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Dormant and Sprouts Generating Isospectral Tree Graphs. I. Facts

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Abstract

A "multiplet dormant" graph is defined as a (tree) graph which can generate infinite series of isospectral (IS) pair graphs by adding the same graph fragments to each of the two sets of "multiplet sprouts" attached to the component vertices in it. In this paper a number of multiplet dormants are introduced. The highest multiplicity which has been found is nine. Almost all the IS tree graph pairs composed of more than eight vertices are shown to be generated from the dormants, among which the smallest one has only five vertices. Thus the conventionally proposed endospectral graph is found to be just a singlet dormant. Almost all the findings in this work have been gained without computer search but by using the *Z* index and *Z*-counting polynomial proposed by the present author.

1. Introduction

Although analysis of isospectral (or cospectral) graphs has been recognized as an important issue not only in graph theory [1,2] but also in mathematical chemistry [3], no dramatic progress has been attained as to explore and widen the concept of endospectral graphs (ESG) [4-7] especially in the domain of tree graphs. For example, although the hitherto known smallest IS tree pair is **1** and **2** of N=8 [8-10], and four and fivc IS pairs were found for N=9 and 10 [10], respectively, only one pair **4** and **5** has been shown to be related to the smallest ESG **3** as shown in Fig. 1 [8].

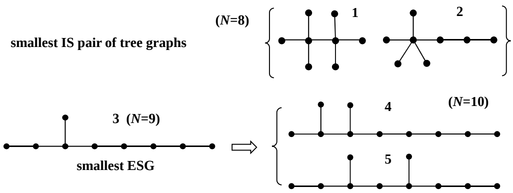


Figure 1. Smallest IS tree pair and smallest ESG.

Furthermore, although so many ESG's have been discovered by computer search, only sporadic discussions have been reported for them [1-9, 11].

However, very recently the present author showed that "topological scrutinization" by the aid of the *Z*-index and *Z*-counting polynomial, $Q_G(x)$ [12,13], is useful and practical for analyzing and unifying chemico-mathematical features of IS graphs [14]. There we found an interesting tree graph **6** with two pairs of "sprout" vertices, * and # (See Fig. 2). By adding an edge at both of * vertices one can obtain graph **7**, which is IS to **8** obtained by adding an edge at both of # vertices of **6**. The *Z*-indices given here are found to have a steering role for this kind of IS analysis. Incidentally these two graphs, **7** and **8**, have been known as the smallest IS conjugated acyclic polyene pair, or in mathematical term, as the smallest pair of "cospectral" trees with a 1-factor [3]. However, they have never been discussed in the conventional theory of ESG's, all of which carry only a pair of endospectral vertices to generate IS pairs.

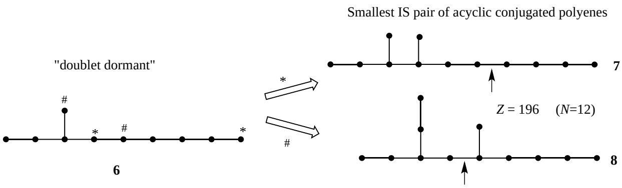


Figure 2. Smallest IS pair of acyclic conjugated polyenes can be derived from "doublet dormant."

Let us call a graph such as **6** "doublet dormant" with two "doublet sprouts." As will be explained in detail in this paper, the smallest IS pair, **1** and **2**, were found to be derived from the triplet dormant of N=5, which eventually works also as quadruplet, sextuplet, and heptuplet dormants. In this sense all the ESG's hitherto have been discussed are nothing else but singlet dormants with a pair of sprouts. Namely, the smallest ESG **3** is now turned out to be the smallest singlet dormant. Thus the concept of the multiplet dormant encompasses that of the conventional ESG and the related discussions.

In this series of papers a number of multiplet dormants with two sets of multiplet (up to nonuplet!) sprouts will be introduced and discussed. In I, "Facts," a variety of multiplet dormants and sprouts are introduced without sophisticated discussion but using only Z-indices and Z-counting polynomial proposed by the present author [12,13]. In II, "Theory," mathematical analysis is given for singlet and doublet dormants, followed by optimistic conjectures and expectations which were found to be useful for discovering highly multiplet dormants with entangled mathematical structure.

