New Method for Constructing Isospectral Graphs

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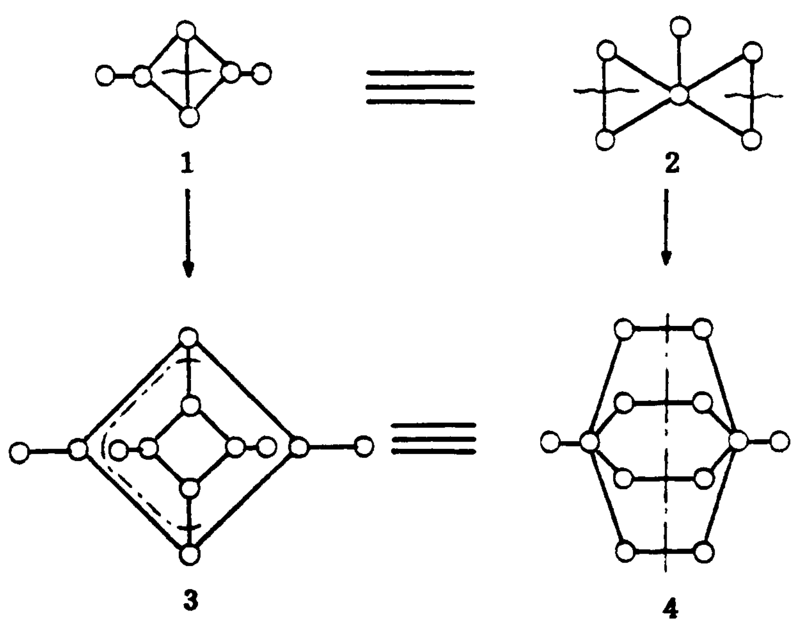
Based on the ring enlargement procedure, a novel method for constructing isospectral graphs is proposed, giving an answer to the conjecture and open problem provided by Randić.

1. INTRODUCTION

There exist several methods available to construct isospectral molecular graphs.[1−10] Recently, M. Randić and his co-workers proposed the ring enlargement process (vide infra) for constructing subspectral graphs.[11] This method can be also used to construct isospectral graphs; however, it may fail sometimes. For example, the isospectral pair **1**, **2** can be enlarged to the isospectral graphs **3**, **4** shown in Figure 1, where the symbol "≡" signifies an isospectral pair and "→" denotes the ring enlargement procedure. Eigenvalues of **3**, **4** are divided into two parts, those in coincidence with that of **1**, **2** are listed on the left, and the remaining ones are put on the right. On the other hand, graph pairs **7**, **8** and **9**, **10** in Figure 2, yielded from isospectral pair **5**, **6**, are not isospectral.

Noticing the difference of the spectrum of graphs **XX**, **XX′** (by "**XX**, **XX′**" we mean that they are generated from subgraph **X** in double size by the enlargement procedure, such as **7**, **8** from **5**; and **9**, **10** from **6**), Randić suggested that if **XX**, **XX′** are bipartite, they should be isospectral, because all eigenvalues now occur in pairs and the difference between **XX** and **XX′** disappears. Hence, he proposed a conjecture below. CONJECTURE: If graph **X** yields nonisomorphic bipartite enlargements **XX**, **XX′**, etc.; the derived graphs are not only superspectral to the parent graph **X** but are also mutually cospectral.

Furthermore, why can isospectral graphs **X**, **Y** sometimes generate isospectral pairs **XX**, **YY** via the ring enlargement procedure, and sometimes they cannot? This inspires the open problem that Randić put forward. OPEN PROBLEM: When, and under what conditions, will a pair of isospectral graphs **X**, **Y** upon enlargement produce isospectral pairs **XX** and **YY**?



1, 2 (with the spectrum):
−1.903, −1.000, −1.000, +0.194,
+1.000, +2.709.

3, 4 (with the spectrum):
−1.903, −1.000, −1.000, +0.194, −2.709, −1.000, −0.194, +1.000,
+1.000, +2.709, +1.000, +1.903.

Figure 1. Isospectral graphs of double size derived from a smaller isospectral pair by the ring enlargement process.

