Vertex and Edge Type Relations of Randić Index for Chemical Trees

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ABSTRACT. Let T be a chemical tree, i.e. a tree with all vertices of degree less than or equal to 4. We find relations for the 0-connectivity and 1-connectivity indices ${}^0\chi(T)$ and ${}^1\chi(T)$, respectively, in terms of the vertices and edges of T. A comparison of these relations with the coefficients of the characteristic polynomial of T associated to its adjacency matrix is established.

1 Introduction and Terminology

A single number which characterizes the graph of a molecule is called a graph-theoretical invariant or topological index. The structure property relationships quantify the connection between the structure and properties of molecules. These relationships are mathematical models that allow the prediction of properties from structural parameter. They are called quantitative structure-property relationships ([9]).

Let T be a tree with set of vertices $\{v_1, \dots, v_n\}$. The 1-connectivity index or Randić index ([7]) of T defined as

$$ {}^1\chi(T) = \sum_{v_i - v_j} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)}} $$

where $v_i - v_j$ runs over all the edges of T and $\delta(v_i)$ denotes the degree of the vertex v_i, is one of the most widely used and most successful in quantitative structure-property relationships ([8], [4] and [5]).

Denote by $\Delta(T) = \max\{\delta(v_i) : i = 1, \dots, n\}$. An $i-vertex$ is a vertex of degree i, $k_i(T)$ is the number of $i-vertices$ and for $i, j \in \mathbb{N}$, $e_{ij}(T)$ denotes the number of edges that joins a $i-vertex$ with a $j-vertex$. Finally, denote by $[v_i, v_j]$ the shortest walk joining v_i with v_j and recall that the number of edges in $[v_i, v_j]$ is called the distance in T between v_i and v_j and is denoted by $d(v_i, v_j)$.

A chemical tree T is a tree such that $\Delta(T) \leq 4$, it is used as a graphical representation of the carbon-atom skeleton of an alkane. We can express the Randić index of T as

$$^1\chi(T) = e_{11} + \frac{e_{12}}{\sqrt{2}} + \frac{e_{13}}{\sqrt{3}} + \frac{e_{14} + e_{22}}{2} + \frac{e_{23}}{\sqrt{6}} + \frac{e_{24}}{\sqrt{8}} + \frac{e_{33}}{3} + \frac{e_{34}}{\sqrt{12}} + \frac{e_{44}}{4}$$

This formula indicates that the Randić index of a chemical tree T is completely determined by e_{ij}, $i \leq j \in \{1,2,3,4\}$. In theorem 2.3 we find a new expression for $^1\chi(T)$ as follows:

$$24 \cdot {}^1\chi(T) = 12n + k_3\rho + k_4\xi + e_{13}\eta + e_{14}\mu + e_{33}\gamma + e_{34}\delta + e_{44}\epsilon + (24\sqrt{2} - 36)$$

where ρ, ξ, η, μ, γ, δ, $\epsilon \in \mathbb{Q}(\sqrt{2}, \sqrt{3})$, the extension field of the rational numbers $\mathbb{Q}$ by adjoining the real numbers $\sqrt{2}$ and $\sqrt{3}$ (see [1]). Comparing with the previous formula, we can see that all e_{ij} where $i = 2$ or $j = 2$ were suppressed and instead, k_3, k_4 and n appeared. This approach has an advantage from the Randić index point of view since k_3, k_4 and n fully determines the 0-connectivity index $^0\chi(T) = \sum_{i=1}^{n} \frac{1}{\sqrt{\delta(v_i)}}$ (see theorem 2.4). In fact, we show in corollary 2.2 that for chemical trees T and T' with the same number of vertices, $^0\chi(T) = {}^0\chi(T')$ if, and only if, $k_3 = k_3'$ and $k_4 = k_4'$. In this case we deduce that

$$24\left({}^1\chi(T) - {}^1\chi(T')\right) = (e_{13} - e_{13}')\,\eta + (e_{14} - e_{14}')\,\mu + (e_{33} - e_{33}')\,\gamma + (e_{34} - e_{34}')\,\delta + (e_{44} - e_{44}')\,\epsilon$$

A natural question arises for chemical trees: is $^1\chi$ completely determined by the numbers e_{ij}?. In other words

$$e_{ij} = e_{ij}' \text{ for every } i \leq j \in \{1,3,4\} \Leftrightarrow {}^1\chi(T) = {}^1\chi(T')?$$

Clearly, $e_{ij} = e_{ij}'$ for every $i \leq j \in \{1,3,4\}$ implies $^1\chi(T) = {}^1\chi(T')$, but in general, the converse does not hold. In example 2.4 we construct trees T and T' such that $^1\chi(T) = {}^1\chi(T')$ although $e_{ij} \neq e_{ij}'$ for every $i \leq j \in \{1,3,4\}$. However, we have an affirmative answer for chemical trees of maximal degree 3: $^1\chi$ is fully determined by the numbers e_{13} and e_{33} (see corollary 2.5).

