sum of the difference in the eigenvalues of the characteristic and matching polynomials yields the topological resonance energy; the latter has been employed as a measure of the relative stabilities of isomers of fullerenes. The isomers that exhibit extremal values of Hosoya's topological Z-index [78] are also of interest. It can thus be inferred that if two isomers of fullerenes exhibit Z-indices close to each other, then they can be viewed as candidates for further investigations by a higher level of computations in order to assess further their relative stabilities. Although many such variants have been proposed, up to now, no similarity measures have been developed for comparing the isomers of fullerenes or other structures. As the first eight coefficients are identical, I have proposed the reduced Z-indices for fullerenes which consider only the differing coefficients of the matching polynomials in deriving the Z-indices. I have further introduced natural logarithms and scaling techniques for deriving the indices proposed in the next section for both the comparison and similarity analysis of fullerenes.

3.2. The Similarity Matrices of Fullerenes and Reduced Z-Indices

As can be seen from Tables 1–12, the matching polynomials of isomers of fullerenes exhibit similarities and, hence, I develop quantitative similarity measures in terms of the similarity matrices that would have the capability to offer a contrast among isomers as well as across the platform of fullerenes. These matrices are defined using the coefficients of the matching polynomials with a scaling incorporated into them. Hence, I define the similarity matrix based on matching polynomials as follows:

$$\mathrm{S_{ij}(M)} = \frac{1}{n_e}\ln(\textstyle\sum_{k=8}^{\frac{n}{2}} \left|\left|p\left(G^i,\lambda_k\right)\right| - \left|p\left(G^j,\lambda_k\right)\right|\right|, \; i \neq j \tag{11}$$

where $p\left(G^i,\lambda_k\right)$ is the k$^{\text{th}}$ coefficient of the matching polynomial of fullerene isomer G^i, while $p\left(G^j,\lambda_k\right)$ is the k$^{\text{th}}$ coefficient of the matching polynomial of fullerene isomer G^j. The absolute differences of the corresponding coefficients are taken and, thus, the difference is always positive so as to maintain this as a true difference without regard for the sign variations of the alternate terms of the matching polynomials. We obtain a matrix element S_{ij} for any two members (*i, j*) among a set of isomers considered for comparison. The diagonal elements of the similarity matrix are set to 0 as the similarity distance between two identical isomers is 0. Consequently, the larger the similarity matrix element, the greater is the dissimilarity between the isomers *i* and *j*, while a small value would then imply that the two isomers are very similar. I have computed the similarity matrices for all of the isomers of fullerenes considered in this study, and the computed similarity matrices are shown in Figure 2 for each fullerene considered here.

As the first eight coefficients of the matching polynomials of isomers of fullerenes are identical, I have introduced a scaled, natural logarithmic version of the reduced Z-index, Z^R, as follows:

$$\mathrm{S} - \ln(Z^R(M)) = \frac{1}{n_e}\ln(\textstyle\sum_{k=8}^{\frac{n}{2}}|p(G,\lambda_k)|) \tag{12}$$

A primary advantage of the reduced-scaled version is that it facilitates a comparison of isomers of fullerenes across the platform. Hence, I have shown in Figure 2 both S-ln(Z^R) as well as Z^R for comparing isomers, where Z^R is simply the sum of the absolute coefficients starting with the eighth coefficient of the matching polynomials.

As seen from Figure 2, the computed similarity measures are in a logarithmic scale and the matrix elements vary between 0.137 and 0.313 where the lowest value corresponding to the most similar structures are for the first two isomers of C_{36} (Figure 1) which are $C_{36}(C_2)$-12 and $C_{36}(C_{2v})$-9. As can be seen from both Figure 1 and Table 3, the two isomers are very similar in multiple ways. Their overall shapes and structural similarities are striking. At a quantitative level, an inspection of Table 3 reveals that the first 10 coefficients in the matching polynomial are identical while the 11th coefficient differs only by unity. Several other subsequent coefficients are also close to each other. This is in turn reflected by the similarity matrix element of 0.137484542 for the two isomers. Likewise, the isomers 5 and 3, which correspond to C_{36}-D_{5h}-15 and C_{36}-D_{2d}-14, exhibit remarkable similarity both in terms of their shape, structures, and matching polynomials. That is, the arrangements of pentagons and hexagons are such that they provide very similar combinatorial matchings. I note that other structures which exhibit such similarities are the two isomers of C_{28} in Figure 1; the two isomers have a similarity measure of 0.1677151 on the basis of their combinatorial matchings. Likewise, two isomers of C_{30} also exhibit comparable similarity measures (see Figure 2). The first isomers of C_{40} (Figure 1) have comparable similarity measures of 0.1627944 and this is corroborated by the corresponding matching polynomials shown in Table 5 where I find that the first 12 coefficients of the two isomers are identical, with the 13th coefficient differing by only 12.

