Topological Twin Graphs. Smallest Pair of Isospectral Polyhedral Graphs with Eight Vertices

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A novel pair of isospectral nonahedral graphs with eight vertices were found, which not only have the same characteristic polynomial, $P_G(x)$, but also have the same distance polynomial, $S_G(x)$, and the same polygonal ($f_3 = 6, f_4 = 3$) and vertex degree ($v_3 = 4, v_4 = 2, v_5 = 2$) distributions, contrary to the observation that almost all the reported pairs of isospectral graphs do not have common topological factors other than $P_G(x)$. Many of their topological indices, such as Z and W, were found to have common values. The only structural difference between this pair of "topological twin graphs" is in the distribution of edge types, namely, the degrees of the two vertices defining an edge. The newly found pair of graphs are the smallest topological twin graphs and also the smallest isospectral polyhedral graphs. The spectra of $P_G(x)$ and $S_G(x)$ of them are also discussed.

INTRODUCTION

Aside from the new wave in fullerene chemistry, a vast number of polyhedral units have long been observed in inorganic molecules and crystals, such as elementary boron and borane families and metal complexes. Most of those polyhedra are composed of a relatively small number of vertices, around ten, and of smaller polygons with three to five edges.[1] Complete catalogues of non-isomorphic convex polyhedra with eight or fewer vertices were published by Britton and Dunitz[2] and Federico.[3,4] Although interesting topological and geometrical features of several classes of polyhedral graphs related to chemical substances and phenomena have been clarified by graph-theoretical analyses,[5] no systematic analysis seems to have been performed for the group of polyhedra, "3,4,5-hedra", whose faces are limited to only 3–5-gons.

During the course of the study on the characterization of the lower numbers of 3,4,5-hedral groups we found such a novel pair of nonahedral graphs, A and B, with eight vertices (see Figure 1) that are isospectral,[6–11] or cospectral,[12,13] with respect not only to the characteristic polynomial, $P_G(x)$, but also to the distance polynomial, $S_G(x)$.[14,15] The pair of isospectral nonahedra were found in 182 3,4,5-polyhedral graphs which were picked up from the catalog of non-isomorphic convex polyhedra with eight or fewer vertices.[2] The nonahedra, A and B, correspond to the 172th and 167th graphs drawn in Figure 4 of ref 2.

As seen in Table 1, both of these two nonahedral graphs have six triangles ($f_3 = 6$) and three tetragons ($f_4 = 3$) and have the same vertex degree distribution, namely, $v_3 = 4$, $v_4 = 2$, and $v_5 = 2$. The topological difference between them is evident from the Schlegel diagrams shown in Figure 1. That is, the two v_5 vertices in A and B are, respectively, adjacent to and separated from each other. Thus, when one denotes the type of an edge with respect to its two terminal vertex degrees of v_j and v_k as $e(j,k)$, A and B have different $e(j,k)$ distributions, as in Table 1.

Despite this difference the newly found pair of graphs also has the same matching polynomial,[16–18] $\alpha_G(x)$, Z-counting polynomial,[19] Z-index,[19] Wiener number,[20] and many other topological indices.[11,21] We call such a pair of highly similar graphs that have common (a) vertex and face distributions, (b) $P_G(x)$, $S_G(x)$, and $\alpha_G(x)$ polynomials, and (c) Z and W indices as topological twin graphs. If more than two non-isomorphic graphs have the above property, they may be called topological multiplet graphs.

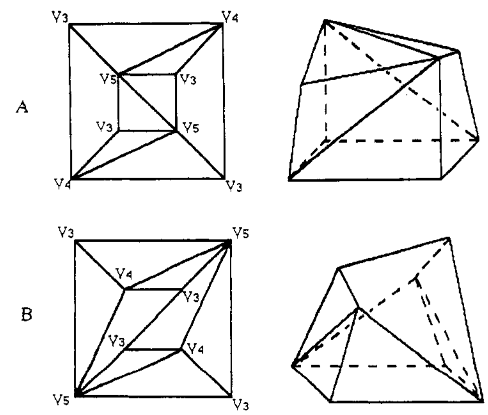

Figure 1. Schlegel diagrams and three-dimensional stereo pictures of the pair of isospectral nonahedra.

