Exhaustive Generation and Analytical Expressions of Matching Polynomials of Fullerenes C$_{20}$–C$_{50}$

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In this paper we consider exhaustive generation of matching polynomials of all fullerenes C$_n$ (n = 20–50, for all even n except C$_{22}$). Matching polynomials thus computed provide a basis for the derivation of an exact analytical formula for the first eight coefficients of the matching polynomials of fullerenes. It is shown that only the ninth coefficient of the matching polynomial can discriminate structural differences of two isomers of fullerenes.

1. INTRODUCTION

Graph polynomials have been the topic of numerous studies[1-23] for several decades. As is well-known, the adjacency matrix of a graph is not unique in that it depends on the labeling. An underlying structural invariant is the characteristic polynomial which is simply the secular determinant of the adjacency matrix. Unfortunately, the characteristic polynomial by itself is not a unique structural invariant in that two nonisomorphic graphs could have the same characteristic polynomials. Nevertheless for fullerenes which by definition contain twelve pentagons and hexagons (except C$_{20}$ which is composed of twelve pentagons), two different structures with the same characteristic polynomials have not been found up to now.

The matching polynomial of a graph[8,9,16,17,18,23] enumerates the number of ways of placing disjoint dimers on the graph. It is also called the acyclic polynomial since the characteristic polynomials of acyclic structures are identical to their matching polynomials. Matching polynomials have several applications in chemical physics, in general. In particular they are useful in estimating the physicochemical properties. They enumerate the number of ways of placing a given number of dimers on a lattice (the Ising problem), the number of Kukulé structures (the constant term in the polynomial), and therefore the resonance energy. The exact computation of the grand canonical partition functions requires the knowledge of matching polynomials.[16,24-25] Matching polynomials also enumerate the number of ways diatomics can be "adsorbed" on a surface. Hosoya[18] formulated an index called the Hosoya index which requires the matching polynomial.

The computation of matching polynomials is certainly a very challenging problem compared to other graph polynomials. While there are elegant algorithms for the characteristic polynomials, the computation of matching polynomials often have to resort to brute-force recursive methods. Often one has to settle for some sort of recursive pruning algorithm. Such algorithms lead to combinatorial explosions due to a larger number of fragments generated in the pruning process, especially for fullerene species.

Fullerene chemistry is a topic of growing importance and has witnessed a significant increase in research contributions in recent years.[26-29] The number of publications in this area has reached a few thousand, and thus an exhaustive literature survey of the topic is no longer possible. However, fortunately there are a few review articles, some of which are cited here.[26-29]

Fueled by the intense activity in fullerene chemistry and intrinsically interesting geometrical and topological features of fullerenes, several studies have focused on the fascinating mathematical properties of fullerenes. These studies included graph theoretical computations of the characteristic polynomials, enumeration of possible structures for a given fullerene formula,[30-32] enumeration of isomers of polysubstituted fullerenes,[33] spectral moments of fullerenes,[34] group theoretical studies concerning the nuclear spin statistics and rovibronic levels,[35] combinatorial techniques for the characterization of the NMR and ESR spectral patterns,[36] and so on. In spite of significant mathematical studies on fullerenes, the computation of the matching polynomials is restricted to the letter of the author[23] in which he considered the matching polynomials of some of the smaller fullerenes.

In the present paper we have combined the results of the matching polynomials of some of the fullerenes obtained before[23] with the new results on fullerenes C$_{32}$, C$_{34}$, C$_{38}$, C$_{42}$, C$_{44}$,(T), C$_{46}$, and C$_{48}$ obtained here for the first time. The matching polynomials of all fullerenes C$_n$ (n = 20–50) for even n with the exception of C$_{22}$ are thus exhaustively obtained. The coefficients were analyzed which resulted in a systematic exact formula for the first several coefficients of the matching polynomials of fullerenes.

2. MATCHING POLYNOMIALS AND THEIR COMPUTATION

The matching polynomial $M_G(x)$ of a graph and the related $Z_G(x)$ are formally defined as

$$M_G(x) = \sum_{k=0}^{m} (-1)^k P(G,k) x^{n-2k}$$

$$Z_G(x) = \sum_{l=0}^{m} (-1)^l P[2l + 1] x^{2l}$$

where n is the number of vertices, the sum terminates with $m = [n/2]$, and $P(G,k)$ is the number of ways of choosing k non-adjacent edges from the graph G. Alternatively $P(G,k)$ is the number of ways of placing k disjoint dimers (dumbbells) on the graph G. Note that $P(G,l)$ is the same as $P[2l + 1]$. For computational convenience we computed results in terms of $P[2l + 1]$.

