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TOPOLOGICAL TWIN GRAPHS II[1]. ISOSPECTRAL POLYHEDRAL GRAPHS WITH NINE AND TEN VERTICES*

Haruo Hosoya,[a] Kyoko Ohta,[b] Masaki Satomi[c]

[a]Department of Information Sciences, Ochanomizu University

Bunkyo-ku, Tokyo 112-8610, Japan

[b] Taisho Pharmaceutical Co. Ltd., 403, Yoshino-Cho,

Omiya, Saitama 330-8530, Japan

[c] Ministry of Land, Infrastructure and Transport,

1-2-1 Kasumigaseki, Chiyoda-ku, Tokyo 100-8950, Japan

Abstract. After searching the characteristic quantities of 2606 and 32300 polyhedral graphs, respectively with nine and ten vertices, three and fifteen pairs of "topological twin graphs" were found, whose characteristic, distance, and Z-counting polynomials together with Z- and Wiener's w and p indices are common among each other. Isospectral triplet and quartet polyhedral graphs with nine and ten vertices were also found.

INTRODUCTION

During the systematic study [1] on the algebraic structure of polyhedral graphs we found a pair of "topological twin graphs" with eight vertices whose characteristic, Z-counting [2], and distance [3] polynomials together with the Z- [2] and Wiener [2,4] indices are all identical (Figure 1) [5]. Although there have been known a number of isospectral [6-13] or cospectral [14-16] graphs with a common characteristic polynomial, the above pair of twin graphs are believed to be the smallest pair of highly similar graphs with such properties. As a matter of fact the smallest pair of twin graphs found by Fischer have fifteen vertices and have three-fold rotational symmetry [17], while the smallest twin tree graphs found by McKay have seventeen vertices

* Dedicated to Professor A. T. Balaban for his 70 th aniversary.

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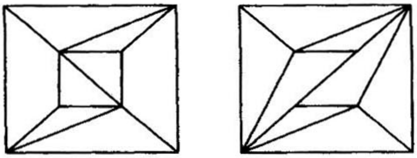


FIGURE 1. Schlegel diagrams of the topological twin polyhedral graphs with eight vertices [5].

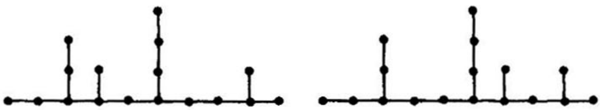


FIGURE 2. The smallest topological twin tree graphs [18]

(Figure 2) [18]. It is interesting to notice that for tree graphs due to the identity between the sets of the coefficients of the characteristic and Z-counting (or matching [19]) polynomials the chance for becoming "twin" seems to be much higher than for non-tree graphs in contrast to their actuality.

In order to analyze the secret of the highly similar property of the twin graphs we have checked our data base of larger polyhedral graphs, and could find three and fifteen pairs of topological twin graphs, respectively, with nine and ten vertices. Rather many isospectral triplet and quartet polyhedral graphs were also found, whereas up to the graphs with ten vertices no topological triplet nor quartet graphs, in the sense of topological twin graphs, was found [20].

In this paper only the network structures and characteristic quantities of the obtained graphs are presented, which provides useful information for the study of isospectral graphs [6-18]. Further, the materials given here have potential relevance to and importance in the enumeration and generation of cyclic graphs in chemistry [21] and regular graphs in graph theory [22]. Graph theoretical analysis on these interesting graphs aimed to the above problems is being under way.

GENERATION AND CALCULATION OF POLYHEDRAL GRAPHS

Generation of polyhedral graphs was performed by our own program, which can reproduce the hitherto known numbers of distinct polyhedral graphs up to eleven vertices [23-26]. The result for twelve vertices was obtained to be 6,384,636 and confirmed later by Brinkmann [27].

In this study the characteristic quantities of polyhedral graphs with nine vertices (2606 graphs) and ten vertices (32300 graphs) were calculated, and their isospectral pairing was checked. The characteristic quantities calculated are the three polynomials, i.e., characteristic, distance, and Z-counting polynomials, and Z- and Wiener's indices (path number w and polarity number p (the number of pairs of vertices connected by three consecutive walks)). Since these are all well known quantifies, their definitions are not given here [2,3,28,29].

ISOSPECTRAL PAIRS, TRIPLETS, AND QUARTETS

In our previous study it was found that there are three smallest isospectral pairs of polyhedral graphs with eight vertices [1]. It was also found that one of them have not only the same characteristic polynomial but also the same distance and Z-counting polynomials, Z-index, and both the Wiener's indices [5]. They were called the topological twin graphs (Figure 1).