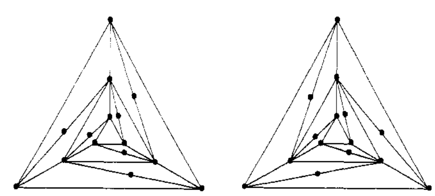

Figure 2. Fisher's smallest topological twin graphs.[22]

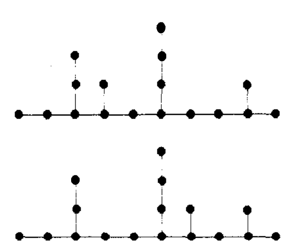

Figure 3. Smallest topological twin tree graphs.[23]

In the classical paper on the isospectral graphs Fisher introduced interesting pairs of graphs with $5n$ ($n \geq 3$) vertices.[22] We found that they are really topological twins, though no one, including Fisher himself, was aware of this fact. In Figure 2 the smallest pair of them are shown. On the other hand,

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Table 1. Topological Parameters of Isospectral Nonahedra

vertices	$V = 8$	$v_3 = 4$	$v_4 = 2$	$v_5 = 2$	
faces	$F = 9$	$f_3 = 6$	$f_4 = 3$		
edges	$E = 15$				
A		$e(3,4) = 6$	$e(3,5) = 6$	$e(4,5) = 2$	$e(5,5) = 1$
B	$e(3,3) = 1$	$e(3,4) = 4$	$e(3,5) = 6$	$e(4,5) = 4$	

non-adjacent number					
k	0	1	2	3	4
$p(G,k)$	1	15	61	65	9

topological index $Z = 1 + 15 + 61 + 65 + 9 = 151$

Z-counting polynomial $Q_G(x) = 1 + 15x + 61x^2 + 65x^3 + 9x^4$

symmetry C_2

distance matrix

$$\mathbf{D}(A) = \begin{bmatrix} 0&1&1&2&2&2&1&2\\ 1&0&1&1&2&2&2&1\\ 1&1&0&1&1&1&2&2\\ 2&1&1&0&2&1&2&2\\ 2&2&1&2&0&1&1&2\\ 2&2&1&1&1&0&1&1\\ 1&2&2&2&1&1&0&1\\ 2&1&2&2&2&1&1&0 \end{bmatrix} \quad \mathbf{D}(B) = \begin{bmatrix} 0&1&1&2&2&2&1&2\\ 1&0&1&1&2&1&2&1\\ 1&1&0&1&2&2&1&2\\ 2&1&1&0&1&2&2&2\\ 2&2&2&1&0&1&1&2\\ 2&1&2&2&1&0&1&1\\ 1&2&1&2&1&1&0&1\\ 2&1&2&2&2&1&1&0 \end{bmatrix}$$

distance polynomial $S_G(x) = x^8 - 67x^6 - 340x^5 - 643x^4 - 436x^3 + 21x^2 + 76x - 7$

Wiener number $W = 1 \times 15 + 2 \times 13 = 41$

characteristics polynomial $P_G(x) = x^8 - 15x^6 - 12x^5 + 41x^4 + 28x^3 - 35x^2 - 12x + 9$

McKay found the smallest pair of tree graphs with 17 vertices having the same distance polynomials (see Figure 3).[23] Interestingly enough, we found that this pair of graphs is also topological twins. From these observations one can say that our newly found pair of graphs is the smallest topological twins. Preliminary but exciting results of them will be described in this paper.

ISOSPECTRAL GRAPHS, TOPOLOGICAL GRAPHS, AND TOPOLOGICAL TWIN GRAPHS

Although it has been known that neither the characteristic polynomial, $P_G(x)$, nor its spectrum uniquely determines the topological structure of a graph, the isospectrality concept has widely attracted the interest of theoretical physicists, mathematical chemists, and applied mathematicians.[11,22,23] In this paper we are concerned only with the connected nondirected graphs without a loop and a multiple or weighted edge.

Connected graphs can be classified into three types: (i) tree, (ii) nontree bipartite, and (iii) nontree nonbipartite graphs. For type i all the isospectral pairs have common Z values and $\alpha_G(x)$, since $\alpha_G(x)$ is exactly equal to $P_G(x)$ in this case. The pair of graphs found by McKay is the smallest topological twin tree graphs. Recently Jiang and Liang[24] extensively studied the algorithm generating the isospectral graphs of type ii, but they all have a branch or branches. Very recently Babic found the family of isospectral polyhex graphs with an odd number of vertices,[25] but they do not have the twin property. Thus it is an open question if there exist topological twin graphs of type ii.