The recurrence relation of Hosoya and co-workers[18] was used. This is similar to the recurrence relation for the rook and king polynomials on a chess board, which can be derived

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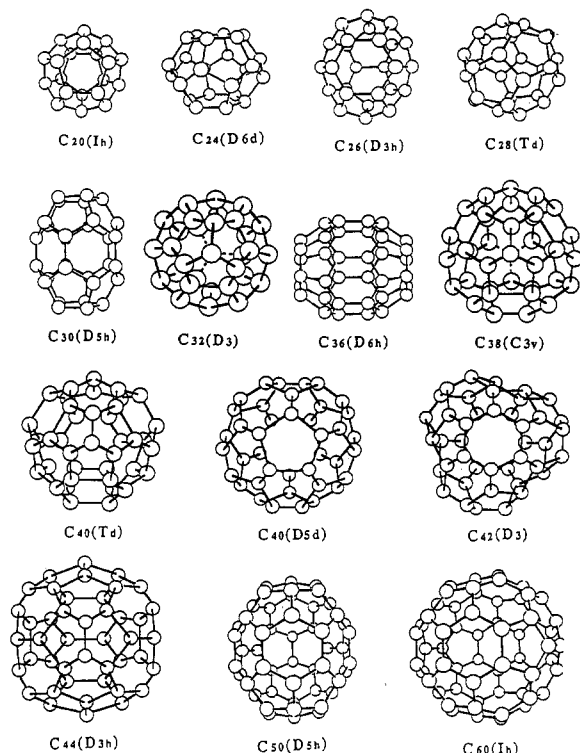
Figure 1. Structures of fullerene cages C_{20}–C_{60} except C_{34}, C_{46}, and C_{48}.

Figure 2. Schlegal diagrams for C_{34} (C_{3v}), C_{38} (D_{3h}), two forms of C_{40}, C_{42} (D_3), two forms of C_{44}, C_{46} (C_3), and C_{48} (D_3).

using the principle of inclusion and exclusion. The recursive relation is as follows.

$$M_G(x) = M_{G-e}(x) - M_{G\ominus e}(x)$$

where $G-e$ is the graph obtained by deleting an edge "e" from G while $G\ominus e$ is the graph obtained by deleting this edge, the vertices composing e, and all the edges connected to the vertices that comprise e. This recursive relation facilitates reduction of the graph G to smaller or simpler graphs.

The matching polynomial of a tree graph is the same as the characteristic polynomial which is readily computed by the code developed by the author[11,12] based on the Leverrier–Frame method. The graph G is thus recursively reduced until all the fragments are trees. Then using the characteristic polynomials of the trees computed using the author's code, the matching polynomials are computed. We used the code developed by Ramaraj and the author[9] for recursive pruning of graphs to trees. This is combined with the author's code[12] for computing the characteristic polynomials to generate the matching polynomials. It was found that as the size of the cage increases, the number of pruning steps astronomically grows.

3. RESULTS FOR FULLERENES AND DISCUSSION

In this investigation new results for the matching polynomials were obtained for fullerenes C_{32} (D_3 symmetry), C_{34} (C_{3v} symmetry), C_{38} (C_{3v} symmetry), C_{42} (D_3 symmetry), C_{44} (T symmetry), C_{46} (C_3 symmetry), and C_{48} (D_3 symmetry). The Schlegal diagrams or full three-dimensional structures of all fullerenes C_{20}–C_{50} are shown in Figures 1 and 2. For the sake of completeness and to provide a complete set of data for further analysis, we also include in tables our previously computed results for other fullerenes from ref 23. We note at the very outset that the computation of matching polynomials of fullerenes is a computationally very intensive problem requiring large amounts of CPU time running into several hours. This is in dramatic contrast with the char-
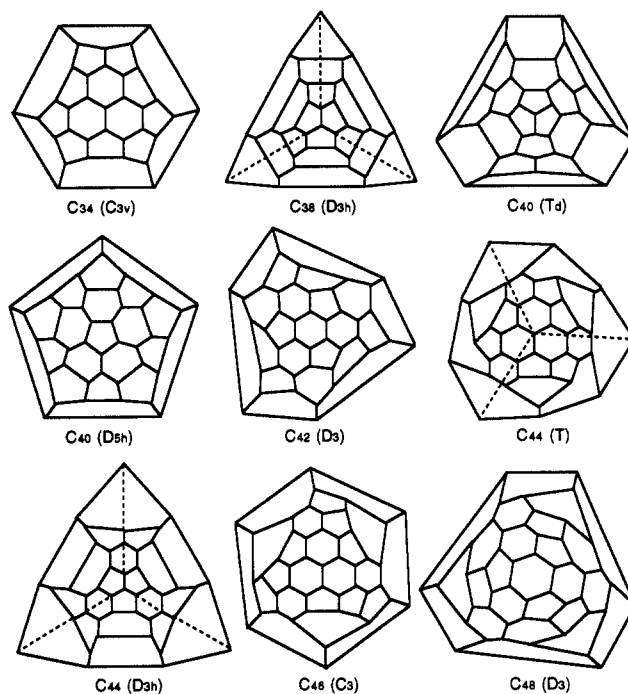
acteristic polynomials which are readily obtained in a few seconds of CPU time for such cages using the author's code based on the Leverrier–Frame method.