Although most of the other isomers of fullerenes exhibit similarity indices close to 0.2, the two isomers of C_{58} are important cases to be noted for the dramatic similarity contrast. First, as noted before, their similarity index is the highest among all the isomers considered here with a striking value of 0.312761 given that this is a logarithmic scale. The contrasting similarity measure is fully consistent with the fact that the first isomer of C_{58} is a true fullerene containing 12 pentagons and hexagons while the second one designated as $C_{58}(C_s)$-hept contains 1 heptagon and 13 pentagons. This contrasting juxtaposition shown in Figure 1 as well as Table 10 is truly echoed in their similarity index measure introduced here. This is a direct validation of the similarity matrix measure that I have developed in that the measure faithfully reflects the variations and dissimilarities as well as similarities among the structures. Moreover, with the values shown in Figure 2, I now have a reference platform to evaluate the similarities among isomers through such quantitative similarity measures.

C_{28}

0.000000000000	0.16771506898
0.16771506898	0.000000000000

Z^{R1}: 8,547,562 S-ln(Z^{R1}): 0.3800275394
Z^{R2}: 8,546,416 S-ln(Z^{R2}): 0.3800243467

C_{30}

0.000000000	0.182398821	0.191308008
0.182398821	0.000000000	0.166690714
0.191308008	0.166690714	0.000000000

Z^{R1}: 31,227,372 S-ln(Z^{R1}): 0.3834845684
Z^{R2}: 31,223,702 S-ln(Z^{R2}): 0.3834819565
Z^{R3}: 31,221,892 S-ln(Z^{R3}): 0.3834806683

C_{36}

0.000000000	0.137484542	0.204370108	0.216672853	0.204890233
0.137484542	0.000000000	0.204174549	0.216772690	0.204700118
0.204370108	0.204174549	0.000000000	0.224360949	0.13847415
0.216672853	0.216772690	0.224360949	0.000000000	0.224539312
0.204890233	0.204700118	0.13847415	0.224539312	0.000000000

Z^{R1}: 1,191,378,824 S-ln(Z^{R1}): 0.387006984
Z^{R2}: 1,191,378,172 S-ln(Z^{R2}): 0.387006974
Z^{R3}: 1,191,316,756 S-ln(Z^{R3}): 0.387006019
Z^{R4}: 1,191,499,436 S-ln(Z^{R3}): 0.387008859
Z^{R5}: 1191314988 S-ln(Z^{R3}): 0.387005992

C_{38}

0.00000000 00	0.21355472 40	0.22335797 44	0.17901818 40
0.21355472 40	0.00000000 00	0.23129277 17	0.21151844 27
0.22335797 44	0.23129277 17	0.00000000 00	0.22442470 08
0.17901818 40	0.21151844 27	0.22442470 08	0.00000000 00

Z^{R1}: 3,867,322,390 S-ln(Z^{R1}): 0.3872952319
Z^{R2}: 3,867,128,970 S-ln(Z^{R2}): 0.3872943544
Z^{R3}: 3,867,660,592 S-ln(Z^{R3}): 0.3872967660
Z^{R4}: 3,867,301,186 S-ln(Z^{R4}): 0.3872951357

C_{40}

0.000000000 0	0.162794463 8	0.183763606 1	0.216601010 9	0.216321298 6
0.162794463 8	0.000000000 0	0.178258068 3	0.217197315 5	0.216927514 0
0.183763606 1	0.178258068 3	0.000000000 0	0.218574807 5	0.218290450 6
0.216601010 9	0.217197315 5	0.218574807 5	0.000000000 0	0.152224322 1
0.216321298 6	0.216927514 0	0.218290450 6	0.152224322 1	0.000000000 0