On the other hand, let $\lambda^n + c_1\lambda^{n-1} + \cdots + c_{n-1}\lambda + c_n$ be the characteristic polynomial of T associated to the adjacency matrix of T. In section 3 we use counting arguments to derive formulas for the coefficients c_4 and c_6 (theorem 3.3) which are closely related to those of ${}^0\chi$ and ${}^1\chi$. In fact, we observe that ${}^0\chi$ and c_4 are determined by the same set of numbers, namely n, k_3 and k_4 while ${}^1\chi$ and c_6 depends on the numbers e_{ij} for every $i \leq j \in \{1,3,4\}$. This analogy allows us to establish a comparison c_4 versus ${}^0\chi$ and c_6 versus ${}^1\chi$. Specifically, we show in corollaries 3.4 and 3.6 that for trees T and T' with the same number of vertices, ${}^0\chi(T) = {}^0\chi(T')$ implies $c_4(T) = c_4(T')$ and ${}^1\chi(T) = {}^1\chi(T')$ implies $c_6(T) = c_6(T')$, but the converse of these do not hold (examples 3.5 and 3.7).

Finally, in [2, Thm 3.4] we consider the set of all cospectral classes of trees with a fixed number of vertices which have a unique vertex of degree greater than 2 and show that over this set, the Randić index is monotone increasing with respect to the (lexicographic) linear order " $\leq$ " defined as follows:

$$T = T' \Leftrightarrow c_i(T) = c_i(T') \text{ for all } i$$

and $T < T' \Leftrightarrow$ there exists $r \in \mathbb{N}$ such that $|c_r(T)| < |c_r(T')|$ and $c_i(T) = c_i(T')$ for $i < r$

Using our previous results we give in corollary 3.8 new sets over which the Randić index is monotone increasing.

2 Randić Index of a Chemical Tree

In this section we derive formulas for ${}^0\chi$ and ${}^1\chi$ of a chemical tree and show that ${}^0\chi$ is completely determined by the numbers k_3 and k_4 (corollary 2.2). Moreover, for trees with maximal degree 3, we show in corollary 2.5 that ${}^1\chi$ is completely determined by the numbers e_{13} and e_{33}.

Theorem 2.1. *Let T be a chemical tree with n vertices. Then*

$$6\chi^0(T) = 3\sqrt{2}n + \alpha k_3 + \beta k_4 + (12 - 6\sqrt{2})$$

where $\alpha = 6 - 6\sqrt{2} + 2\sqrt{3}$ and $\beta = 15 - 9\sqrt{2}$.

Proof: We know that

$$\chi^0(T) = k_1 + k_2\frac{\sqrt{2}}{2} + k_3\frac{\sqrt{3}}{3} + k_4\frac{1}{2}$$

The result follows from the relations

$$k_3 + 2k_4 + 2 = k_1$$
$$k_1 + k_2 + k_3 + k_4 = n.$$

□

In our next result we show that ${}^0\chi$ is completely determined by the numbers k_3 and k_4:

Corollary 2.2. *Let T and T' be chemical trees with n vertices. The following conditions are equivalent:*

(a) $\chi^0(T) = \chi^0(T')$;

(b) $k_3 = k_3'$ *and* $k_4 = k_4'$.