Table 1 shows the matching polynomials of all fullerenes C_{20}–C_{40} (for C_n, n = even number), while Table 2 shows the matching polynomials of C_{42}, C_{44}, C_{46}, C_{48}, and C_{50} fullerenes. In each case we considered the most attractive structures from the standpoint of strain energy and other considerations. Feyereisen et al.[37] have considered *ab initio* studies of some of these fullerenes. The most favorable structures considered by these authors for the fullerenes are included in our study.

The constant coefficients in the matching polynomials yield the number of Kekulé structures. Thus these numbers can be used as a primary measure of stability. Further we note that even if a fullerene cage by itself is not very stable, the introduction of a metal atom can significantly stabilize it. This is the case with the C_{28} fullerene cage which is stabilized by the introduction of a tetravalent metal atom.[29]

Figure 3 shows the plot of the constant coefficient (we call this K) in the matching polynomial divided by n as a function of n for C_{20}–C_{50}. As seen from Figure 3, we find a sudden jump in the constant coefficient in the matching polynomial in moving from C_{28} to C_{30} (coefficient doubles). The coefficients change very little in moving from 30 to 34, while it increases in moving from C_{34} to C_{36}. Another jump is seen in going from 38 to 40. Again we see a sharp increase from C_{48} to C_{50} which is suggestive of the enhanced stability of C_{50} compared to other smaller fullerenes.

This increase in K/n for $n = 30$ is consistent with the change in the SCF energy/carbon in moving from C_{28} to C_{30}.[37] The C_{30} cluster exhibits a local maximum in the SCF energy per carbon. From C_{30} to C_{32}, we see a drop in the energy per carbon for the fullerene structure. There has to be a large rise in K/n for larger values of n since K is a nonlinear function of n. It is thus interesting that a simple plot of K/n as a function of n correlates reasonably with the *ab initio* predictions.

Let us compare the matching polynomials of two isometric fullerenes. As a first example, consider two C_{38} fullerene

Table 1. Matching Polynomials of Fullerene Clusters C$_{20}$–C$_{40}$

Matching Polynomial of the Dodecahedral C$_{20}$ Fullerene

P[1]	1	P[9]	10 155	P[17]	10 260
P[3]	-30	P[11]	-24 474	P[19]	-1 400
P[5]	375	P[13]	34 805	P[21]	36
P[7]	-2 540	P[15]	-27 300		

Fullerene Cluster C$_{24}$ with D$_{6d}$ symmetry
Matching Polynomial

P[1]	1	P[11]	-93 876	P[19]	-1 49 020
P[3]	-36	P[13]	216 026	P[21]	37 704
P[5]	558	P[15]	-3 18 960	P[23]	-3 552
P[7]	-4 884	P[17]	2 89 458	P[25]	54
P[9]	26 613				

Fullerene Cluster C$_{26}$ with D$_{3h}$ Symmetry
Matching Polynomial

P[1]	1	P[11]	-163 632	P[21]	3 24 012
P[3]	-39	P[13]	451 187	P[23]	-69 078
P[5]	663	P[15]	-8 32 773	P[25]	5 477
P[7]	-6 461	P[17]	10 03 968	P[27]	-63
P[9]	39 936	P[19]	-7 53 490		

Fullerene Cluster C$_{28}$ with T$_{d}$ symmetry
Matching Polynomial

P[1]	1	P[11]	-269 628	P[21]	1 859 652
P[3]	-42	P[13]	868 440	P[23]	-678 312
P[5]	777	P[15]	-1 932 444	P[25]	123 387
P[7]	-8 344	P[17]	2 932 008	P[27]	-8 274
P[9]	57 708	P[19]	-2 944 708	P[29]	75

