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The Computation of the Matching Polynomials of Fullerene Graphs

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A new formula for the evaluation of the matching polynomials of fullerene graphs is presented.

INTRODUCTION

The relation between the stability of fullerenes and the topological resonance energy (TRE) has been studied by several authors.[1–6] TRE is computed from the difference in roots of the characteristic polynomials and the matching polynomials of fullerenes. The matching polynomial of a graph G is defined as

$$M(\mathrm{G}; X) = \sum_{k=0}^{\frac{n}{2}} (-1)^k \, p(\mathrm{G}; k) \, x^{n-2k} \,, \tag{1}$$

where n is the number of vertices, and $p(\mathrm{G}; k)$ is the number of ways of choosing k disjoint edges from graph G.

It is well known that the matching polynomial can be obtained by using the recurrence relation,[7, 8]

$$M(\mathrm{G}; x) = M(\mathrm{G} - e; x) - M(\mathrm{G} - (e); x) \,, \tag{2}$$

where G – e is the subgraph of graph G obtained by removing edge e from G, while G – (e) is the subgraph obtained by deleting edge e and incident vertices. Using the recurrence formula (2) repeatedly, we can obtain the

matching polynomial of a fullerene graph G by computing the matching polynomials of a series of trees. The matching polynomial for a tree graph is readily achieved because it is the same as the characteristic polynomial.

Recently, Herndon, Radhakrishnan and Živković[9] developed a different strategy which is to specify at the beginning all edges which will be removed during the computation. By deleting some edges of G, one can obtain a spanning tree, T(G). Another subgraph constituted by the edges not contained in the spanning tree T(G) is called a cotree of T(G), coT(G).[5] The Hosoy index[10] of coT(G) is denoted by Z. There exist Z subgraphs $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_i, \ldots, \varepsilon_z$ in coT(G), such that ε_i ($i = 1, 2, \ldots, z$) contain k disjoint edges only. Thus, the matching polynomial of G may be rewritten as

$$M(\mathrm{G}; x) = \sum_{i}^{z} (-1)^k M[\mathrm{T}(\mathrm{G} - \{\varepsilon_i\}); x], \tag{3}$$

where $\{\varepsilon_i\}$ denotes a set of vertices incident to edges in ε_i. Using formula (3), Babić and Ori [6] wrote the program and obtained the matching polynomial of fullerene C_{70}.

Using formulae (2) and (3) to obtain the matching polynomial of a fullerene graph, one has to compute very large numbers of characteristic polynomials of trees. Thence, the computation of a matching polynomial is a laborious procedure which consumes a great amount of CPU time. Quite recently, a remarkably efficient algorithm for calculating the matchings of a fullerene graph was developed by Babić.[11] Use of this algorithm enabled massive computation of all fullerene isomers with up to 70 atoms. The results[12–13] showed some distinct and interesting properties of the topological resonance energy of fullerene and of the matching polynomials.

A complex problem in the spanning tree algorithm is finding the optimal cotree, with the minimum Hosoya index, in a general fullerene graph. In the first part of this work, we discuss the optimal cotrees of fullerene graphs C_{60} and C_{70}. The Hosoya indices of the cotrees in the two graphs are somewhat smaller than those of the path – cotrees, which were incorrectly claimed as the optimal ones.[14] In the second part, we present another algorithm for computation of the matching polynomial in which some edges of a graph are deleted to yield a subgraph with no two cycles sharing the same edge, instead of the spanning tree in the previous algorithm. The matching polynomial can be obtained by computing the characteristic polynomials of the subgraphs with complex weights put on certain edges.[2,15–20] The number of characteristic polynomials of the subgraphs which need to be computed in this way is significantly smaller than in the spanning tree algorithm.

THE OPTIMAL coT(G) OF A FULLERENE GRAPH

A fullerene molecule C_n is a trivalent polyhedral cage which shares 12 five-membered rings and $n/2-10$ six-membered rings.[21] One can produce its T(G) by opening $n/2+1$ rings. In other words, its coT(G) has $n/2+1$ edges. For a fullerene graph, its coT(G) consists of path fragments and cyclic fragments. The number of cycle edges in coT(G) can be five or six. The Hosoya indices of paths and cycles with a different number of edges are given in Appendix. These data were obtained by Hosoya in 1971.[10] Let Z_i denote the Hosoya index of i^{th} fragment in coT(G). The value Z can be obtained by

$$Z = \prod_i Z_i \tag{4}$$

The coT(G) of a fullerene graph can take the different forms. In order to make the Hosoya index of coT(G) arrive at the minimum value, Herndon *et al.*[9] showed that the edges of coT(G) should share common vertices, as far as possible. And Babić *et al.* emphasized[5] that coT(G) should be compact. In