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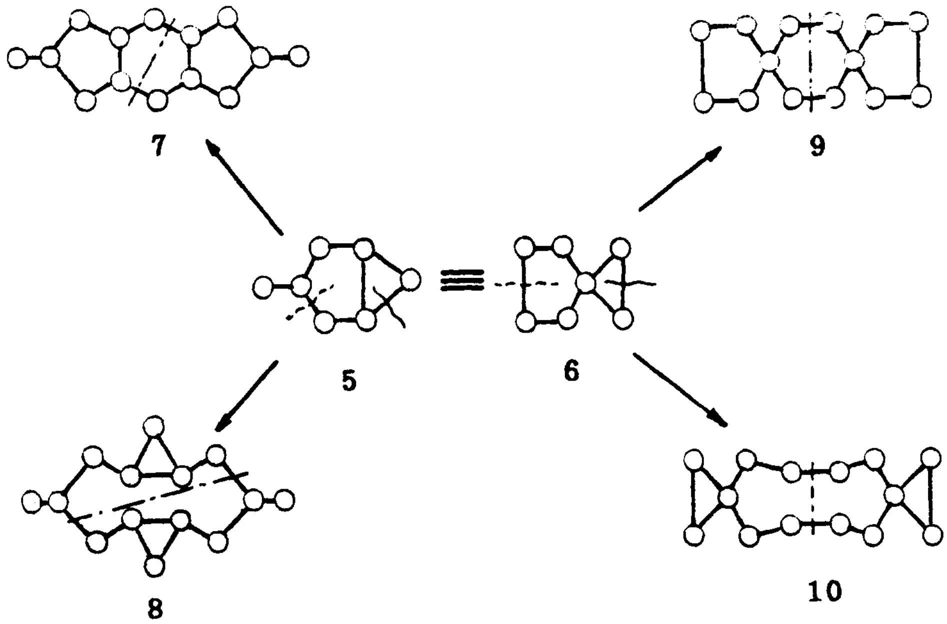

5, 6 (with the spectrum):
-1.953, -1.618, -1.000, 0,
+0.618, +1.463, +2.473,
7 (with the spectrum):
-1.953, -1.618, -1.000, 0, -2.303, -1.861, -0.254, 0,
+0.618, +1.463, +2.473, +1.000, +1.303, +2.115.
8 (with the spectrum):
-1.953, -1.618, -1.000, 0, +2.303, +1.861, +0.254, 0,
+0.618, +1.463, +2.473, -1.000, -1.303, -2.115.
9 (with the spectrum):
-1.953, -1.618, -1.000, 0, +2.164, +1.000, +1.000, +0.618,
+0.618, +1.463, +2.473, -0.773, -1.618, -2.391.
10 (with the spectrum):
-1.953, -1.618, -1.000, 0, -2.164, -1.000, -1.000, -0.618,
+0.618, +1.463, +2.473, +0.773, +1.618, +2.391.

Figure 2. Ring enlargement, having failed to produce an isospectral pair.

In this paper, we try to find regularities of isospectral graphs generated by the ring enlargement. At first in section **2**, we review the theoretical basis of Randić's ring enlargement procedure[11] and the extended Sachs theorem. Then in section **3**, a theorem is inferred, which can be used to reduce enlarged graphs. Moreover two corollaries are deduced from the reduction theorem in section **4** in order to analyze Randić's conjecture and his open problem. Thus, a novel method for constructing isospectral graphs is formulated.

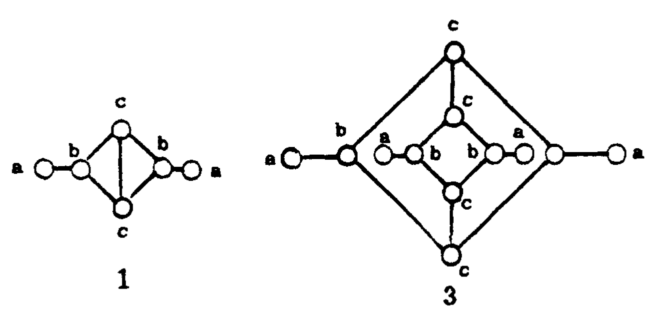

Figure 3. An example for illustrating VNSR.