As almost all the results introduced here have been obtained by back-of-envelope calculations using the Z-index, the present author is longing for the full support by computer search and refinement by rigorous analysis in order to mature this incomplete but throbbing problem. Extension to non-tree graphs is the next important target leading to the basic discussion on the origin of aromaticity.

2. Analysis of dormant families by the *Z*-index and *Z*-counting polynomial

The spectrum of a graph is defined as the set of eigenvalues $\{x: P_G(x)=0\}$, where $P_G(x)$ is the characteristic polynomial defined in terms of the adjacency matrix **A** and unit matrix **E** of graph G as

$$P_G(x) = (-1)^N \det(\mathbf{A} - x\mathbf{E}) . \tag{1}$$

In 1971 the present author showed that for tree graphs $P_G(x)$ can be expressed in terms of the non-adjacent number, $p(G,k)$, or k-matchings for G [12,13] as

$$P_G(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(G,k)\, x^{N-2k} \quad (G \in \text{tree}). \tag{2}$$

By adding all the $p(G,k)$'s for G the topological index (here we call Z-index) is defined as

$$Z = \sum_{k=0}^{\lfloor N/2 \rfloor} p(\mathrm{G}, k). \tag{3}$$

In order to discuss the isospectrality of tree graphs Z is found to be very useful, but the Z-counting polynomial

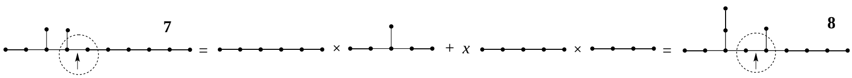
$$Q_{\mathrm{G}}(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} p(\mathrm{G}, k)\, x^k \tag{4}$$

is crucial, since Eqs. (2) and (4) are mathematically equivalent for tree graphs, while Z is subordinate to $Q_{\mathrm{G}}(x)$ as

$$Z = Q_{\mathrm{G}}(1). \tag{5}$$

Now for checking the isospectrality of tree graphs we will use Z as a steering role and Q function as the decisive role instead of being bothered by $P_{\mathrm{G}}(x)$ and the set of its eigenvalues.

As an example consider the graphs **6**~**8**. Luckily in this case the isospectrality of **7** and **8** can immediately be proved by noticing the two edges indicated by an arrow, because the Q functions (mathematically equivalent to the later proposed matching polynomial [15-17]) of this pair of graphs are shown to be the same by applying the recursion formula [12,13] as follows.



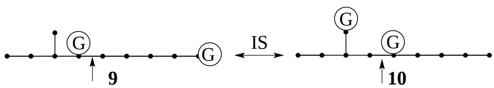
Then we have

$$Q_7(x) = Q_8(x) = (1+5x+6x^2+x^3)(1+5x+5x^2+x^3) + x(1+4x+3x^2)(1+3x+x^2)$$
$$= 1 + 11x + 43x^2 + 73x^3 + 53x^4 + 14x^5 + x^6. \tag{6}$$

By putting x=1 their Z-indices can be obtained as

$$Z_7 = Z_8 = 1 + 11 + 43 + 73 + 53 + 14 + 1 = 196. \tag{7}$$

Further we can safely assert that infinite pairs of IS graphs can be generated from **9** and **10** by adding any tree or non-tree graph G.



Although details will be explained in Appendix 1, the Q-functions of the IS pair of **9** and **10** for any G can be given by

$$Q_G(x) = (1+3x+x^2)^2\, G^2 + x\,(1+3x+x^2)\,(3+5x)\, GH + x^2\,(1+x)\,(2+5x+x^2)\, H^2, \quad (8)$$

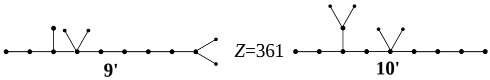
where G represents the Q of G, and H is the Q of graph H obtained from G by deleting its root, the attaching vertex. In the case of **7** and **8**, G=1+x and H=1, yielding Eq. (6).

The corresponding expression for the Z-index of graph G can be obtained by putting x=1 in Eq. (8) as

$$Z_G = (5\,G + 4\,H)^2. \quad (9)$$

However, in this case G and H are the Z-indices of graphs G and H. Namely, Z_7=Z_8=196 can be derived by putting G=2 and H=1into Eq. (9).