Proof: $(a) \Rightarrow (b)$ Assume that $\chi^0(T) = \chi^0(T')$. Then by theorem 2.1,

$$\begin{aligned} 0 = \chi^0(T) - \chi^0(T') &= \alpha(k_3 - k_3') + \beta(k_4 - k_4') \\ &= [6(k_3 - k_3') + 15(k_4 - k_4')] + \sqrt{2}\,[-6(k_3 - k_3') - 9(k_4 - k_4')] \\ &\quad + \sqrt{3}\,[2(k_3 - k_3')] \end{aligned}$$

Since $\{1, \sqrt{2}, \sqrt{3}\}$ is a linearly independent set over $\mathbb{Q}$, we conclude that $k_3 = k_3'$ and $k_4 = k_4'$. $(b) \Rightarrow (a)$ is an immediate consequence of theorem 2.1. □

Theorem 2.3. *Let T be a chemical tree with n vertices. Then*

$$\begin{aligned} 24 \cdot {}^1\chi(T) = 12n + k_3\rho + k_4\xi + e_{13}\eta + e_{14}\mu + e_{33}\gamma \\ + e_{34}\delta + e_{44}\varepsilon + (24\sqrt{2} - 36) \end{aligned}$$

where $\rho = 12\sqrt{2} + 12\sqrt{6} - 48$, $\xi = 48\sqrt{2} - 72$, $\eta = 8\sqrt{3} - 12\sqrt{2} - 4\sqrt{6} + 12$, $\mu = 24 - 18\sqrt{2}$, $\gamma = 20 - 8\sqrt{6}$, $\delta = -4\sqrt{6} - 6\sqrt{2} + 4\sqrt{3} + 12$ *and* $\varepsilon = 18 - 12\sqrt{2}$.

Proof: This is a consequence of the fact that

$$\begin{aligned} {}^1\chi(T) = e_{12}\frac{\sqrt{2}}{2} + e_{13}\frac{\sqrt{3}}{3} + e_{22}\frac{1}{2} + e_{23}\frac{\sqrt{6}}{6} + e_{33}\frac{1}{3} + \\ e_{14}\frac{1}{2} + e_{24}\frac{\sqrt{8}}{8} + e_{34}\frac{\sqrt{12}}{12} + e_{44}\frac{1}{4} \end{aligned}$$

bearing in mind that

$$\begin{aligned} e_{12} + e_{13} + e_{14} &= k_3 + 2k_4 + 2 \\ e_{23} &= 3k_3 - e_{13} - 2e_{33} - e_{34} \\ e_{24} &= 4k_4 - e_{14} - 2e_{44} - e_{34} \\ e_{22} &= n - 3 + e_{33} + e_{34} + e_{44} + e_{13} + e_{14} - 6k_4 - 4k_3. \end{aligned}$$

□

Now, assume that T and T' are chemical trees with n vertices and further assume that $k_3 = k_3'$ and $k_4 = k_4'$, or equivalently, ${}^0\chi(T) = {}^0\chi(T)$ (corollary 2.2). Then, by our previous theorem,

$$\begin{aligned} 24 \cdot [{}^1\chi(T) - {}^1\chi(T')] = \eta(e_{13} - e_{13}') + \mu(e_{14} - e_{14}') + \gamma(e_{33} - e_{33}') + \\ + \delta(e_{34} - e_{34}') + \epsilon(e_{44} - e_{44}') \end{aligned}$$

where η, μ, γ, δ and ϵ are defined as in theorem 2.3. The following question arises naturally for chemical trees: is ${}^1\chi$ determined by the numbers e_{ij}? That is,

$$e_{ij} = e'_{ij} \text{ for every } i \leq j \in \{1,3,4\} \Leftrightarrow {}^1\chi(T) = {}^1\chi(T')?$$

Clearly, $e_{ij} = e'_{ij}$ for every $i \leq j \in \{1,3,4\}$ implies ${}^1\chi(T) = {}^1\chi(T')$ but in general this is not true since the numbers $\eta,\mu,\gamma,\delta,\epsilon \in \mathbb{Q}(\sqrt{2},\sqrt{3})$ are not linearly independent over $\mathbb{Q}$: $6\eta - 4\mu + 3\gamma - 12\delta + 6\epsilon = 0$

Example 2.4: *Let T and T' be trees such that $e_{13} - e'_{13} = 6$, $e_{14} - e'_{14} = -4$, $e_{33} - e'_{33} = 3$, $e_{34} - e'_{34} = -12$ and, $e_{44} - e'_{44} = 6$. Then ${}^1\chi(T) = {}^1\chi(T')$ although $e_{ij} \neq e'_{ij}$ for every $i \leq j \in \{1,3,4\}$ (see figure 1).*