2. THEORETICAL BASIS

(1) Ring Enlargement.[11] The ring enlargement can be used to construct a larger graph **G** from a smaller sub-one **g**. The graph **G** is of double size, sharing all eigenvalues of **g**, known as "vertex neighbor sum rule" (VNSR) as follows. VNSR (Randić): Graph **G** for whose vertices one can assign labels a, b, c ... of a smaller **g** such that for each vertex the same vertex neighbor sum rule holds, or the sum rule can be obtained by linear combinations of the vertex sum rules of **g**, will necessarily have the eigenvalues of **g**.

For example, in Figure 3 if labels a, b, and c are assigned to the equivalent vertices of **1**, the neighbor sums of vertices a, b, and c are b, a + 2c, and 2b + c, respectively. According to VNSR, on opening the central edge, the graph grows in succession on connecting three pairs of c-, b-, and a-type vertices, respectively, thus a new graph **3** characterized by similar neighborships is yielded. As shown in Figure 1, graph **3** contains the spectrum of graph **1**.

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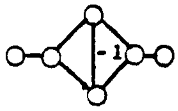

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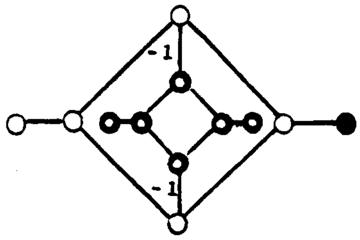

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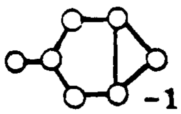
Figure 4. Examples of a definition of Möbius and hypo-Möbius graphs.



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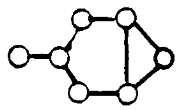

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14 (with the spectrum):
+2.115, +1.303, +1.000, 0,
-0.254, -1.861, -2.303.
15 (with the spectrum):
-2.115, -1.303, -1.000, 0,
+0.254, +1.861, +2.303.

Figure 5. Two Möbius graphs having contrary eigenvalues.

(2) Extension of Sachs Theorem to Möbius Graphs. A critical problem encountered in this work is to evaluate the characteristic polynomials and the spectra of Möbius graphs. By a Möbius graph, we mean a graph for which

(1) at least one edge weight is -1;

(2) at least along one circuit the product of edge weights is equal to -1.

If a graph meets condition (1) only, then it is called hypo-Möbius, *i.e.*, a Hückel graph. For example (see Figure 4), **11** is Möbius, but **12** is Hückel, because in **12** there are two edges with weight -1, and the product of edge weights along any circuits is equal to **1**. Now we introduce the following lemma in order to show the equivalence of graphs, for example, **12** and **3** are equivalent. LEMMA **1**. If graph **G′** results from changing the sign of weight for each incident edge of a vertex of graph **G**, then **G′** and **G** are equivalent. Its validity is proved in the Appendix.

Based on Lemma **1**, it is a direct way to distinguish Möbius graphs and Hückel graphs, illustrating many useful deductions. For example, a Möbius cyclic graph involves a single edge with weight -1 arbitrarily. Odd and even edges with the weight -1 for a cycle result in Möbius and Hückel graphs, respectively. Acyclic graphs with any number of edges of weight -1 are eventually Hückel-type, etc. On changing the weights from 1 to -1 for edges incident to the **6** vertices marked by bold circles in **12**, **3** is generated, *i.e.*, **12** and **3** are equivalent.