Fullerene C$_{30}$ with D$_{5h}$ Symmetry
Matching Polynomial

P[1]	1	P[13]	1 566 065	P[23]	-4 388 255
P[3]	-45	P[15]	-4 091 265	P[25]	1 377 420
P[5]	900	P[17]	7 524 770	P[27]	-217 960
P[7]	-10 560	P[19]	-9 568 000	P[29]	13 265
P[9]	80 820	P[21]	8 137 551	P[31]	-151
P[11]	-424 392				

Fullerene C$_{32}$ with D$_{3}$ symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[13]	2 677 550	P[23]	-21 366 846
P[3]	-48	P[15]	-8 048 208	P[25]	9 954 461
P[5]	1 032	P[17]	17 458 041	P[27]	-2 711 652
P[7]	-13 136	P[19]	-27 041 484	P[29]	371 775
P[9]	110 244	P[21]	29 269 326	P[31]	18 904
P[11]	-643 044			P[33]	140

Fullerene Cluster C$_{34}$ with C$_{3v}$ Symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[13]	4 379 124	P[25]	53 685 020
P[3]	-51	P[15]	-14 906 664	P[27]	-21 843 978
P[5]	1 173	P[17]	37 348 041	P[29]	5 224 707
P[7]	-16 099	P[19]	-68 510 278	P[31]	-632 716
P[9]	147 033	P[21]	90 732 108	P[33]	28 623
P[11]	-943 539	P[23]	-84 691 494	P[35]	-19

C$_{36}$ Fullerene with D$_{6h}$ Symmetry
Matching Polynomial

P[1]	1	P[15]	-26 255 052	P[27]	-129 746 178
P[3]	-54	P[17]	74 743 467	P[29]	46 494 021
P[5]	1 323	P[19]	-158 920 874	P[31]	-9 821 428
P[7]	-19 476	P[21]	250 185 213	P[33]	1 050 468
P[9]	192 321	P[23]	-286 861 644	P[35]	-42 288
P[11]	-1 346 910	P[25]	233 449 135	P[37]	272
P[13]	6 898 019				

Fullerene C$_{38}$ with C$_{3v}$ Symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[15]	-44 311 485	P[29]	303 147 594
P[3]	-57	P[17]	141 457 329	P[31]	-96 498 792
P[5]	1 482	P[19]	-342 789 924	P[33]	18 186 867
P[7]	-23 294	P[21]	627 517 788	P[35]	-1 745 700
P[9]	247 323	P[23]	-858 202 755	P[37]	63 675
P[11]	-1 877 511	P[25]	860 997 544	P[39]	-378
P[13]	10 521 461	P[27]	-616 692 840		

Table 1 (Continued)

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

$P[1]$	1	$P[15]$	-44 311 485	$P[29]$	303 435 693
$P[3]$	-57	$P[17]$	141 457 335	$P[31]$	-96 787 471
$P[5]$	1 482	$P[19]$	-342 790 103	$P[33]$	18 348 216
$P[7]$	-23 294	$P[21]$	627 520 038	$P[35]$	-1 788 042
$P[9]$	247 323	$P[23]$	-858 218 370	$P[37]$	67 274
$P[11]$	-1 877 511	$P[25]$	861 063 321	$P[39]$	-456
$P[13]$	10 521 461	$P[27]$	-616 866 771		

Fullerene C_{40} with D_{5d} Symmetry
Matching Polynomial

$P[1]$	1	$P[15]$	-72 094 680	$P[29]$	1 568 572 975
$P[3]$	-60	$P[17]$	255 308 425	$P[31]$	-686 949 378
$P[5]$	1 650	$P[19]$	-695 619 640	$P[33]$	195 473 975
$P[7]$	-27 580	$P[21]$	1 455 391 002	$P[35]$	-33 022 120
$P[9]$	313 335	$P[23]$	-2 321 337 100	$P[37]$	2 849 295
$P[11]$	-2 563 260	$P[25]$	2 786 373 750	$P[39]$	-94 470
$P[13]$	15 606 390	$P[27]$	-2 468 180 640	$P[41]$	562