Among the topological twin graphs found by Fisher[22] the smallest ones have 3-fold symmetry, as shown in Figure 2. By factoring out their component units with five vertices, he showed that all the derived twins of n-fold symmetry ($n \geq 3$) are isospectral. Since there is a mistype in his paper, the corrected result is given here.

$$P_G(x) = (x^2 - 2(\cos(k\theta))x - 1)\{x^3 - 4(\cos(k\theta))x^2 + (4(\cos^2(k\theta)) - 5)x + 2\cos(k\theta)\}$$

with

$$\theta = 2\pi/n \quad k = 1, 2, ..., n$$

From the structure of their distance matrices all the higher members are also expected to be topological twins. For $n = 2$ some edges are forced to have weight 2, and these twins jump out from our category. Note that both Fisher's and our twins have a common homeomorphic skeleton, C, or two fused triangles. By using n C's as units, one can construct a pair of larger graphs with n-fold symmetry as Fisher did. However, it was shown that the topological twins are born only when $n = 2$ in this case. From these considerations it is highly probable that A and B are the smallest topological twin graphs.

Another interesting feature of our topological twin graphs is that they are the only observed isospectral pairs of graphs that can represent polyhedra. A polyhedral graph is a planar graph whose vertex degrees are all equal to or larger than 3. We can say that our topological twins are the only known polyhedral isospectral pairs of graphs.

PROPERTIES OF THE SMALLEST TOPOLOGICAL TWIN GRAPHS

In Figure 1 the three-dimensional stereoviews of A and B are also drawn together with their Schlegel diagrams, from which one can easily discern the C_2 axes of and the topological difference between the twin graphs.

The characteristic polynomial, $P_G(x)$, for graph G with N vertices has been defined in terms of the adjacenty matrix **A** and unit matrix **E** as

$$P_G(x) = (-1)^N \det(\mathbf{A} - x\mathbf{E}) = \sum_{k=0}^{N} a_k x^{N-k}$$

In analogy with $P_G(x)$ the distance polynomial, $S_G(x)$, was proposed to be defined by one of the present authors[14] in terms of the distance matrix, **D**, as

$$S_G(x) = (-1)^N \det(\mathbf{D} - x\mathbf{E}) = \sum_{k=0}^{N} b_k x^{N-k}$$

where the D_{jk} element is the number of the shortest steps between vertices j and k.

By using the C_2 symmetry of A and B, both $P_G(x)$ and $S_G(x)$ can be factored out into the products of the symmetrically and antisymmetrically modified skeletons of C as follows:

$$P_A(x) = P_B(x) = (x^4 + x^3 - 3x^2 - x + 1)(x^4 - x^3 - 11x^2 - 3x + 9)$$

$$S_A(x) = S_B(x) = (x^4 + 7x^3 + 15x^2 + 9x - 1)(x^4 - 7x^3 - 33x^2 - 13x + 7)$$

The Z-counting polynomial $Q_G(x)$ and matching polynomial $\alpha_G(x)$ are defined in terms of the non-adjacent numbers, $p(G,k)$'s, as[19]

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

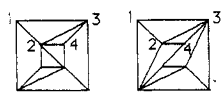
$$\alpha_G(x) = \sum_{k=0}^{[N/2]} p(G,k)x^{N-2k}$$

The topological index Z has been defined also by using p-

Table 2. Spectra and Eigenvectors of the Topological Twin Graphs[a]