Now consider graph as G whose bottom vertex is chosen as its root. Then the Z-indices of G and H become, respectively, to be 3 and 1, yielding Z_G=361, which are the Z-indices of the IS pair **9**' and **10'**.



We have found a number of doublet dormants like **6**, some of which are already introduced in Ref. 14.

Now notice graph **11** in Fig. 3 with a pair of triplet sprouts (See **11'** and **11"**), which are found to generate the famous smallest tree pair of IS graphs [1-3,9], **1** and **2**.

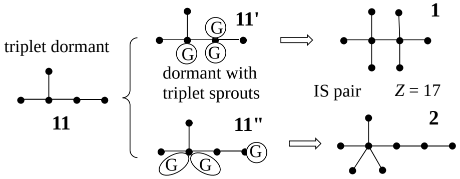


Figure 3. The smallest IS tree pair is generated from the triplet dormant of N=5.

Here as will be shown in Appendix 2 the Q-functions and Z-indices of **11**' and **11**" are obtained to be

$$Q_{11'} = Q_{11''} = 2\,G^2H + (5x-1)\,GH^2 + x(2x-1)\,H^3 \quad (10)$$

and

$$Z_{11'} = Z_{11''} = 2\,G^2H + 4\,GH^2 + H^3. \quad (11)$$

3. Small IS graphs generated from dormants

As already mentioned, the above (**1**,**2**) is the smallest IS tree pair of N=8, and can be generated from the dormant **11**. Similarly all the five and four IS pairs of N=9 and 10, respectively, were found to be generated from dormants as shown in Figs. 4 and 5.

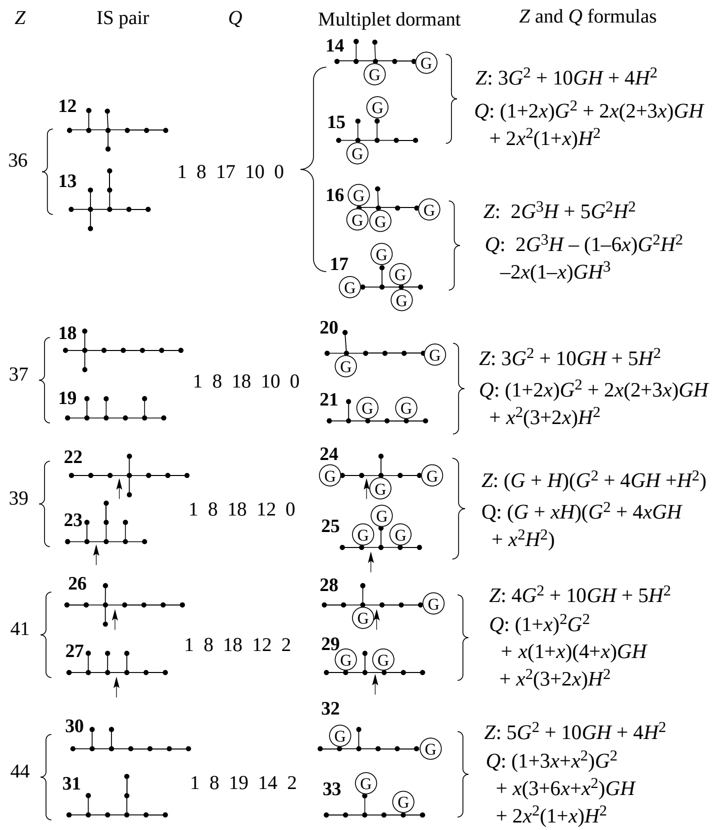


Figure 4. All the five IS pairs of N=9 can be generated from their dormants. Z=36 pair has two dormants. The arrows indicate that an intrinsic IS pair can be generated. The general expressions for Z-indices and Q-functions are given.