Fullerene C_{40} with T_d Symmetry
Matching Polynomial

$P[1]$	1	$P[15]$	-72 094 680	$P[29]$	1 568 795 676
$P[3]$	-60	$P[17]$	255 308 427	$P[31]$	-687 273 224
$P[5]$	1 650	$P[19]$	-695 619 704	$P[33]$	195 781 161
$P[7]$	-27 580	$P[21]$	1 455 391 878	$P[35]$	-33 195 276
$P[9]$	313 335	$P[23]$	-2 321 343 852	$P[37]$	2 897 204
$P[11]$	-2 563 260	$P[25]$	2 786 406 318	$P[39]$	-98 592
$P[13]$	15 606 390	$P[27]$	-2 468 284 212	$P[41]$	576

isomers, one with C_{3v} symmetry and the other with D_{3h} symmetry (see Figures 1 and 2). The structure with C_{3v} symmetry has a slightly smaller constant coefficient (378) compared to the D_{3h} cage which has 456 resonance structures. It is also seen that the Hosoya Z index as defined below

$$Z = \sum_k P(G,k)$$

is larger for the D_{3h} cage compared to the C_{3v} cage. Thus on the basis of the number of Kekulé structures and the Z index alone, one may be tempted to conclude that the D_{3h} cage will be more stable than C_{3v}. However two factors come in. The Kekulé count has to be substantially larger other things being the same. The more important feature governing the instability is the existence of several fused pentagons. The larger the number of fused pentagons, the less stable a structure would be. The D_{3h} structure has 18 eight-membered circuits arising from 2 fused pentagons. On the other hand the C_{3v} structure has only 12 eight-membered circuits arising from 2 fused pentagons. Consequently based on this the C_{3v} fullerene is more stable than D_{3h} for C_{38}. Note that the constant coefficient is only 20% larger for D_{3h} compared to C_{3v}.

The other striking feature we note, in comparing the matching polynomials of two isomeric fullerenes, is that the first eight coefficients in the matching polynomials are identical. [Compare the matching polynomial of C_{38} (C_{3v}) with C_{38} (D_{3h}).] This trend is noted for C_{40} (D_{5d}) and C_{40} (T_d) as well as C_{44} (T) and C_{44} (D_{3h}). This is a consequence of the fact that the first eight coefficients of the matching polynomials depend only on n, the number of vertices in the fullerene. It is the ninth coefficient in the polynomial which introduces structural dependence.

The characteristic polynomial of a graph is defined in terms of the adjacency matrix A of the graph shown below:

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

The characteristic polynomial P_G of the graph G is defined as

$$P_G = |A - xI| = C_0 x^n + C_1 x^{n-1} + C_2 x^{n-2} + ... + C_n$$

The celebrated Sach theorem provides a structural interpretation for the coefficients C_k in the characteristic polynomial and hence their relation to the coefficients in the matching polynomial. According to Sach's theorem

$$C_k = \sum_{H_k} (-1)^h 2^c$$

where H_k is a union of distinct subgraphs containing k vertices in G such that the components of H_k are composed only of edges or cycles (circuits) and c is the number of such circuits in H_k (an edge is not counted as a circuit). Consequently the coefficients C_k in the characteristic polynomials include the net contribution from disjoint edges and circuits in the graph that span k vertices, while the coefficients in the matching polynomials contain only the contributions from the edges.

The $P[3]$ coefficient in the matching polynomials is readily seen to be $-3n/2$. The $P[5]$ coefficient in the matching polynomial is the number of ways of choosing two disjoint dimers from the carbon cage. Since fullerene cages have no four-membered rings, the only surviving contribution in C_4 is due to two disjoint edges. Since the number of edges for a fullerene cage is $3n/2$, it is readily seen that the number of ways of choosing two disjoint edges from the fullerene cage is

$$P[5] = 3n(3n - 10)/8$$

Note that the $P[7]$ coefficient of the matching polynomial is related to the C_6th coefficient of the characteristic polynomial, which is composed of three disjoint edges (partition 2^3 of 6) and hexagons (6) as there are no four-membered rings for a fullerene cage. Hence

$$P[7] = C_6 - n + 20$$

Since $P[7]$ is the number of ways of choosing three disjoint edges from the fullerene cage, thus it has to be less than the

Table 2. Matching Polynomials of C$_{42}$–C$_{50}$ Fullerene Cages

Fullerene C$_{42}$ with D_3 Symmetry
Matching Polynomial

P[1]	1	P[17]	442 349 103	P[31]	-3857 643 550
P[3]	-63	P[19]	-1 340 120 611	P[33]	1515 265 230
P[5]	1 827	P[21]	3 160 264 869	P[35]	-387 943 698
P[7]	-32 361	P[23]	-5 775 791 133	P[37]	59 144 903
P[9]	391 734	P[25]	8 107 383 539	P[39]	-4 623 135
P[11]	-3 435 882	P[27]	-8 616 572 229	P[41]	138 936
P[13]	22 589 909	P[29]	6 792 255 882	P[43]	-680
P[15]	-113 623 299				