Z^{R1}: 12,469,598,020 S-ln(Z^{R1}): 0.3874426560
Z^{R2}: 12,469,615,304 S-ln(Z^{R2}): 0.3874426791
Z^{R3}: 12,469,659,460 S-ln(Z^{R3}): 0.3874427381
Z^{R4}: 12,469,164,072 S-ln(Z^{R4}): 0.3874420760
Z^{R5}: 12,469,173,332 S-ln(Z^{R5}): 0.3874420884

C_{44}

0.0000000000	0.2468108664	0.2463780569
0.2468108664	0.0000000000	0.1927300435
0.2463780569	0.1927300435	0.0000000000

Z^{R1}: 128,498,921,114 S-ln(Z^{R1}): 0.3875634295
Z^{R2}: 128,510,791,024 S-ln(Z^{R2}): 0.3875648290
Z^{R3}: 128,510,456,752 S-ln(Z^{R3}): 0.3875647896

Figure 2. *Cont.*

C_{48}

0.0000000000	0.2589370959
0.2589370959	0.0000000000

Z^{R1}: 1,318,197,267,571
S-ln(Z^{R1}): 0.387601197
Z^{R2}: 1,318,322,223,405
S-ln(Z^{R2}): 0.3876025139

C_{50}

0.0000000000	0.2783002779	0.2610747109	0.2662630442	0.2850277531
0.2783002779	0.0000000000	0.2815354907	0.2828349970	0.2726842541
0.2610747109	0.2815354907	0.0000000000	0.2511735066	0.2870732104
0.2662630442	0.2828349970	0.2511735066	0.0000000000	0.2879451010
0.2850277531	0.2726842541	0.2870732104	0.2879451010	0.0000000000

Z^R	S-ln(Z^R)
4,218,555,026,432	0.3876068503
4,219,715,995,440	0.3876105192
4,218,236,211,684	0.3876058426
4,218,084,725,292	0.3876053638
4,220,477,890,248	0.3876129264

C_{52}

0.0000000000	0.2547814446	0.2652650595	0.2657065483
0.2547814446	0.0000000000	0.2578899560	0.2586812417
0.2652650595	0.2578899560	0.0000000000	0.2225806760
0.2657065483	0.2586812417	0.2225806760	0.0000000000

Z^R	S-ln(Z^R)
13,503,792,382,988	0.3876152779
13,503,369,805,438	0.3876148767
13,502,825,284,708	0.3876143597
13,502,790,617,918	0.3876143268

C_{58}

0.0000000000	0.3127607739
0.3127607739	0.0000000000

Z^R	S-ln(Z^R)
442,762,963,217,720	0.387632823805
442,106,464,006,600	0.387615768251

C_{60}

0.0000000000	0.2949084894
0.2949084894	0.0000000000

Z^R	S-ln(Z^R)
1,417,033,687,086,496	0.387637134765
1,417,370,147,605,744	0.387639772675

C_{72}

0.0000000000	0.2885597755
0.2885597755	0.0000000000

Z^R	S-ln(Z^R)
1,244,877,071,455,144,960	0.385792300566
1,244,845,236,328,149,760	0.385792063777

Figure 2. Similarity matrices and reduced Z-indices and scaled reduced ln(Z-indices) of fullerene isomers considered in this study.

To shed further light into the similarity matrix invariants, let us consider the five isomers of C_{50} shown in Figure 1 with their matching polynomials displayed in Table 8. Let us consider the computed similarity matrix which is highlighted below for the five isomers of C_{50} in the order:

$C_{50}(C_2)$-269, $C_{50}(C_{2v})$-13, $C_{50}(D_3)$-270, $C_{50}(D_{5h})$-271, and $C_{50}(D_{3h})$-3.

	$C_{50}(C_2)$-269	$C_{50}(C_{2v})$-13	$C_{50}(D_3)$-270	$C_{50}(D_{5h})$-271	$C_{50}(D_{3h})$-3
$C_{50}(C_2)$-269	0.0000000000	0.2783002779	0.2610747109	0.2662630442	0.2850277531
$C_{50}(C_{2v})$-13	0.2783002779	0.0000000000	0.2815354907	0.2828349970	0.2726842541
$C_{50}(D_3)$-270	0.2610747109	0.2815354907	0.0000000000	0.2511735066	0.2870732104
$C_{50}(D_{5h})$-271	0.2662630442	0.2828349970	0.2511735066	0.0000000000	0.2879451010
$C_{50}(D_{3h})$-3	0.2850277531	0.2726842541	0.2870732104	0.2879451010	0.0000000000

The above array suggests that the smallest matrix element (0.251174) is between the isomers 3 and 4, while the largest matrix element is between the isomers 4 and 5 (0.2879451010). I now refer to Figure 1, where indeed I find the isomers 3 and 4, $C_{50}(D_3)$-270 and $C_{50}(D_{5h})$-271, which are quite similar in their shapes and overall structural features.