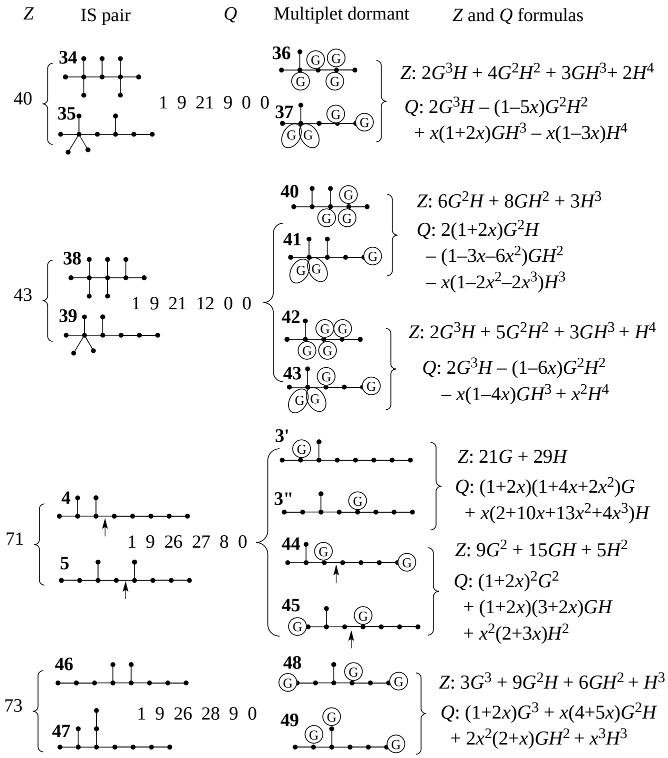


Figure 5. All the four IS pairs of N=10 can be generated from their dormants. Z=43 and 71 pairs have two dormants. The arrows indicate that an intrinsic IS pair can be generated.

Now we have realized that so many different dormants generate small IS tree pairs. Then the results obtained up to now were carefully summarized as in Fig. 6 just by excluding the larger graphs **6**~**8**, where an italic number indicates the multiplicity and the parenthesized gothic numbers are those assigned to IS pairs. For later discussion tentative codes for these dormants are given.

One can immediately imagine that (i) dormants are generally non-linear and asymmetric. (ii) Several dormants can generate more than two different IS pairs, whereas (iii) several IS pairs, such as (**4**, **5**), (**12**, **13**), and (**38**, **39**), can be generated from different dormants.

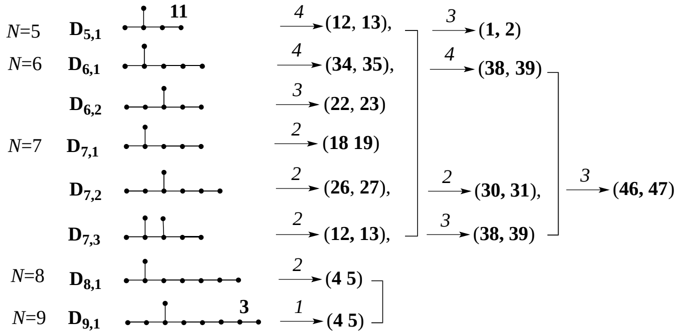
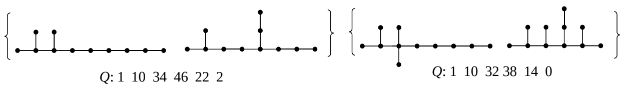


Figure 6. Illustrative summary of the dormants introduced here. Itallic: multiplicity of dormants.

The items (i) and (ii) will be discussed in more detail in the following sections. However, before extending the discussion let us make a brief comment on the dormant. According to our survey, out of about two hundreds of N=11 trees 50 form two IS trios and 22 IS pairs, but about ten pairs cannot be related to a common dormant, such as the pairs below:



This means that behind the isospectrality of a pair of isomer graph so many complicated factors seem to be entangled.

4. A dormant can generate many different series of IS pairs

The smallest dormant $\mathbf{D_{5,1}}$(=**11**) already explained in Fig. 3 was found to generate many other series of IS graphs as illustrated in Figure 7, where the general expressions for giving the Z-indices are also shown. Namely **11** can work not only as a triplet dormant but also as quadruplet, sextuplet and septuplet dormants.