Fullerene C$_{44}$ with T Symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[17]	739 662 345	P[33]	9 210 020 709
P[3]	-66	P[19]	-2 468 621 666	P[35]	-3 266 975 370
P[5]	2 013	P[21]	6 487 126 077	P[37]	758 493 495
P[7]	-37 664	P[23]	-13 393 722 960	P[39]	-105 468 900
P[9]	483 978	P[25]	21 594 114 326	P[41]	7 588 950
P[11]	-4 531 152	P[27]	-26 905 576 992	P[43]	-212 136
P[13]	32 000 462	P[29]	25 514 074 656	P[45]	864
P[15]	-174 145 908	P[31]	-18 024 278 416		

Fullerene C$_{44}$ with D_{3h} Symmetry
Matching Polynomial

P[1]	1	P[17]	739 662 342	P[33]	9 205 872 024
P[3]	-66	P[19]	-2 468 621 548	P[35]	-3 263 413 578
P[5]	2 013	P[21]	6 487 124 046	P[37]	756 639 056
P[7]	-37 664	P[23]	-13 393 702 806	P[39]	-104 943 960
P[9]	483 978	P[25]	21 593 986 461	P[41]	7 523 484
P[11]	-4 531 152	P[27]	-26 905 033 434	P[43]	-210 480
P[13]	32 000 462	P[29]	25 512 497 241	P[45]	960
P[15]	-174 145 908	P[31]	-18 021 154 632		

Fullerene Cluster C$_{46}$ with C_3 Symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[17]	1 198 817 862	P[33]	46 264 981 725
P[3]	-69	P[19]	-4 373 291 348	P[35]	-21 377 190 444
P[5]	2 208	P[21]	12 685 070 817	P[37]	6 873 356 805
P[7]	-43 516	P[23]	-29 244 168 333	P[39]	-1 448 331 729
P[9]	591 606	P[25]	53 376 352 572	P[41]	182 577 150
P[11]	-5 889 138	P[27]	-76 553 899 758	P[43]	-11 819 157
P[13]	44 469 741	P[29]	85 295 234 247	P[45]	288 978
P[15]	-260 403 741	P[31]	-72 646 698 403	P[47]	-1 032

Fullerene C$_{48}$ with D_3 Symmetry
Coefficients in the Matching Polynomial

P[1]	1	P[19]	-7 486 059 786	P[35]	-115 286 996 736
P[3]	-72	P[21]	23 775 564 096	P[37]	48 432 339 830
P[5]	2 412	P[23]	-60 611 132 058	P[39]	-14 196 268 002
P[7]	-49 944	P[25]	123 759 759 689	P[41]	2 734 176 903
P[9]	716 238	P[27]	-201 338 447 622	P[43]	-315 951 696
P[11]	-7 554 444	P[29]	258 752 431 728	P[45]	18 833 124
P[13]	60 745 322	P[31]	-259 492 544 072	P[47]	-429 648
P[15]	-380 928 456	P[33]	199 691 703 636	P[49]	1 575
P[17]	1 890 083 478				

Fullerene C$_{50}$ with D_{5h} Symmetry
Matching Polynomial

P[1]	1	P[19]	-12 430 405 330	P[37]	279 429 116 630
P[3]	-75	P[21]	42 930 477 279	P[39]	-107 155 471 120
P[5]	2 625	P[23]	-120 030 323 355	P[41]	28 728 154 280
P[7]	-56 975	P[25]	271 474 997 635	P[43]	-5 070 966 660
P[9]	859 575	P[27]	-494 945 313 135	P[45]	538 792 490
P[11]	-9 576 453	P[29]	722 820 579 630	P[47]	-29 762 020
P[13]	81 704 030	P[31]	-837 675 911 840	P[49]	642 645
P[15]	-546 377 070	P[33]	760 448 826 260	P[51]	-2 343
P[17]	2 907 494 480	P[35]	-531 467 488 160		

total number of ways of choosing three edges which is n^3 in order. The author[23] found that a cubic fit for the P[7] coefficient using the computed values for C$_{20}$, C$_{24}$, C$_{26}$, and C$_{28}$ yielded

$$P[7] = -(9n^3 - 90n^2 + 232n)/16$$

These formulas for P[5] and P[7] can be derived from the work of Dias[19,20] on the characteristic polynomial coefficients a_4 and a_6 by eliminating the ring term and substituting for q = $3n/2$ and $e(3,3)$ = q.[19,20]