Among the 2606 polyhedral graphs with nine vertices there were found 53 isospeetral pairs (See Table 1). Besides them an isospectral triplet and quartet were found. They are the smallest triplet and quartet among the polyhedral graphs.

TABLE 1. The numbers of isospectral pairs, triplets, and quartets of polyhedral graphs with eight to ten vertices.

	Isospectral		
No. of vertices	Pair	Triplet	Quartet

8	3	0	0
9	53	1	1
10	622	9	2

Their Schlegel diagrams (with a few exceptions) are shown in Figures 3 and 4, where bold lines represent the difference in the network structure within the pair of isospectral graphs. The isospectral triplet with seven vertices reported by Harary et al. [15] seems to be the smallest, but no quartet has ever been reported.

As seen in Figure 3 among the above triplet Nos. 995 and 1602 differ in only one edge bridging, while the difference between Nos. 1571 and 1602 is doubled. Then three edge moving is necessary for interchanging between the graphs Nos. 995 and 1571.

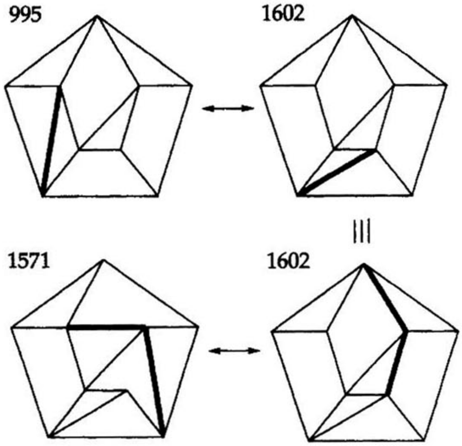


FIGURE 3. Schlegel diagrams of and similarity relations among the isospectral triplet polyhedral graphs with nine vertices. The numbers are the serial numbers generated by the authors'

algorithm. Bold lines are drawn so that the difference between a pair of graphs can be clarified.

Similarly one can observe and measure the degree of similarity or difference between each pair among the isospectral quartet graphs.

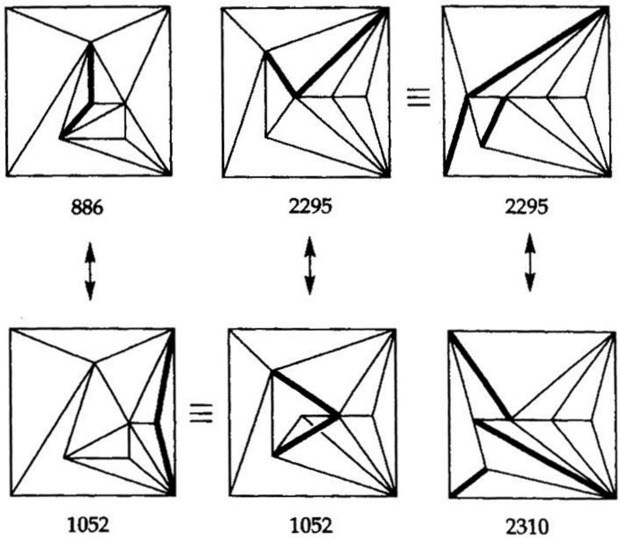
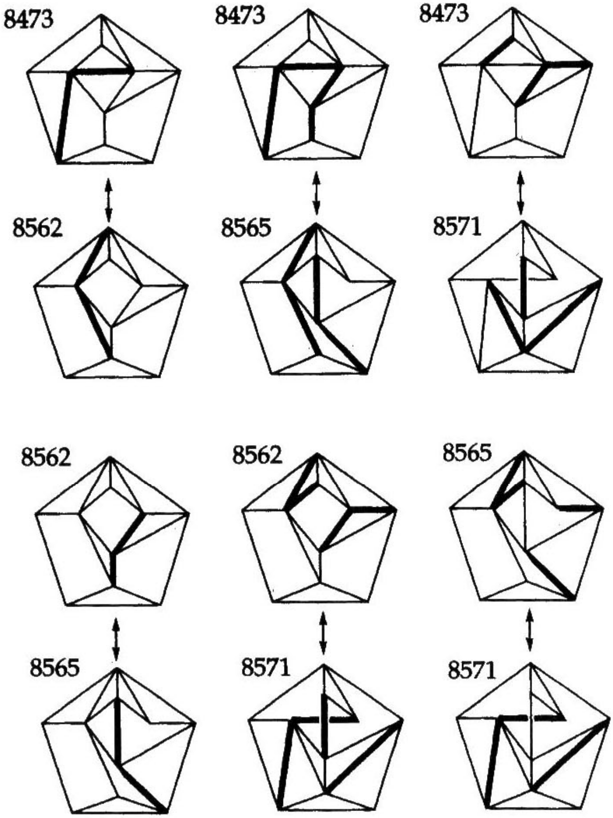
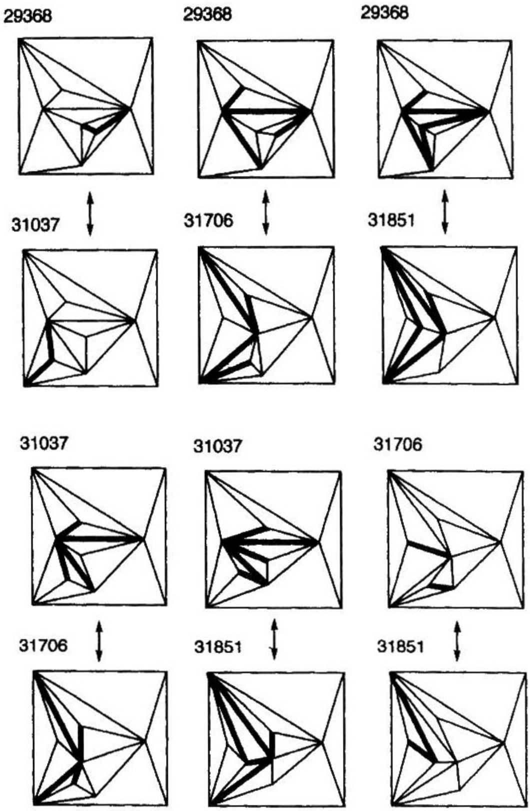