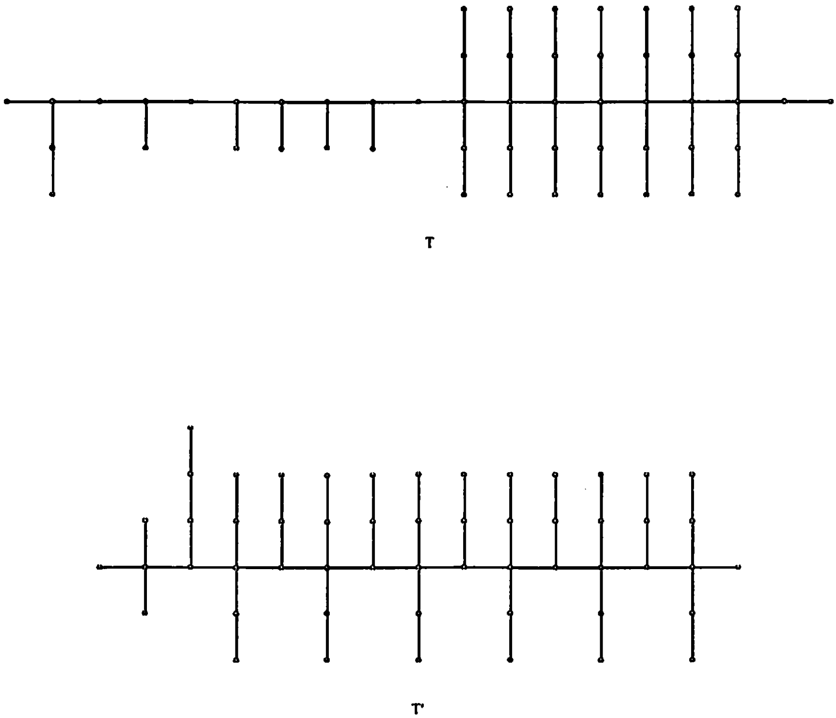

Figure 1

Note that $k_3 = k'_3$ and $k_4 = k'_4$.

However, ${}^1\chi$ is completely determined by the e_{ij} for chemical trees of maximal degree 3 as we can see in the following result:

Corollary 2.5. *Let T and T' be chemical trees with n vertices such that $\Delta(T) \leq 3$, $\Delta(T') \leq 3$ and $k_3 = k'_3$. The following conditions are equivalent:*

(a) ${}^1\chi(T) = {}^1\chi(T')$;

(b) $e_{13} = e'_{13}$ *and* $e_{33} = e'_{33}$.

Proof: (a)$\Rightarrow$(b). If ${}^1\chi(T) = {}^1\chi(T')$ then, by theorem 2.3, $0 = \eta(e_{13} - e'_{13}) + \gamma(e_{33} - e'_{33})$. Consequently,

$$\begin{aligned} 0 &= \eta(e_{13} - e'_{13}) + \gamma(e_{33} - e'_{33}) \\ &= [12(e_{13} - e'_{13}) + 20(e_{33} - e'_{33})] + [-12(e_{13} - e'_{13})]\sqrt{2} + \\ &\quad [8(e_{13} - e'_{13})]\sqrt{3} + [-8(e_{33} - e'_{33})]\sqrt{6} \end{aligned}$$

Now, since $\{1, \sqrt{2}, \sqrt{3}, \sqrt{6}\}$ is a linearly independent set over $\mathbb{Q}$, we conclude that $e_{13}(T) = e_{13}(T')$ and $e_{33}(T) = e_{33}(T')$. (b)$\Rightarrow$(a) follows immediately from theorem 2.3. □

3 Randić Index and Lexicographic Order for Chemical Trees

In this section we determine the coefficients $c_4(T)$ and $c_6(T)$ of the characteristic polynomial $\lambda^n + c_1(T)\lambda^{n-1} + \cdots + c_{n-1}(T)\lambda + c_n(T)$ associated to the adjacency matrix of a chemical tree T in terms of the degree structure of T (theorem 3.3) and establish a comparison with ${}^0\chi$ and ${}^1\chi$ (corollaries 3.4 and 3.6). As a consequence, we define in corollary 3.8 new sets over which the Randić index is monotone increasing with respect to the lexicographic order.

It is well known (see [3]) that the odd coefficients $c_{2r+1}(T)$ are zero, and the even coefficients $c_{2r}(T)$ are given by the rule that $(-1)^r c_{2r}$ is the number of ways of choosing r disjoint edges in the tree T. This result will be used in the sequel.