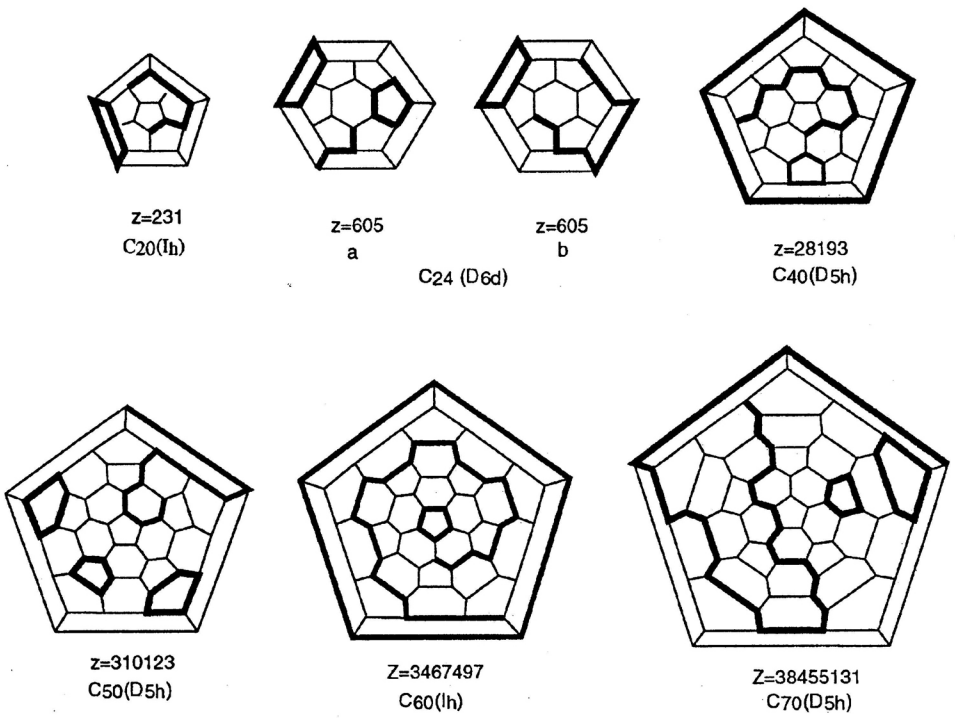

Figure 1. The optimal coT(G)s of several fullerenes, indicated by bolded lines, and their Hosoya indices.

their publication, a path with 36 edges was chosen as the coT(G) of C_{70}. Based on formula (4) and two tables in the Appendix, we arrived at the following conclusions:

The optimal coT(G) of a fullerene should satisfy three conditions. (i) The number of paths in coT(G) should be as small as possible. (ii) The path contained by the coT(G) shares at least three edges. (iii) The coT(G) should contain as many as possible five-membered cycles, providing that conditions (i) and (ii) are met.

The optimal coT(G)s of several fullerene graphs are showed in Figure 1. Figure 1 gives also the Hosoya indices of these coT(G)s. One can find another coT(G) of C_{20} (I_h) that contains two five-membered cycles, and a path with one edge. Though this case meets conditions (i) and (iii), it does not fulfil condition (ii). In fact, the Hosoya index of this coT(G) is 2402 ($= 11^2 \times 2$), which is greater than that of the optimal coT(G) showed in Figure 1. It is interesting that in fullerene $C_{24}(D_{5d})$ we can find two optimal coT(G)s. One possesses two five-membered cycles and one path of three edges, the other has one five-membered cycle and one path with eight edges. Their Hosoya indices are 605 ($= 11^2 \times 5$; $= 11 \times 55$). We note that the paths chosen as coT(G)s produce somewhat greater Hosoya indices than those of the optimal coT(G)s.

A NEW FORMULA FOR THE COMPUTATION OF FULLERENE GRAPHS

Several authors have investigated the relation between the matching polynomials of a graph and the characteristic polynomials of the associated edge-weighted graph.[2, 15–20]

If a graph contains cycles and no edge is shared by any two cycles, the graph is called the bridge tree, B. It is well known that the matching polynomial, $M(B, x)$, of B is equal to the characteristic polynomial, $P(B', x)$, of graph B'. B' is obtained by changing one edge of each cycle in B into the directed edge with weights of $\pm i$, where the plus and minus signs stand for two possible directions. Let B(G) be a bridge tree existing in graph G and coB(G) be the set of edges which belong to graph G but do not belong to B(G). Then, the matching polynomial of G can be expressed by

$$M(G; x) = \sum_{i}^{z} (-1)^k M[B(G - \{\varepsilon_i\}); x] \tag{5}$$

Using formula (5), the matching polynomial of G can be obtained by computing Z characteristic polynomials. Here value Z is the Hosoya index of coB(G).