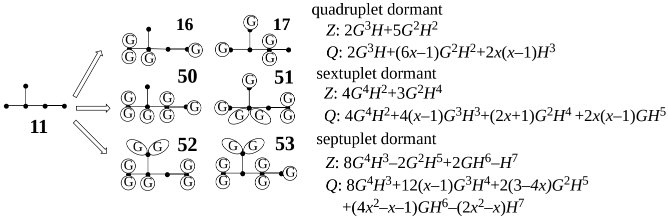


Figure 7. The smallest dormant can work also as quadruplet, sextuplet, and heptuplet dormants.

In the next paper "Theory" how these IS pairs were found will be explained.

Similarly, to the case of **11** the smallest ESG **3** (**=D$_{9,1}$**) was also found to work as many different multiplet dormants with multiplicity of 3, 4, 5, and 6 as shown in Fig. 8. As a matter of fact, since further research is not yet finished at this stage, there remains a possibility of still higher multiplicity for this graph.

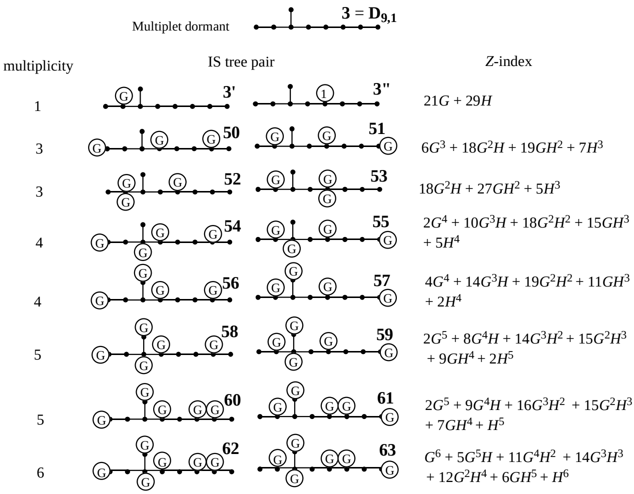


Figure 8. The smallest ESG **D$_{9,1}$** can work as a dormant with many different multiplicities.

In this case the structures of the pairs, (**54**, **55**), (**56**, **57**), (**58**, **59**), (**60**, **61**), and (**62**, **63**), are closely related among each other. Their mathematical relations can be explained well by following the discussion expanded in the next paper, "Theory."

The next example is a small dormant $\mathbf{D_{6,1}}$ of N=6 with many different multiplicities up to two kinds of nonuplet.

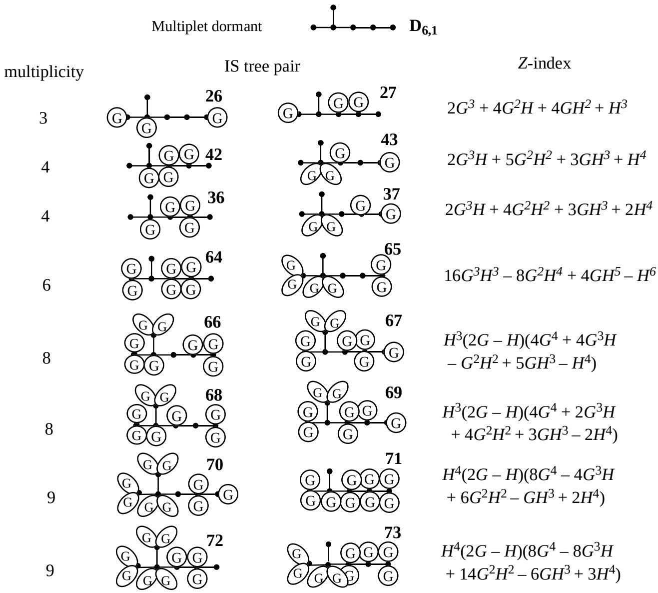
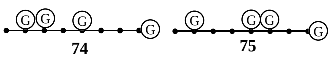


Figure 9. A small dormant $\mathbf{D_{6,1}}$ of N=6 but with many different multiplicities.

It is interesting to observe that the graph **71**, especially when G is substituted by an edge, is IS to a rather asymmetric isomer **70**.

5. Linear and symmetric dormants

As far as we have checked, the shortest linear dormant is found to be the path graph S_8 working as quadruplet as shown below.



$$2G^4 + 8G^3H + 12G^2H^2 + 9GH^3 + 3H^4$$

Possibilities of its higher multiplicity and longer linear dormants are expected to be found. Anyway existence of linear dormant seems to be rare.