FIGURE 4. Schlegel diagrams of and similarity relations among the isospectral quartet polyhedral graphs with nine vertices. The numbers are the serial numbers generated by the authors' algorithm. Bold lines are drawn so that the difference between a pair of graphs can be clarified.

It is inferred from Table 1 that the numbers of isospectral pairs and triplets increase quite rapidly with the size of graphs, whereas there were found only two isospectral quartets with ten vertices as given in Figures 5a and 5b.



(a)



(b)

FIGURE 5. Schlegel diagrams of and similarity relations among the two sets (a) and (b) of the isospectral quartet polyhedral graphs with ten vertices.

TOPOLOGICAL TWIN GRAPHS

Among the isospectral pairs of polyhedral graphs with nine and ten vertices, respectively, three and fifteen pairs of topological twin graphs were found, whose structures and characteristic quantities are given, respectively, in Figures 6 and 7 and Tables 2 and 3. Except for one case Schlegel diagrams are drawn so that the difference of the structure within each twin can be detected. Up to this size no topological triplet nor quartet graphs was found.

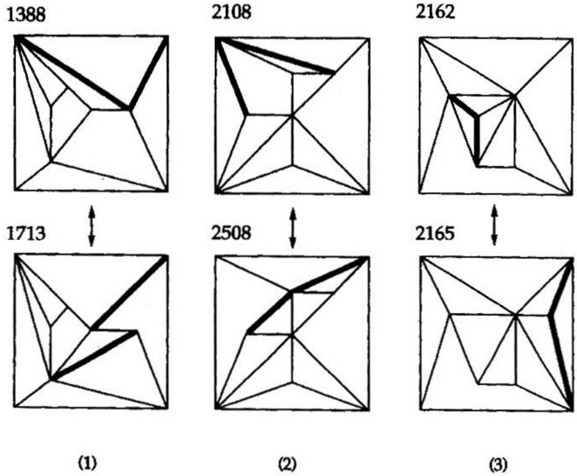


FIGURE 6 Schlegel diagrams of and similarity relations among the three sets of the topological twin polyhedral graphs with nine vertices.

TABLE 2. Characteristic quantities of topological hat' polyhedral graphs with nine vertices.