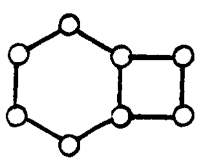
The extended Sachs theorem embraces the characteristic polynomials of the Möbius graphs. EXTENDED SACHS THEOREM:[1,12-14] The characteristic polynomial of a Möbius graph **G** is

$$P_G(x) = x^n + a_1x^{n-1} + ... + a_jx^{n-j} + ... + a_n \quad (1)$$

The coefficients $a_j(1 \le j \le n)$ are computed from the following expression:

$$a_j = \sum_{S \in S_j} (-1)^{c(s) + p(r)_2 r(s)} \quad (2)$$

where S_j denotes a set of graphs each comprising j vertices, $S \in S_j$ means that S is a member of the set S_j, and in S there



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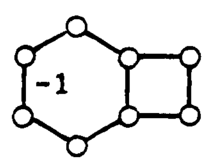

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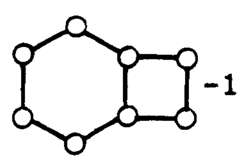

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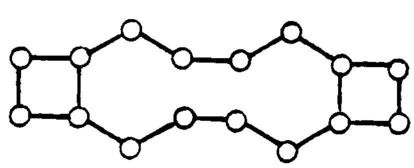

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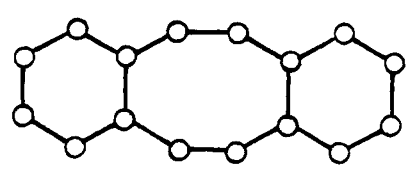

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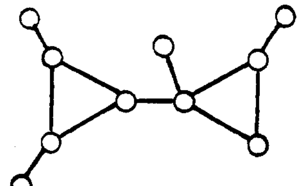
16 (with spectrum):
+2.356, +1.477, +1.095, +0.262.
17 (with spectrum):
+2.284, +1.751, +0.785, +0.318.
18 (with spectrum):
+2.127, +1.576, +1.197, +0.747.
19 (with spectrum):
+2.356, +1.477, +1.095, +0.262, +2.284, +1.751, +0.785, +0.318.
20 (with spectrum):
+2.356, +1.477, +1.095, +0.262, +2.127, +1.576, +1.197, +0.747.

Figure 6. An example unconformable to Randić conjecture.



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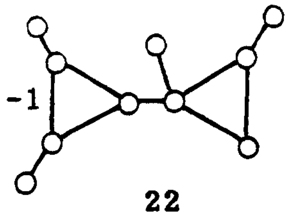

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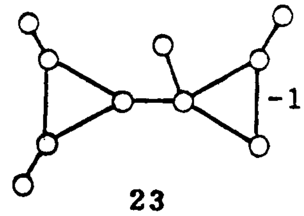

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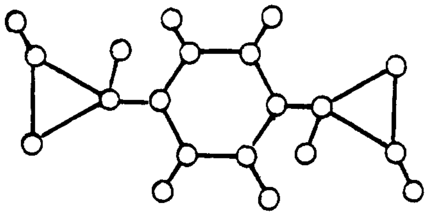

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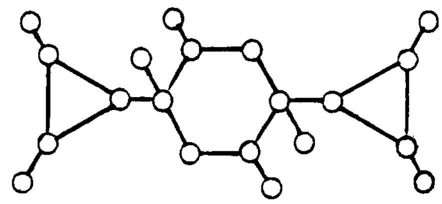

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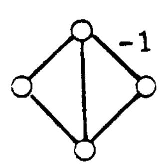
```
21 (with spectrum):
+2.658, +2.085, +0.695, +0.618,
 0,      0,     -1.000, -1.405,
-1.618, -2.033.
22 and 23 (with spectrum):
+2.497, +1.618, +1.328, +0.618,
 0,      0,     -0.618, -1.328,
-1.618, -2.497.
24 and 25 (with spectrum):
+2.658, +2.085, +0.695, +0.618,
 0,      0,     -1.000, -1.405,
-1.618, -2.033,
+2.497, +1.618, +1.328, +0.618,
 0,      0,     -0.618, -1.328,
-1.618, -2.497.
```

Figure 7. An example showing corollary 1.

are only components with all degrees of vertices equal to one or all degrees of vertices equal to two, $c(S)$ is the number of components in the graph S, $p(r)$ is the number of edges with weight -1 in the ring component of the graph S, and $r(S)$ is the number of rings in S. With the Möbius graph **13**,