Given a tree T such that $\Delta(T) \leq 3$, a 3-vertex w_0 of T and w_i $(i = 1, 2, 3)$ the adjacent vertices of w_0, we can define the following subtrees of T :

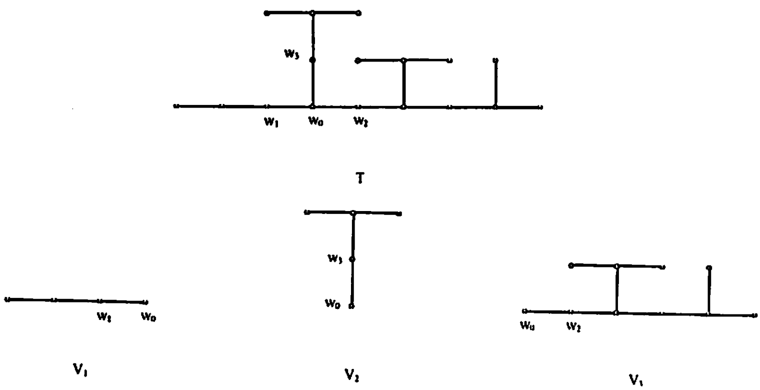

Figure 2

where $w_i \in V_i$. Note that it is possible to choose w_0 such that $\Delta(V_i) \leq 2$ for some $i \in \{1, 2, 3\}$. Define $W_i = Vi \backslash [w_0, w_i]$ for $i = 1, 2, 3$.

Theorem 3.1. *Let T be a chemical tree with n vertices and $\Delta(T) \leq 3$. Then*

$$2c_4(T) = (n-1)^2 - 3(n-1) - 2(k_3(T) - 1)$$

Proof: We use induction on $k_3(T)$. If $k_3(T) = 0$ then $T = P_n$, the path tree of n vertices, and so

$$\begin{aligned} 2c_4(T) &= (n-3)(n-2) = n^2 - 5n + 6 \\ &= (n-1)^2 - 3(n-1) + 2(0-1) \end{aligned}$$

Now, assume that the result is true for trees with k 3-vertices, $k \geq 0$ and let T be a tree with n vertices such that $k_3(T) = k + 1$. Choose w_0 as in figure 2 and assume that $\Delta(V_1) \leq 2$. Let v_0 be the 1-vertex of V_1 and $d = d(v_0, w_0)$. Consider now the subtree $S = T \backslash V_1$ of T. Clearly, $k_3(S) = k$ so by our inductive hypothesis,

$$2c_4(S) = (n-d-1)^2 - 3(n-d-1) - 2(k-1)$$

To find $c_4(T)$ we look at the following table which indicates every possible way of choosing two disjoint edges in T :

edges in S	edges in $V_1 = P_{d+1}$	Formula
2	0	$c_4(S)$
0	2	$c_4(P_{d+1})$
1	1	$c_2(S)c_2(W_1) + c_2(W_2) + c_2(W_3)$

Hence,

$$\begin{aligned} 2c_4(T) &= 2c_4(S) + 2c_4(P_{d+1}) + 2c_2(S)c_2(W_1) + 2(c_2(W_2) + c_2(W_3)) \\ &= (n-d-1)^2 - 3(n-d-1) - 2(k-1) + (d-2)(d-1) \\ &\quad + 2(n-d-1)(d-1) + 2(n-d-3) \\ &= (n-1)^2 - 3(n-1) - 2k. \end{aligned}$$

□

Theorem 3.2. *Let T be a chemical tree with n vertices and $\Delta(T) \leq 3$. Then*

$$\begin{aligned} -6c_6(T) = (n-1)^3 - 9(n-1)^2 + (26 - 6k_3(T))(n-1) \\ - 6(4 + e_{13}(T) - e_{33}(T) - 6k_3(T)) \end{aligned}$$

Proof: We use induction on $k_3(T)$. If $k_3(T) = 0$ then $T = P_n$, $e_{13}(T) = e_{33}(T) = 0$ and

$$-6c_6(P_n) = (n-5)(n-4)(n-3) = n^3 - 12n^2 + 47n - 60$$
$$= (n-1)^3 - 9(n-1)^2 + 26(n-1) - 24$$