Pair 9-1

$Q_G(x) = 1 + 17x + 84x^2 + 132x^3 + 46x^4$

$\Sigma = 280 = Z \qquad w = 56 \qquad p = 1$

$P_G(x) = x^9 - 17x^7 - 12x^6 + 58x^5 + 44x^4 - 56x^3 - 40x^2 + 12x + 8$

Σ " $(\pm) = 144 = Z''$

$S_G(x) = x^9 - 98x^7 - 616x^6 - 1502x^5 - 1422x^4 + 78x^3 + 834x^2 + 268x - 48$

$\Sigma' = 2506 = Z'$

Pair 9-2

$Q_G(x) = 1 + 18x + 94x^2 + 151x^3 + 52x^4$

$\Sigma = 316 = Z \qquad w = 54 \qquad p = 0$

$P_G(x) = x^9 - 18x^7 - 18x^6 + 66x^5 + 84x^4 - 55x^3 - 78x^2 + 12x + 18$

Σ " $(\pm) = 152 = Z''$

$S_G(x) = x^9 - 90x^7 - 554x^6 - 1378x^5 - 1544x^4 - 591x^3 + 146x^2 + 96x - 10$

$\Sigma' = 3925 = Z'$

Pair 9-3

$Q_G(x) = 1 + 18x + 92x^2 + 148x^3 + 53x^4$

$\Sigma = 312 = Z \qquad w = 54 \qquad p = 0$

$P_G(x) = x^9 - 18x^7 - 20x^6 + 62x^5 + 86x^4 - 58x^3 - 94x^2 + x + 12$

$\Sigma''(\pm) = 140 = Z''$

$S_G(x) = x^9 - 90x^7 - 560x^6 - 1426x^5 - 1694x^4 - 810x^3 + 10x^2 + 97x + 12$

$\Sigma' = 4461 = Z'$

Z - ***Counting polynomial***

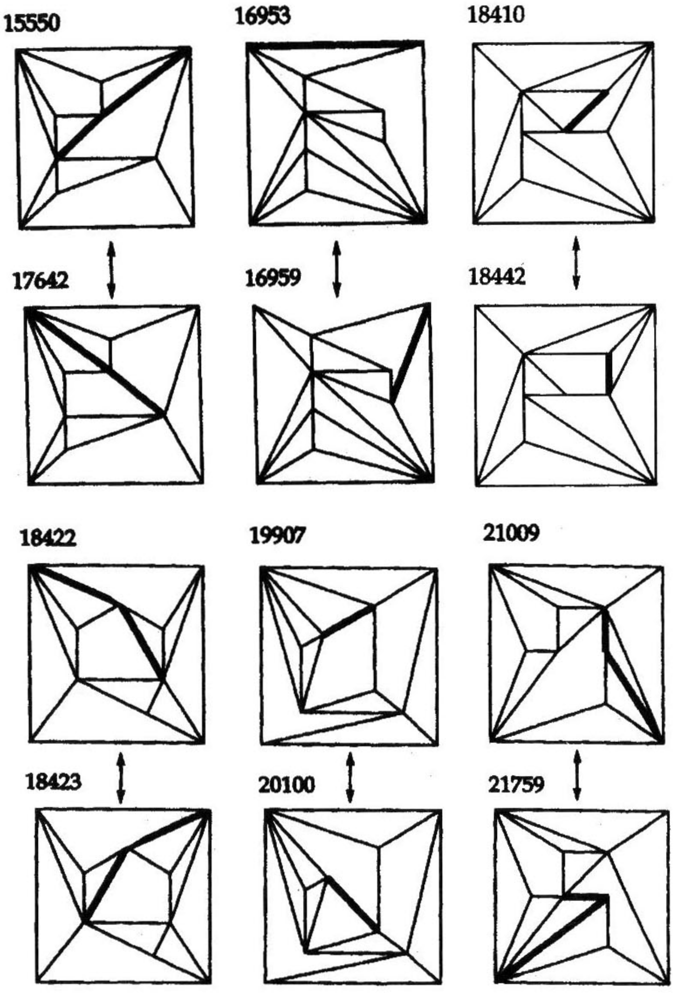
$$Q_G(x) = \sum_{k=0}^{[N/2]} p(G,k)x^k \qquad \Sigma = \sum_{k=0}^{[N/2]} p(G,k) = Q_G(1)$$

Characteristic polynomial

$$P_G(x) = (-1)^N \det(A - xE) = \sum_{k=0}^{N} a_k x^{N-k} \qquad \Sigma''(\pm) = \sum_{k=0}^{[N/2]} (-1)^k a_{2k} = \tilde{Z}$$