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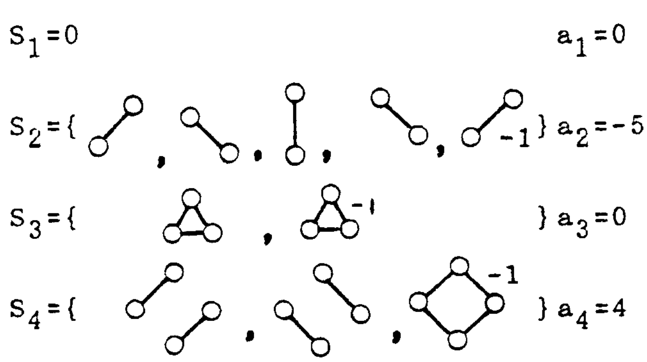
we have S_j, and a_j are evaluated as follows



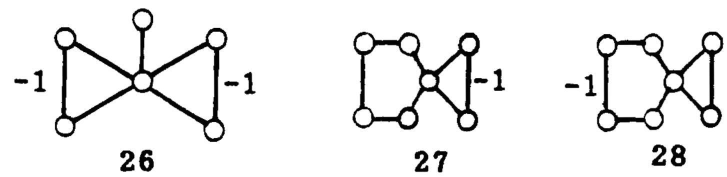
whence, $P_G(x) = x^4 - 5x^2 + 4$, with the spectrum ± 2 and ± 1.

The extended Sachs theorem states that energy levels of a Möbius graph with odd-membered rings, such as **13**, are symmetrically distributed about $x = 0$ just as in alternant hydrocarbons. On the other hand, two Möbius graphs with different arrangement of the edge weighted -1 as shown, for instance, in **14** and **15** in Figure 5 may have eigenvalues inversely equal each other.

3. REDUCTION THEOREM

We have seen that in the case of the ring enlargment, the spectrum of **G** always contains the equal set of the spectrum of **g**. But what is the meaning of the remaining half eigenvalues of **G**?

Möbius graph **11** and **1** are almost the same except they differ in the weight of their central edges. By the ring enlargement procedure, **12** is obtained from cutting the central edge of **11**. As shown in section **2**, **12** and **3** are equivalent; therefore, they have identical spectrum. Thus, **3** can be reduced to **1** and **11**. Obviously, this deduction is true in general, hence one can state a theorem as follows. REDUCTION THEOREM: If **G** is derived from enlarging a smaller graph **g**, then **G** can be reduced to **g** and $\mathbf{g}_{\text{Mö}}$, where $\mathbf{g}_{\text{Mö}}$ is Möbius with respect to **g** in which the weight of the cutting edge(s) in the ring enlargement process is -1.