	1 S	2 A	3 S	4 A	5 A	6 S	7 A	8 S
				spectrum (eigenvalue)				
	3.880 14	1.355 67	0.773 17	0.477 26	–0.737 64	–1.246 42	–2.095 29	–2.406 89
				Eigenvectors of A				
b								
1	0.292 04	0.220 68	0.441 37	0.542 85	0.299 16	0.202 83	0.259 08	–0.422 81
2	0.441 37	0.299 16	–0.292 04	0.259 08	–0.220 68	0.422 81	–0.542 85	0.202 83
3	0.345 89	0.484 06	0.316 65	–0.160 12	–0.357 06	–0.337 81	0.335 50	0.407 41
4	0.316 65	0.357 06	–0.345 89	–0.335 50	0.484 06	–0.407 41	–0.160 12	–0.337 81
				Eigenvectors of B				
b		*		*	*		*	
1	0.316 65	0.357 06	0.345 89	–0.335 50	0.484 06	–0.407 41	–0.160 12	–0.337 81
2	0.373 64	0.484 06	0.005 99	–0.160 12	–0.357 06	0.529 69	0.335 50	–0.282 46
4	0.278 16	0.299 16	–0.602 69	0.259 08	–0.220 68	–0.230 92	–0.542 85	–0.077 87
3	0.427 49	0.220 68	0.130 72	0.542 85	0.299 16	–0.010 94	0.259 08	0.547 76

[a] Symmetry type of the eigenvector with respect to C_2 axis: S (symmetric), A (antisymmetric). [b] Vertex numbers are given below. Note the bold faced number of B, and the symmetrical patterns of the vectors for A and B marked with an asterisk. See also the pairing patterns between the vectors joined together with arrows.



(G,k)'s as

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

The Wiener number W has been defined[20] as the half-sum of the off-diagonal elements of **D**, or

$$W = \sum_{j<k} D_{jk}$$

A number of topological indices have been proposed to distinguish or characterize the topological nature of graphs.[11,21] The topological index which is derived or related to the adjacency or distance matrix would be the same within the pair of the topological twin graphs. However, such an index that is calculated from the edge types $e(j,k)$'s may discriminate the twins. Actually this is the case with the connectivity index, $\chi_R(G) = \sum_{j<k} e(j,k)^{-1/2}$, proposed by Randic.[26] Namely, for this pair of graphs $\chi_R(A) = 3.9285$ and $\chi_R(B) = 3.9317$, but still the difference is very small.

Johnson and Newman[27] proposed to distinguish isospectral pairs by substituting $(x,0,1)$ in $(\mathbf{A} - x\mathbf{E})$ with $(\lambda,1,x)$. However, one could not distinguish between A and B by this substitution but got

$$P_G(\lambda,x) = (1 - 8x - 4x^2 + 74x^3 - 62x^4 - 108x^5 + 157x^6 - 66x^7 + 9x^8) - (4 + 32x - 168x^2 + 72x^3 + 300x^4 - 208x^5 + 4x^6 + 12x^7)\lambda - (28 - 138x + 54x^2 + 156x^3 + 223x^4 - 218x^5 + 35x^6)\lambda^2 + (16 + 60x - 128x^2 - 256x^3 + 56x^4 + 28x^5)\lambda^3 + (34 - 88x - 65x^2 - 132x^3 + 41x^4)\lambda^4 - (8 + 40x + 52x^2 + 12x^3)\lambda^5 - (13 + 15x^2)\lambda^6 + \lambda^8$$

which also shows that our twin graphs are strongly similar to each other.

SIMILARITY OF EIGENVECTORS FOR THE TOPOLOGICAL TWINS

The eigenvalues (spectra) and eigenvectors of A and B are given in Table 2, where the order of the row numbers for B is intentionally changed. The eigenvectors are either symmetric (S) or antisymmetric (A) with respect to the C_2 rotation. One can observe the highly symmetrical structure in them as follows: (i) All the A-type eigenvectors with the same eigenvalue of the twins are composed of the same set of coefficients but differ only in the distribution over the vertices. Namely, the coefficients for B can be obtained as the mirror image of A with respect to the asterisk. (ii) All the A-type vectors of A and B can find their counterpart within the vectors of the same graph, as the pair of bonding and antibonding MO's of a heteropolar diatomic molecule. (iii) For the graph A but not for B similar relation can be found in the S-type vectors.

Although detailed analysis of these pairing relations is not yet complete, one can say that for a symmetrical pair of eigenvectors of A and B the magnitude of the coefficient is strongly dependent on the vertex degree. Namely, the symmetrical relation of the vectors between A and B always appears at vertices with the same degree.

At present the newly found topological twin graphs cannot find promising application to chemical problems, they might have strongly shaken the famous problem of "Can one hear the shape of a drum?" raised by Kac.[22,28,29]

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