On the other hand, the isomers $C_{50}(D_{5h})$-271 and $C_{50}(D_{3h})$-3 are extremely dissimilar in that the latter is an oblate spheroid while the former is more spherical. Likewise, as can be seen from the fifth row of the similarity matrix, the oblate spheroidal $C_{50}(D_{3h})$-3 stands out in having larger matrix elements with the entire array of other isomers of C_{50} considered here. This is consistent with the fact that the $C_{50}(D_{3h})$-3 isomer is conspicuous among the five isomers of C_{50} in being an oblate spheroid while the other four isomers are closer to spherical structures (See Figure 1).

I note from Figure 2 that although Z^R increases rapidly as a function of the number of atoms in fullerenes, the scaled-logarithmic version can be used to make comparisons. As pointed out by Hosoya [78], the Z-index by itself does not correlate with the aromaticity or stability of polycyclic aromatics. However, the reduced index Z^R can provide first-order information on the total number of resonance structures and possible full and partial matchings. If I consider the two isomers of C_{60}, their Z^R values are 1,417,033,687,086,496 and 1,417,370,147,605,744 for the I_h and D_3 isomers, respectively. Although the numbers of the resonance structures of the I_h and D_3 structures are 12,500 and 9622, respectively, their Z^R indices exhibit an opposite trend with the I_h isomer exhibiting an overall lower Z^R index. The lower overall Z^R for the I_h isomer together with the greater number of resonance structures for the I_h structure suggests a considerably enhanced stability for the I_h isomer. This is consistent with the DFT quantum chemical studies on these isomers which reveal that the D_3 isomer of C_{60} is higher in energy [76]. I find a similar correlation for other fullerenes such as C_{50} and C_{36} with the cautionary note that there is no direct correlation between the relative stability and the Z^R indices as well as the total number of resonance structures.

Finally, there appears to be a correlation between the shapes of fullerene structures and the combinatorial matching-based similarity indices. For example, nearly spherical structures have very close similarity indices while a fullerene isomer with an oblate spheroid structure exhibits a numerically larger value of the similarity index when compared to more spherical structures. Likewise, two oblate spheroid isomers have closer similarity and, thus, a smaller similarity matrix element. The subject matter of quantifying shapes and QShAR has received attention over the years [79,80]. Consequently, the present similarity matrices derived from the matchings add yet another novel dimension to the shape similarity problem. The similarity indices derived here based on combinatorial matchings could find applications in water clusters [81] where the hydrogen bonds between any two water molecules could become matchings. Moreover, dimer covers could also model placing dimers such as transition metal dimers [82] that avoid being neighbors and, thus, could also serve as models for the chemisorption or substitution of dimeric molecules on fullerene cages and nanotubes.

4. Conclusions

In retrospect, I have developed powerful similarity measures using matrix invariants derived from the matching polynomials. These similarity matrices were applied to isomers of fullerenes, and it was demonstrated that the similarity matrix measures are quite robust in providing quantitative measures of similarity of two fullerene isomers. It also seems that the techniques provide some indirect measures of shape similarities of fullerene isomers. There are a few limitations that should be pointed out. The techniques developed might not provide much contrast for isospectral graphs and isospectral trees. In particular, for isospectral trees, the matching polynomials and characteristic polynomials become degenerate. Likewise, some isospectral structures that contain rings with pending fragments might not be contrasted by the matching polynomial-based methods. Babić [83] has shown the existence of isospectral benzenoid graphs containing 33 vertices and 9 hexagons. Likewise, the author and Basak [84] have illustrated isospectral benzenoid graphs with pendant bonds. Yet, the techniques based on matching polynomials appear to provide considerable promise for molecular structures containing several rings, three-dimensional fullerene cages, and carbon nanotubes. Graph theoretical techniques analogous to the ones developed here in conjunction with group theory and combinatorics can also be applied to NMR, ESR, and vibrational spectroscopies [85], thus paving the way for the applications of the emerging field of artificial intelligence.

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