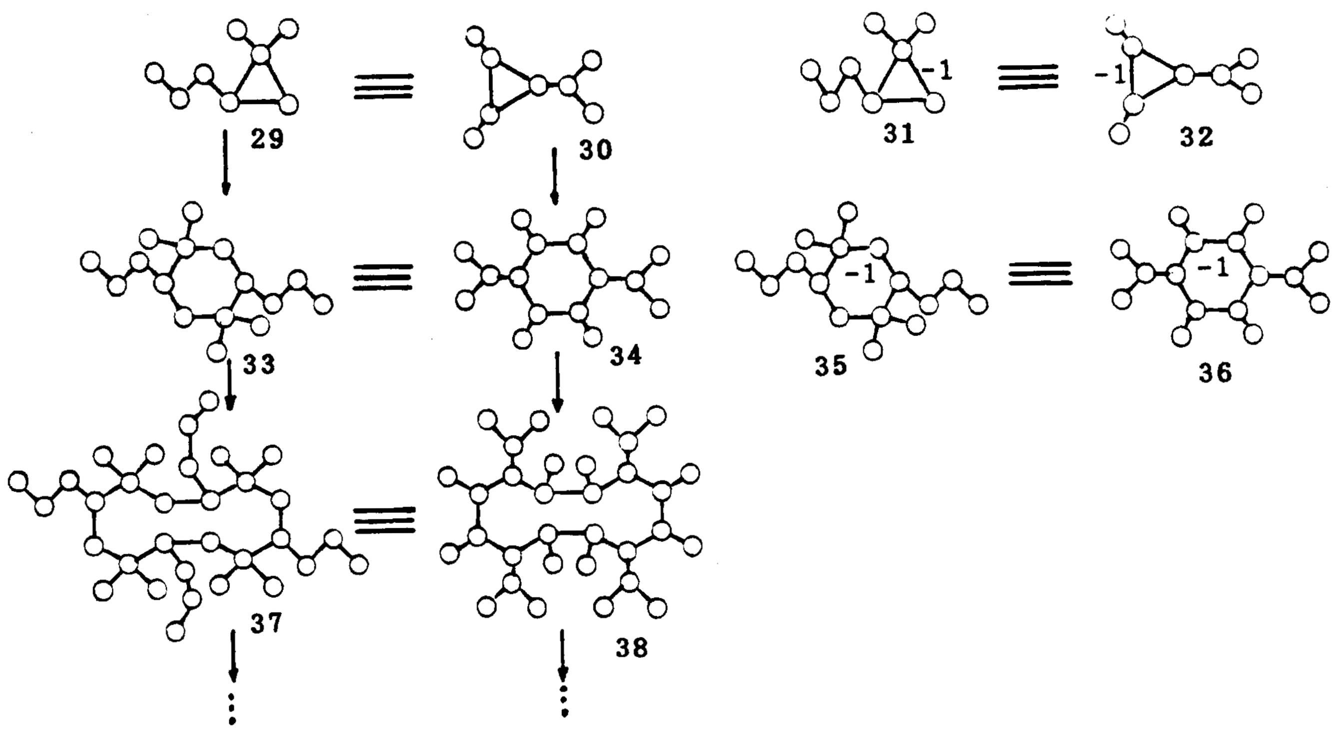


11 and 26 (with spectrum):
+1.903, +1.000, +1.000, -0.194,
-1.000, -2.709.

27 (with spectrum):
-2.391, -1.618, -0.773, +0.618,
+1.000, +1.000, +2.164.

28 (with spectrum):
+2.391, +1.618, +0.773, -0.618,
-1.000, -1.000, -2.164.

Figure 8. Spectrum of Möbius graphs **26**, **27**, and **28**.



29 and 30 (with spectrum):
+2.473, +1.463, +0.618, 0,
0, -1.000, -1.618, -1.935.

31 and 32 (with spectrum):
-2.473, -1.463, -0.618, 0,
0, +1.000, +1.618, +1.935.

33 and 34 (with spectrum):
+2.473, +1.463, +0.618, 0,
0, -1.000, -1.618, -1.935,
-2.473, -1.463, -0.618, 0,
0, +1.000, +1.618, +1.935.

35 and 36 (with spectrum):
±2.272, ±2.272, ±1.492, ±1.492,
±0.780, ±0.780, 0, 0,
0, 0.

37 and 38 (with spectrum):
±2.473, ±1.935, ±1.618, ±1.463,
±1.000, ±0.618, 0, 0,
0, 0,
±2.272, ±2.272, ±1.492, ±1.492,
±0.780, ±0.780, 0, 0,
0, 0.

Figure 9. A series of doubly larger isospectral pairs induced from a known isospectral pair.

The reduction theorem shows that half of the eigenvalues of the enlarged graph **G** comes from its Hückel precursor **g** (listed on the left in Figure 1 and 2) and the remaining half (the right side in Figure 1 and 2) refer to the Möbius species $\mathbf{g}_{\text{Mö}}$.

4. DISCUSSION

It follows from the reduction theorem that one can obtain two corollaries below.

COROLLARY 1: Let $\mathbf{G}'$, $\mathbf{G}''$ be nonisomorphic, obtained from enlarging **g**, then $\mathbf{G}'$, $\mathbf{G}''$ are isospectral, if and only if $\mathbf{g}_{\text{Mö}}'$, $\mathbf{g}_{\text{Mö}}''$ are isospectral, where $\mathbf{g}_{\text{Mö}}'$, $\mathbf{g}_{\text{Mö}}''$ are Möbius alternatives of **g** with some edge weight equal to -1.