Distance polynomial

$$S_G(x) = (-1)^N \det(D - xE) = \sum_{k=0}^{N} b_k x^{N-k} \qquad \Sigma = -\sum_{k=0}^{N} b_k$$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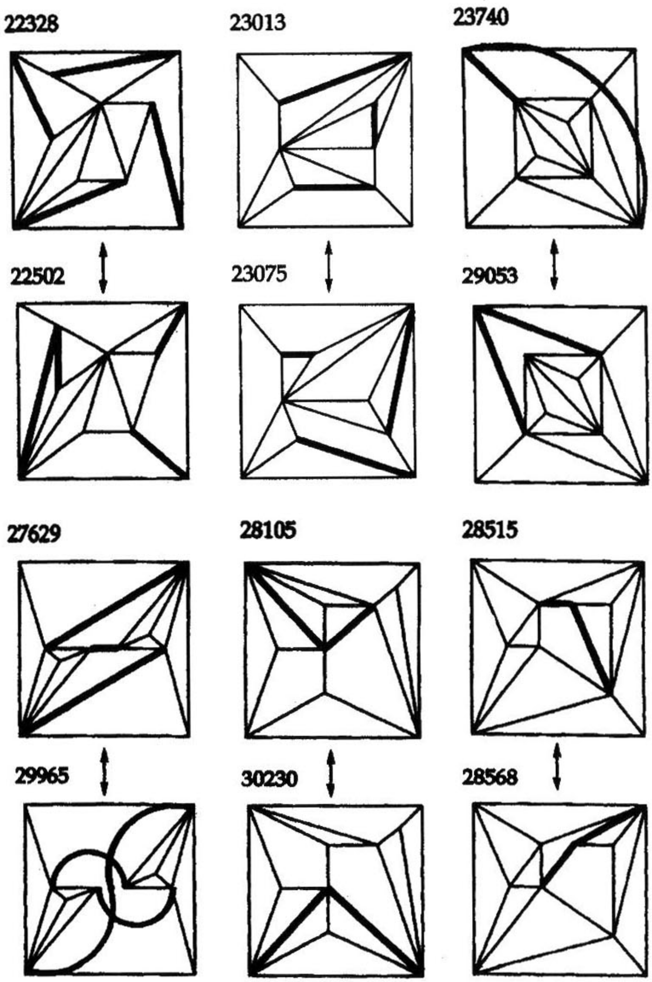
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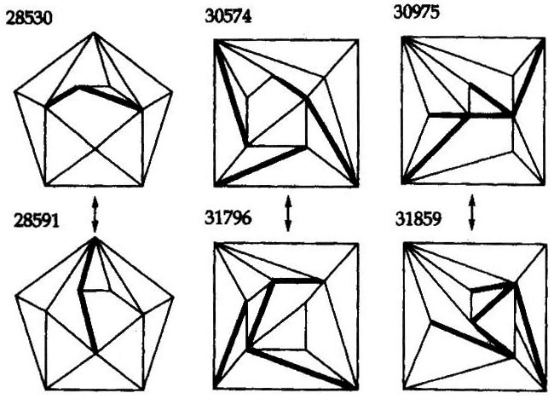

FIGURE 7. Schlegel diagrams of and similarity relations among the fifteen sets of the topological twin polyhedral graphs with ten vertices.

CALCULATION OF HÜCKEL MOLECULAR ORBITALS

In general it is rather difficult to draw proper Schlegel diagrams for clarifying the difference in the network structure of a pair of non-tree graphs with many faces as given in Figures 3-7. In order to draw these figures the "bond order matrix" was utilized, which is almost routinely calculated by available programs of the Hückel molecular orbital (HMO) method [30]. Note that almost all the polyhedral graphs are non-bipartite. Then the charge density distribution of each graph formally obtained from HMO calculation is not uniform. Inspection of the results for isospectral pair of graphs reveals that for each pair the charge densities on the vertices of topologically similar environment tend to take exactly the same value. Further analysis of the origin of the highly similar properties of these isospectral and twin graphs is in progress along this line.

TABLE 3. Characteristic quantities of topological twin polyhedral graphs with ten vertices.