Assume that the result holds for every $k \geq 0$ and let T be a tree with n vertices such that $k_3(T) = k+1$. With the same notation as in the previous theorem, the following table shows how to find $c_6(T)$:

edges in $V_1 = P_{d+1}$	edges in S	Formula
3	0	$-c_6(P_{d+1})$
0	3	$-c_6(S)$
2	1	$c_4(P_{d+1})(-c_2(S)-2) + 2c_4(W_2)$
1	2	$c_4(S)(-c_2(W_2)) + c_4(W_2) + c_4(W_3) + c_2(W_2)c_2(V$

Assume first that $d > 1$ (in particular, $e_{13}(S) = e_{13}(T)$). We have the formulas

$$-6c_6(P_{d+1}) = (d-4)(d-3)(d-2) = d^3 - 9d^2 + 26d - 24,$$
$$6c_4(P_{d+1}) = 3(d-2)(d-1) = 3d^2 - 9d + 6,$$
$$12c_4(W_2) = 6(d-3)(d-2) = 6d^2 - 30d + 36 \text{ and}$$
$$-c_2(W_2) = d-1$$

On the other hand, $k_3(S) = k$. The number of 3-vertices in W_2 and W_3, $k_3(W_2)$ and $k_3(W_3)$, and $e_{33}(S)$ depends on the degree of w_2 and w_3:

$\delta(w_2)$	$\delta(w_3)$	$e_{33}(S)$	$k_3(W_2) + k_3(W_3)$
2	2	$e_{33}(T)$	k
2	3	$e_{33}(T) - 1$	$k-1$
3	3	$e_{33}(T) - 2$	$k-2$

We have all data needed to calculate $c_6(T)$. In the first case, by induction,

$$-6c_6(S) = (n-d-1)^3 - 9(n-d-1)^2 + (26-6k)(n-d-1)$$
$$- 6(4 + e_{13}(T) - e_{33}(T) - 6k)$$

Set $-c_2(W_2) = a_2$ and $-c_2(W_3) = a_3$. By our previous theorem,

$$6c_4(W_2) = 3a_2^2 - 9a_2 - 6(k_3(W_2) - 1)$$

and

$$6c_4(W_3) = 3a_3^2 - 9a_3 - 6(k_3(W_3) - 1)$$

Set $x = n-d-1$. Since $a_2 + a_3 = x - 2$ and $k_3(W_2) + k_3(W_3) = k$

$$6c_4(W_2) + 6c_4(W_3) + 6c_2(W_2)c_2(W_3) = 3(a_2^2 + a_3^2 + 2a_2a_3) - 9(a_2 + a_3)$$
$$- 6(k_3(W_2) + k_3(W_3) - 2)$$
$$= 3(x-2)^2 - 9(x-2) - 6(k-2)$$
$$= 3x^2 - 21x + 30 - 6(k-2).$$

It follows that

$$\begin{aligned}
-6c_6(T) &= d^3 - 9d^2 + 26d - 24 + x^3 - 9x^2 + (26-6k)x \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) - 6k) \\
&\quad + (3d^2 - 9d + 6)(x-2) + 6d^2 - 30d + 36 \\
&\quad + (3x^2 - 9x - 6(k-1))(d-1) + 3x^2 - 21x + 30 - 6(k-2) \\
&= (d+x)^3 - 9(d+x)^2 + (20-6k)(d+x) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) - 6k - 6) \\
&= \quad (n-1)^3 - 9(n-1)^2 + (26 - 6(k+1))(n-1) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) - 6(k+1)).
\end{aligned}$$

In the second case,

$$\begin{aligned}
-6c_6(S) &= (n-d-1)^3 - 9(n-d-1)^2 + (26-6k)(n-d-1) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) + 1 - 6k),
\end{aligned}$$

$6c_4(W_2)$ and $6c_4(W_3)$ are exactly the same as above except that $k_3(W_2) + k_3(W_3) = k-1$. Thus, the only difference from the previous case is the constant term in the $(n-1)$-polynomial which in this case is $-6(4+e_{13}(T)-e_{33}(T)+1-6k)+6(k-1)-6(k-3)+30 = -6(4+e_{13}(T)-e_{33}(T)-6(k+1))$.

In the last case,

$$\begin{aligned}
-6c_6(S) &= (n-d-1)^3 - 9(n-d-1)^2 + (26-6k)(n-d-1) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) + 2 - 6k)
\end{aligned}$$

and the rest is as above but $k_3(W_2) + k_3(W_3) = k-2$. Therefore, the constant term in the $(n-1)$-polynomial is $-6(4 + e_{13}(T) - e_{33}(T) + 2 - 6k) + 6(k-1) - 6(k-4) + 30 = -6(4 + e_{13}(T) - e_{33}(T) - 6(k+1))$.