Corollary 1 indicates that Randić's conjecture may not always be valid. For example (see Figure 6), bipartite graphs **19** and **20** are constructed from enlarging **16**; meanwhile, the reduction theorem shows **19**, **20** can be reduced to **16**, **17** and **16**, **18**, respectively. However, the extended Sachs theorem gives unequal coefficients, a_4's, of the characteristic polynomials of **17** and **18** which indicates **17**, **18** are nonisospectral and **19**, **20** likewise.

For further understanding of corollary 1, we illustrate another example (see Figure 7). Graphs **24**, **25** can be constructed from enlarging **21** and in terms of the reduction theorem, both of them can be reduced to **21**, **22** and **21**, **23**, respectively. It is not quite difficult to confirm the isospectrality of the graphs **22** and **23** by extended Sachs theorem, since only the coefficients of their characteristic polynomials, relevant to three-membered Möbius rings, need to be compared. Thus, one can see that **22** and **23** are indeed isospectral, thus **24** and **25** are isospectral too. The following corollary of the reduction theorem may answer Randić's open problem.

COROLLARY 2: Let $\mathbf{g}'$, $\mathbf{g}''$ be an isospectral pair, and let $\mathbf{G}'$, $\mathbf{G}''$ be obtained from enlarging $\mathbf{g}'$, $\mathbf{g}''$; $\mathbf{G}'$, $\mathbf{G}''$ are isospectral, if and only if $\mathbf{g}_{\text{Mö}}'$, $\mathbf{g}_{\text{Mö}}''$ are isospectral, where $\mathbf{g}_{\text{Mö}}'$, $\mathbf{g}_{\text{Mö}}''$ are Möbius alternatives of $\mathbf{g}'$, $\mathbf{g}''$ with the weight of relevant edges equal to -1.

Corollary 2 provides the argument as to why graphs **1** and **2** in Figure 1 can be enlarged to an isospectral pair (but **5** and **6** in Figure 2 cannot), which is attributed to the fact that graphs **11** and **26** (Möbius forms of **1** and **2**) are isospectral, whereas **14**, **15**, **27**, and **28** (Möbius forms of **5** and **6**) are not (see Figure 8).

Finally we cite an interesting example (see Figure 9) in illustration of corollary 2. Graphs **29**, **30** are a known isospectral pair. The isospectrality of their Möbius species **31** and **32**, which contain only one ring can be easily verified by the extended Sachs theorem; therefore, they can be enlarged to an isospectral pair **33** and **34**. Furthermore **35** and **36** (Möbius forms of **33** and **34**) are also isospectral, thereby **33**, **34** can again be enlarged to an isospectral pair **37**, **38**. This procedure can be repeated, and a series of larger and larger isospectral graphs can be constructed.

ACKNOWLEDGMENT

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APPENDIX

The secular determinant of **G** is defined as follows

$$\det|x\mathbf{I} - \mathbf{A}| = 0 \tag{3}$$

where **I** is the identity matrix and x is a variable. The adjacency matrix **A** in eq 3 is typically sparse with entries in the ith row and jth column:

$$a_{ij} = \begin{cases} = 1 & \text{if vertices } i \text{ and } j \text{ are connected} \\ = 0 & \text{otherwise} \end{cases} \tag{4}$$

Let each element of both ith row and ith column of the determinant (3) be multiplied by -1, and the secular determinant of $\mathbf{G}'$ is obtained.

$$\det|x\mathbf{I} - \mathbf{A}'| = 0 \tag{5}$$

Linear algebra states that the determinants (3) and (5) are equivalent, namely, they have not only the same eigenvalues but also equal eigenvectors. The difference between the eigenvector (c_1, c_2,...c_i...) of **G** and the eigenvector (c_1, c_2,... $-c_i$...) of $\mathbf{G}'$ is caused by the inverse phases of their ith $2P_z$ orbitals. Thus, Lemma 1 is proved.

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