Pair 10-1

$Q_G(x) = 1 + 20x + 125x^2 + 279x^3 + 188x^4 + 16x^5$

$\Sigma = 629 = Z \quad w = 72 \quad p = 2$

$P_G(x) = x^{10} - 20x^8 - 16x^7 + 97x^6 + 94x^5 - 149x^4 - 144x^3 + 48x^2 + 32x$

$\Sigma''(\pm) = 315 = Z''$

$S_G(x) = x^{10} - 130x^8 - 964x^7 - 2892x^6 - 3890x^5 - 1541x^4 + 1320x^3 + 1204x^2 + 96x - 80$

$\Sigma' = 6877 = Z'$

Pair 10-2

$Q_G(x) = 1 + 21x + 134x^2 + 301x^3 + 201x^4 + 18x^5$

$\Sigma = 676 = Z \quad w = 71 \quad p = 2$

$P_G(x) = x^{10} - 21x^8 - 26x^7 + 92x^6 - 168x^5 - 61x^4 - 288x^3 - 71x^2 + 30x + 8$

$\Sigma''(\pm) = 96 = Z''$

$S_G(x) = x^{10} - 127x^8 - 932x^7 - 2859x^6 - 4336x^5 - 3126x^4 - 696x^3 + 244x^2 + 108x + 7$

$\Sigma' = 11717 = Z'$

Pair 10-3

$Q_G(x) = 1 + 20x + 125x^2 + 278x^3 + 184x^4 + 16x^5$

$\Sigma = 624 = Z \quad w = 71 \quad p = 1$

$P_G(x) = x^{10} - 20x^8 - 16x^7 + 99x^6 + 94x^5 - 170x^4 - 160x^3 + 84x^2 + 80x + 12$

$\Sigma''(\pm) = 362 = Z''$

$S_G(x) = x^{10} - 125x^8 - 924x^7 - 2803x^6 - 3872x^5 - 1668x^4 + 1180x^3 + 1119x^2 + 92x - 68$

$\Sigma' = 7069 = Z'$

Pair 10-4

$Q_G(x) = 1 + 20x + 125x^2 + 278x^3 + 186x^4 + 16x^5$

$\Sigma = 626 = Z \qquad w = 72 \qquad p = 2$

$P_G(x) = x^{10} - 20x^8 - 16x^7 + 97x^6 + 98x^5 - 142x^4 - 168x^3 + 24x^2 + 56x + 12$

$\Sigma^{''}(\pm) = 272 = Z''$

$S_G(x) = x^{10} - 130x^8 - 960x^7 - 2849x^6 - 3746x^5 - 1409x^5 + 1210x^3 + 1020x^2 + 64x - 68$

$\Sigma^{'} = 6868 = Z^{'}$

Pair 10-5

$Q_G(x) = 1 + 20x + 125x^2 + 278x^3 + 186x^4 + 18x^5$

$\Sigma = 628 = Z \qquad w = 72 \qquad p = 2$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 97x^6 + 120x^5 - 122x^4 - 176x^3 + 32x^2 + 72x + 12$

$\Sigma^{''}(\pm) = 260 = Z''$

$S_G(x) = x^{10} - 130x^8 - 966x^7 - 2935x^6 - 4138x^5 - 2099x^4 + 920x^3 + 1452x^2 + 536x + 60$

$\Sigma^{'} = 8377 = Z^{'}$

Pair 10-6

$Q_G(x) = 1 + 20x + 124x^2 + 270x^3 + 172x^4 + 14x^5$

$\Sigma = 601 = Z \qquad w = 72 \qquad p = 2$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 96x^6 + 118x^5 - 130x^4 - 196x^3 + 8x^2 + 56x + 12$

$\Sigma^{''}(\pm) = 243 = Z''$

$S_G(x) = x^{10} - 130x^8 - 966x^7 - 2935x^6 - 4138x^5 - 2099x^4 + 920x^3 + 1452x^2 + 536x + 60$

$\Sigma^{'} = 7300 = Z^{'}$

Pair 10-7

$Q_G(x) = 1 + 20x + 121x^2 + 256x^3 + 159x^4 + 12x^5$

$\Sigma = 569 = Z \qquad w = 71 \qquad p = 1$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 85x^6 + 94x^5 - 102x^4 - 116x^3 + 31x^2 + 32x$

$\Sigma^{''}(\pm) = 239 = Z''$

$S_G(x) = x^{10} - 125x^8 - 934x^7 - 2900x^6 - 4186x^5 - 1995x^4 + 1342x^3 + 1600x^2 + 296x - 68$

$\Sigma^{'} = 6970 = Z^{'}$

Pair 10-8

$Q_G(x) = 1 + 20x + 121x^2 + 257x^3 + 163x^4 + 14x^5$

$\Sigma = 576 = Z \qquad w = 71 \qquad p = 1$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 85x^6 + 92x^5 - 111x^4 - 130x^3 + 23x^2 + 32x$