A little lower symmetric than linear but a series of interesting mirror-symmetric triplet dormants which derive also mirror-symmetric IS pairs were found as in Fig. 10.

Incidentally all of them were found to be intrinsic as the arrows indicate.

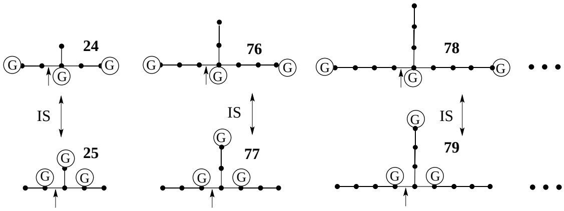


Figure 10. A series of intrinsic and mirror symmetric triplet dormants which generate also mirror symmetric IS pair graphs.

Although we have not yet grasped complete mathematical structure of the dormant family, in the following paper let us disclose as honestly as possible our successful strategy for discovering these interesting dormants without recourse to computer search.

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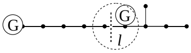
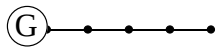
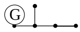
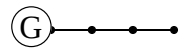
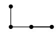
Appendix 1 How to derive the *Q* function for **9** containing graph fragment G.

We are now going to obtain the *Q* function for **9** containing graph fragments G's. Edge *l* to be deleted from **9** is the one indicated by the arrow. The recursion formula can formally be written down as

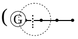
$$Q(\mathbf{9})=Q(\mathbf{9}-l)+xQ(\mathbf{9}\Theta l), \qquad \text{(A1)}$$

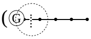
where **9**–*l* is the subgraph of **9** obtained by deleting edge *l*, while 9Θ*l* is obtained further by deleting all the edges incident to *l*. Note that in this case one graph fragment G is also cut to yield H (See the dotted circle in LHS of Eq. (A2)).

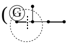
 =  $\times$  $+\ x$  $\times$ 

Q (**9**) *Q* (**9–*l***) *Q* (**9Θ*l***) (A2)

The Q functions of the three graphs containing graph fragment G can be degraded into as follows.

Q () $= (1+2x)\,G + x(1+x)\,H$

Q () $= (1+3x+x^2)\,G + x(1+2x)\,H$

Q () $= (1+3x+x^2)\,G + x(1+x)\,H$

Now by putting them into Eq. (A2) one gets

$$Q(9) = (1+3x+x^2)^2\,G^2 + x\,(1+3x+x^2)\,(3+5x)\,GH + x^2\,(1+x)\,(2+5x+x^2)\,H^2, \quad \text{(A3)}$$

which is equal to Eq. (8). Exactly the same result can be obtained also for IS **10**.

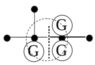
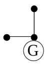
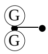
The Z-indices for **9** and **10** can be obtained just by putting x=1 into Eq. (A3) as $Z_9 = Z_{10} = (5G+4H)^2$. Further by putting G=1+x and H=1 into Eq. (A3) one gets Eq. (6), which eventually gives Eq. (7), or the Z-indices of **4** and **5**, by putting x=1.

The Q functions of **9’** and **10’** can be derived by putting G=1+2x and H=1 to be

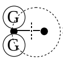
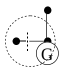
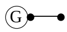
$$Q(9') = Q(10') = 1 + 13x + 61x^2 + 127x^3 + 116x^4 + 39x^5 + 4x^6. \quad \text{(A4)}$$

Appendix 2 How to derive the Q function for **11’** containing graph fragment G.

In this case formally the Q function can be degraded into

 =  $\times$  $+\ x\,H^3.$ (A5)

In calculating this we need to know

 =  $+\ x\,H^2 = 2GH + (x-1)\,H^2$ and  =  $+\ x\,H = G + 2x\,H.$ (A6)

In order to get the Q function of the twin G in the above-left equation, the following relation is necessary.

 $= HG + GH - H^2 = 2GH - H^2.$ (A7)

However, the above derivation can be obtained by Eq. (1) of the next paper.

By putting Eq. (A6) into Eq. (A5) we get Eq. (10).