The C$_8$ coefficient in the characteristic polynomial for fullerene cages consists of octagonal circuits generated by two fused pentagons, hexagon + a disjoint edge and the terms arising from four disjoint dimers. By eliminating the cyclic terms from C$_8$ we find that

$$P[9] = C_8 - (3n - 24)(n - 20)/4 + 2n_5^{(2)}$$

where $n_5^{(2)}$ is the number of ways of choosing two fused pentagons. Hence if the exact formula can be computed for
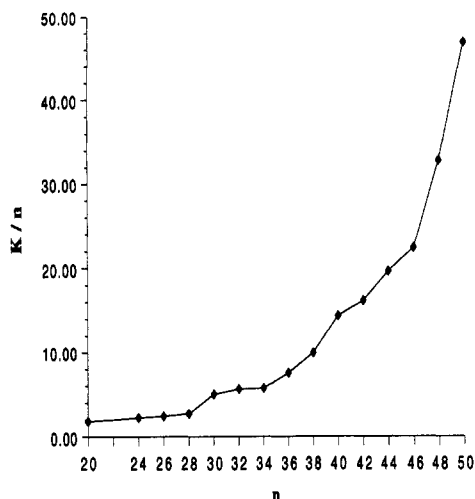
Figure 3. Plot of K/n versus n.

C_8 and $n_5^{(2)}$ for fullerenes, one can obtain $P[9]$. The computation of C_8 can be achieved through the method of moments. For example, it can be seen that there are 30 ways to choose 2 fused pentagons for C_{20}. The C_8 coefficient of the characteristic polynomial of C_{20} is computed as 10 095 and thus $P[9]$ for the C_{20} cage is 10 155. This is exactly what we compute independently using the recursive formula for the matching polynomials. For the C_{24} cage, $n_5^{(2)} = 18$. The C_8 coefficient of the characteristic polynomial is computed as 26 661. Hence $P[9]$ is computed for C_8 as 26 613. The exact analytical expressions for the moments of fullerene cages have been recently obtained.[38] The exact formulas for $P[9]$ and C_8 are given below:

$$P[9] = {}^1/_{128}(27n^4 - 540n^3 + 3684n^2 - 8688n)$$

$$C_8 = {}^1/_{128}(27n^4 - 540n^3 + 3876n^2 - 14\,064n) + 240$$

The C_{10} coefficient of the characteristic polynomial is composed of 10-membered rings arising from two fused hexagons and two disjoint pentagons, 8-membered rings arising from two fused pentagons plus a disjoint edge, and finally five disjoint edges. The following formulas for $P[11]$ and C_{10} are thus derived:

$$P[11] = C_{10} + 2n_6^{(2)} - 4n'_5^{(2)} - n_5^{(2)}(3n - 30)$$

$$C_{10} = -\frac{1}{1280}[81n^5 - 2700n^4 + 35820n^3 - 256560n^2 +$$
$$1152384n] + 2556$$

where $n_6^{(2)}$ is the number of fused hexagons, $n_5^{(2)}$ is the number of fused pentagons, and $n'_5^{(2)}$ is the number of disjoint pentagons. Consequently the $P[11]$ coefficient is a polynomial in n of order 5. We fit the $P[11]$ coefficients of the matching polynomials to the following exact expression.

$$P[11] = -\frac{1}{1280}[81n^5 - 2700n^4 + 34380n^3 - 199920n^2 +$$
$$453504n - 15360]$$

It is quite interesting that the first two leading coefficients in $P[11]$ are identical to the corresponding coefficients C_{10} in the characteristic polynomial. In fact, the denominator 1280 obtained for C_{10} is the key motivating factor to fit $P[11]$ with the factor 1280 in the denominator.