$\Sigma''(\pm) = 240 = Z''$

$S_G(x) = x^{10} - 125x^8 - 934x^7 - 2896x^6 - 4164x^5 - 1950x^4 + 1386x^3 + 1620x^2 + 296x - 68$

$\Sigma' = 6835 = Z'$

Pair 10-9

$Q_G(x) = 1 + 22x + 148x^2 + 346x^3 + 236x^4 + 20x^5$

$\Sigma = 733 = Z \qquad w = 70 \qquad p = 2$

$P_G(x) = x^{10} - 22x^8 - 28x^7 + 96x^6 + 176x^5 - 72x^4 - 256x^3 - 80x^2 + 32x$

$\Sigma''(\pm) = 111 = Z''$

$S_G(x) = x^{10} - 124x^8 - 896x^7 - 2667x^6 - 3824x^5 - 2310x^4 + 280x^3 + 1076x^2 + 480x + 64$

$\Sigma' = 7921 = Z'$

Pair 10-10

$Q_G(x) = 1 + 21x + 136x^2 + 303x^3 + 193x^4 + 13x^5$

$\Sigma = 667 = Z \qquad w = 70 \qquad p = 1$

$P_G(x) = x^{10} - 21x^8 - 24x^7 + 100x^6 + 176x^5 - 63x^4 - 228x^3 - 45x^2 + 72x + 27$

$\Sigma''(\pm) = 113 = Z''$

$S_G(x) = x^{10} - 122x^8 - 888x^7 - 2719x^6 - 4116x^5 - 2900x^4 - 492x^3 + 352x^2 + 96x - 12$

$\Sigma' = 10801 = Z'$

Pair 10-11

$Q_G(x) = 1 + 20x + 124x^2 + 270x^3 + 172x^4 + 14x^5$

$\Sigma = 601 = Z \qquad w = 71 \qquad p = 1$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 96x^6 + 114x^5 - 134x^4 - 188x^3 + 16x^2 + 56x + 12$

$\Sigma''(\pm) = 255 = Z''$

$S_G(x) = x^{10} - 125x^8 - 926x^7 - 2846x^6 - 4130x^5 - 2267x^4 + 640x^3 + 1020x^2 + 136x - 68$

$\Sigma' = 8566 = Z'$

Pair 10-12

$Q_G(x) = 1 + 21x + 138x^2 + 321x^3 + 222x^4 + 20x^5$

$\Sigma = 723 = Z \quad w = 70 \quad p = 1$

$P_G(x) = x^{10} - 21x^8 - 20x^7 + 104x^6 + 128x^5 - 149x^4 - 202x^3 + 40x^2 + 80x + 16$

$\Sigma^{''}(\pm) = 299 = Z''$

$S_G(x) = x^{10} - 122x^8 - 880x^7 - 2584x^6 - 3422x^5 - 1406x^4 + 850x^3 + 684x^2 + 24x - 36$

$\Sigma^{'} = 6892 = Z^{'}$

Pair 10-13

$Q_G(x) = 1 + 20x + 125x^2 + 276x^3 + 182x^4 + 16x^5$

$\Sigma = 620 = Z \quad w = 71 \quad p = 1$

$P_G(x) = x^{10} - 20x^8 - 18x^7 + 101x^6 + 126x^5 - 156x^4 - 246x^3 + 20x^2 + 112x + 32$

$\Sigma^{''}(\pm) = 266 = Z''$

$S_G(x) = x^{10} - 125x^8 - 918x^7 - 2776x^6 - 3952x^5 - 2237x^4 + 276x^3 + 723x^2 + 208x + 16$

$\Sigma^{'} = 8785 = Z^{'}$

Pair 10-14

$Q_G(x) = 1 + 21x + 138x^2 + 321x^3 + 222x^4 + 20x^5$

$\Sigma = 723 = Z \quad w = 70 \quad p = 1$

$P_G(x) = x^{10} - 21x^8 - 20x^7 + 104x^6 + 130x^5 - 155x^4 - 242x^3 + 16x^2 + 104x + 28$

$\Sigma^{''}(\pm) = 269 = Z''$

$S_G(x) = x^{10} - 122x^8 - 876x^7 - 2541x^6 - 3292x^5 - 1300x^4 + 810x^3 + 639x^2 + 12x - 36$