To exemplify the application of formula (5), an example is given in Figure 2 for triphenylene.

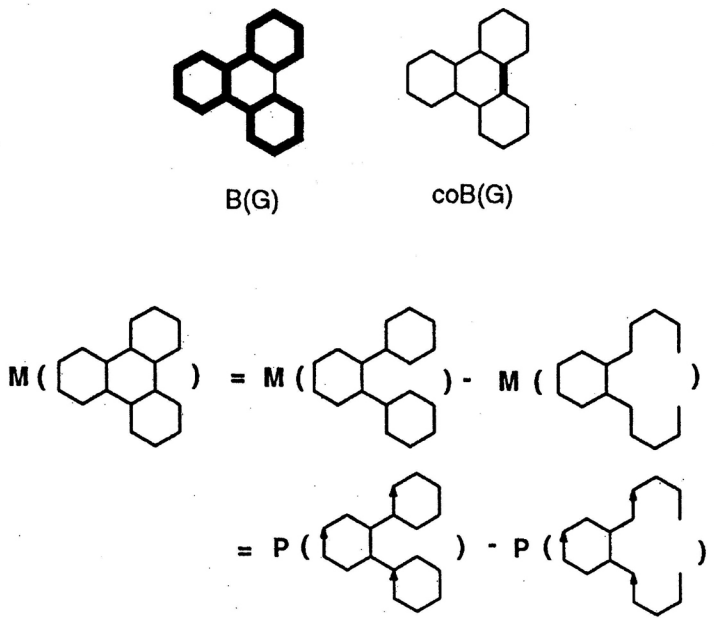

Figure 2. The matching polynomial of the triphenylene graph, obtained by formula (5). B(G) and coB(G) are indicated by bolded lines.

The coB(G) of this graph has only one path fragment with one edge, whose Hosoya index is 2. Thence, using formula (5), the matching polynomial of the triphenylene molecule can be obtained by the linear combination of two characteristic polynomials. However, one easily verify that by using formula (3) this matching polynomial is given by the linear combination of at least eight characteristic polynomials.

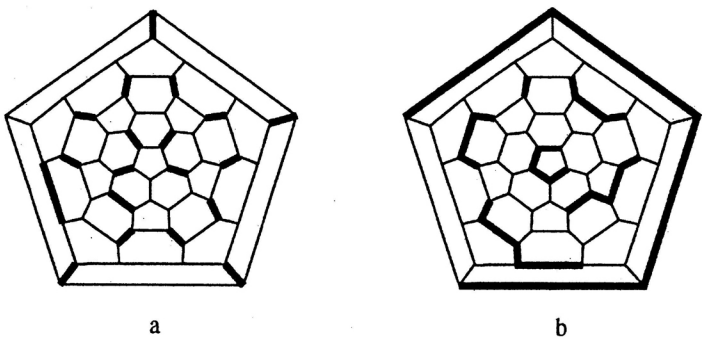

Figure 3. Two possible coB(G)s of C_{60}.

When B(G) of a fullerene graph contains r rings, its coB(G) possesses $n/2 - r + 1$ edges. The B(G) of C_{60} (I_h) can have 12 rings. The associated coB(G), shown in Figure 3a, consists of 19 disjoint edges. Its Hosoya index is 524288 (= 2^{19}). A better coB(G) (see Figure 3b) is constructed by four paths with 4 edges, two paths with 3 edges and one path with 1 edge. The Hosoya index of this coB(G) is 204800 (= $8^4 \times 5^2 \times 2$). For C_{60} the ratio between the Hosoya indices of the coB(G) showed in Figure 3b and the optimal coT(G) in Figure 1 is about 0.059.

Finally, we point out that there is still an interesting open problem: How to find the optimal coT(G) and coB(G) in a general fullerene graph?

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APPENDIX

TABLE I

The Hosoya index Z of a path with N edges

N	Z	N	Z	N	Z	N	Z
0	1	10	144	20	17711	30	2178309
1	2	11	233	21	28657	31	3524578
2	3	12	377	22	46368	32	5702887
3	5	13	610	23	75025	33	9227465
4	8	14	987	24	121393	34	14930352
5	13	15	1597	25	196418	35	24157817
6	21	16	2584	26	317811	36	39088169
7	34	17	4181	27	514229	...	...
8	55	18	6765	28	832040	...	...
9	89	19	10946	29	1346369	...	...

TABLE II

The Hosoya index Z of a cycle with N edges

N	Z	N	Z	N	Z
3	4	5	11	7	29
4	7	6	18	.....	.....

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SAŽETAK

Izračunavanje polinoma sparivanja za fullerenske grafove

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Prikazana je nova formula za dobivanje polinoma sparivanja za fullerenske grafove.