The $P[13]$th coefficient is the matching polynomial is related to the C_{12} coefficient, and thus they should not appear in the

matching polynomial. The $P[13]$ coefficient of the matching polynomial is given by

$$P[13] = C_{12} - \text{cyclic contributions}$$

Hence $P[13]$ is a sixth-order polynomial in n. A numerical fit to $P[13]$ was sought with a common denominator of 5120. The result is shown as follows:

$$P[13] = \frac{1}{5120}[81n^6 - 4050n^5 + 82260n^4 - 1853560n^3 +$$
$$4562464n^2 - 10254080n + 1177600]$$

The $P[15]$ coefficient of the matching polynomial is related to the C_{14} coefficient of the characteristic polynomial. Using the method of moments, Zhang and the author showed that the C_{12} coefficient of the characteristic polynomials of fullerenes is given by

$$C_{12} = -\frac{1}{5120}[81n^6 - 4050n^5 + 85140n^4 - 1009080n^3 +$$
$$7680544n^2 - 40830720n] + 25970 - 10p - 2q$$

where p and q are structure-dependent factors. That is, p is the number of bonds connecting two pentagons, while q is the number of hexagons lying between two pentagons. However p and q factors contribute only as cyclic contributions to the C_{12} coefficient of the characteristic polynomial. The $P[15]$ coefficient in the matching polynomial is given by

$$P[15] = C_{14} - \text{cyclic contributions}$$

Zhang and the author showed that C_{14} is given by

$$C_{14} = -\frac{1}{71680}(243n^7 - 17010n^6 + 517860n^5 -$$
$$9155160n^4) + 146500032n^3 - 875226240n^2 +$$
$$5213230080n + 217630 + 15np + 3nq + 63q -$$
$$137r - 137s$$

where p, q, r, and s are structure-dependent factors which contribute only to the characteristic polynomial (cyclic contributions). Hence $P[15]$ is a seventh-order polynomial in n. A numerical fit with 71 680 as common denominator yielded

$$P[15] = -\frac{1}{71680}[243n^7 - 17010n^6 + 502740n^5 -$$
$$8066520n^4 + 74548992n^3 - 38015040n^2 + 865336320n -$$
$$206438400]$$

All the exact expressions thus obtained for $P[1] - P[15]$ are shown in Table 3.

Finally we would like to address the CPU time required to generate the matching polynomials of fullerene cages by the algorithms of removing an edge at a time. The computation of the matching polynomial of the C_{34} (C_{3v}) fullerene took 4

Table 3. Exact Formulas for the Coefficients $P[1]-P[11]$ of the Matching Polynomials of Fullerene Cages

$P[1]$	1
$P[3]$	$-3n/2$
$P[5]$	$3n(3n - 10)/8$
$P[7]$	$-(9n^3 - 90n^2 + 232n)/16$
$P[9]$	${}^1/_{128}[27n^4 - 540n^3 + 3684n^2 - 8688n]$
$P[11]$	$-{}^1/_{1280}[81n^5 - 2700n^4 + 34380n^3 - 199920n^2 +$ $453504n - 15360]$
$P[13]$	${}^1/_{5120}[81n^6 - 4050n^5 + 82260n^4 - 853560n^3 +$ $4562464n^2 - 10254080n + 1177600]$
$P[15]$	$-{}^1/_{71680}[243n^7 - 17010n^6 + 502740n^5 -$ $8066520n^4 + 74548992n^3 - 38015040n^2 +$ $865336320n - 206438400]$

MATCHING POLYNOMIALS OF FULLERENES C_{20}–C_{50}

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min and 34 s of CPU time on an IBM RS6000/560 model. The C_{38} (C_{36}) fullerene took 13 min and 55 s of CPU time on the same system. On the other hand the computation of the matching polynomial of C_{50} took 7 h and 22 min of CPU time on the same computer. It is clear that the factor of CPU time between C_{38} and C_{34} is roughly 3. The factor of CPU time between C_{50} and C_{38} is $\sim$32. Thus the CPU time increases as n^{10-13} for smaller fullerenes (C_{30}–C_{50}) where n is the number of vertices. For larger fullerenes the CPU time should increase by n^m, where $m \geq 13$. On the basis of this we obtain a very conservative estimate of the CPU time required for computing the matching polynomial of the Bucky ball as 113 h on IBM RS6000/560 or roughly 5 days of CPU time using the algorithm of removing one edge at a time. However, the more practical problem that needs to be dealt with is attributed to Pascal Compiler's overflow problem which results in a core dump for such large fullerenes. Therefore we suggest that more elegant algorithms be developed for the computation of the matching polynomials of fullerenes larger than C_{60}. A possible algorithm could be to obtain more powerful recursive relations which remove one ring at a time instead of one edge at a time. Such powerful algorithms for obtaining the matching polynomials of large fullerene cages and the computation of their topological resonance energies which depend on the eigenvalues of the matching polynomials could be the topics of further investigations.

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