$\Sigma^{'} = 6706 = Z^{'}$

Pair 10-15

$Q_G(x) = 1 + 21x + 136x^2 + 303x^3 + 190x^4 + 14x^5$

$\Sigma = 665 = Z \quad w = 69 \quad p = 0$

$P_G(x) = x^{10} - 21x^8 - 22x^7 + 102x^6 + 148x^5 - 135x^4 - 270x^3 - 16x^2 + 108x + 36$

$\Sigma^{''}(\pm) = 207 = Z''$

$S_G(x) = x^{10} - 117x^8 - 850x^7 - 2598x^6 - 3876x^5 - 2551x^4 + 174x^3 + 472x^2 + 92x - 20$

$\Sigma^{'} = 9622 = Z^{'}$

REFERENCES

[1] M. Omote, M. Wakamatsu, S. Hyugaji, U. Nagashima, H. Hosoya, *Natl. Sci. Rept. Ochanomizu University,* **1994**, *45*, 29-65.

[2] H. Hosoya, *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332-2339.

[3] H. Hosoya, M.Murakami, M. Gotoh, *Natl. Sci. Rept. Ochanomizu Univ.* **1973**, *24*, 27-34.

[4] H. Wiener, *J. Am. Chem. Soc.* **1947**, *69*, 17-20.

[5] H. Hosoya, U. Nagashima, S. Hyugaji, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 428-431.

[6] K. Mizutani, K. Kawasaki, H. Hosoya, *Natl. Sci. Rept. Ochanomziu Univ.* **1971**, *22*, 39-58.

[7] K. Kawasaki, K. Mizutani, H. Hosoya, *Natl. Sci. Rept. Ochanomziu Univ.* **1971**, *22*, 181-214.

[8] A. T. Balaban, F. Harary, *J. Chem. Doc.* **1971**, *11*, 258-259.

[9] I. Gutman, N. Trinajstić, *Top. Curr. Chem.* **1973**, *42*; 49-93.

[10] W. C. Herndon, *Tetrahedron Lett.* **1974**, 671-674.

[11] T. Živković, N. Trinajstić, M. Randić, *Mol. Phys.* **1975**, *30*, 517-533.

[12] M. Randić, N. Trinajstić, T. Živković, *J. Chem. Soc. Faraday Trans.* 2, **1976**, *72*, 244-256.

[13] Y. Jiang, C. Liang, *Croat. Chem. Acta,* **1995**, *68*, 343-357.

[14] V. L. Collatz, U. Sinogowitz, *Abh. Math. Sem. Univ. Hamburg,* **1957**, *21*, 6~77.

[15] F. Harary, C. King, A. Mowshowitz, R.C. Read, *Bull. London Math. Soc.* **1971**, *3*, 321-328.

[16] D. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs: Theory and Application,* Academic Press, Berlin (1980).

[17] M. E. Fischer, *J. Comb. Theory, B.* **1966**, 105-125.

[18] B. D. McKay, *Ars. Combinatorica,* **1977**, *3*, 219-232.

[19] E. Farrell, *J. Comb.* Theory, B. **1979**, *26*, 75-86 .

[20] Preliminary results were presented in 19th Symposium on Information Chemistry, Osaka, Japan (1996), and in 7th International Symposium on Mathematical Chemistry, Girona, Spain (1997).

[21] A. T. Balaban, Enumeration of cyclic graphs, in *Chemical Applications of Graph Theory,* A. T. Balaban, Ed., Academic Press, London, 1976, pp.63-105.

[22] A.T. Balaban, *J. Comb. Theory,* B. **1972**, *12*, 1-5.

[23] A. A. Britton, J.D. Dunitz, *Acta Crystallogr. A.* **1973**, *29*, 362-371.

[24] P J. Federico, *Geom. Dedicata, B*, **1975**, *3*, 469-481.

[25] P. Engel, *Discrete Math.* **1982**, *41*, 215-218.

[26] R. C. Read, R. J. Wilson, *An Atlas of Graphs,* Oxford Univ. Press, New York, 1998.

[27] C. Brinkmann, Private communication. See also C. Brinkmann, *J. Graph Theory,* **1996**, *23*, 139-149.

[28] L. B. Kier, L. H Hall, *Molecular Connectivity in Chemistry and Drug Research,* Academic Press, New York, 1976.

[29] N. Trinajstić, *Chemical Graph Theory,* CRC Press, Boca Raton, FL, 1983.

[30] A. Streitwieser, Jr., *Molecular Orbital Theory for Organic Chemists,* John Wiley, New York, 1961.