If $d = 1$

$$-6c_6(T) = -6c_6(S) + 6c_4(W_2) + 6c_4(W_3) + 6c_2(W_2)c_2(W_3)$$

where $e_{13}(S) = e_{13}(T) - 1$. Again we analyze each of the three cases. In the first case

$$\begin{aligned}
-6c_6(T) &= x^3 - 9x^2 + (26-6k)x - 6(4 + (e_{13}(T) - 1) - e_{33}(T) - 6k) \\
&\quad + 3x^2 - 21x + 30 - 6(k-2) \\
&= \quad x^3 - 6x^2 + (5-6k)x - 6(4 + e_{13}(T) - e_{33}(T) - 5k - 8) \\
&= (x+1)^3 - 9(x+1)^2 - (26 - 6(k+1))(x+1) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) - 6(k+1)) \\
&= (n-1)^3 - 9(n-1)^2 - (26 - 6(k+1))(n-1) \\
&\quad - 6(4 + e_{13}(T) - e_{33}(T) - 6(k+1))
\end{aligned}$$

The second and third case for $d = 1$ are similar to those of $d > 1$ and are left to the reader. □

Similar arguments as in the proof of theorems 3.4 and 3.2 using induction on $k_4(T)$ (note that $k_4(T) = 0$ implies $\Delta(T) \leq 3$) allows us to extend theorems 3.1 and 3.2 to chemical trees:

Theorem 3.3. *Let T be a chemical tree with n vertices. Then*

$$2c_4(T) = (n-1)^2 - 3(n-1) - 2(k_3(T) + 3k_4(T) - 1)$$

and

$$\begin{aligned}-6c_6(T) = (n-1)^3 - 9(n-1)^2 + [26 - 6(k_3(T) + 3k_4(T))](n-1) - \\ 6(4 + 2e_{14}(T) + e_{13}(T) - e_{33}(T) - 2e_{34}(T) - 4e_{44}(T) \\ - 6k_3(T) - 20k_4(T)).\end{aligned}$$

□

It is feasible at this point to establish a comparison $c_4(T)$ versus ${}^0\chi(T)$ and $c_6(T)$ versus ${}^1\chi(T)$ for a chemical tree T (see theorems 2.1, 2.3 and 3.3).

Corollary 3.4. *Let T and T' be chemical trees with n vertices. If ${}^0\chi(T) = {}^0\chi(T')$ then $c_4(T) = c_4(T')$*

Proof: If ${}^0\chi(T) = {}^0\chi(T')$ then, by corollary 2.2, $k_3 = k_3'$ and $k_4 = k_4'$. The result follows applying theorem 3.3. □

Example 3.5: *In general, the converse of corollary 3.4 is false. Consider the following trees:*

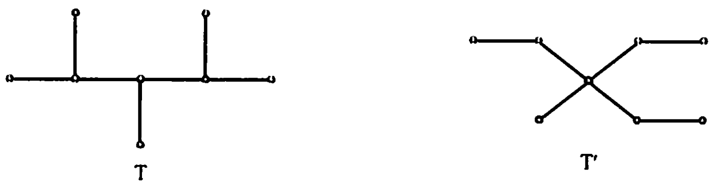

Figure 3

Since $k_3 + 3k_4 = k'_3 + 3k'_4$ we know, by theorem 3.3, that $c_4(T) = c_4(T')$. However, ${}^0\chi(T) \neq {}^0\chi(T')$ by corollary 2.2.

Corollary 3.6. *Let T and T' be chemical trees with n vertices, $\Delta(T) \leq 3$, $\Delta(T') \leq 3$ and $k_3 = k'_3$. If ${}^1\chi(T) = {}^1\chi(T')$ then $c_6(T) = c_6(T')$.*

Proof: If ${}^1\chi(T) = {}^1\chi(T')$ then, by corollary 2.5, $e_{13} = e'_{13}$ and $e_{33} = e'_{33}$. Therefore, by theorem 3.3, we conclude that $c_6(T) = c_6(T')$. □

Example 3.7: *In general, the converse of corollary 3.6 does not hold. For example, consider the following trees*

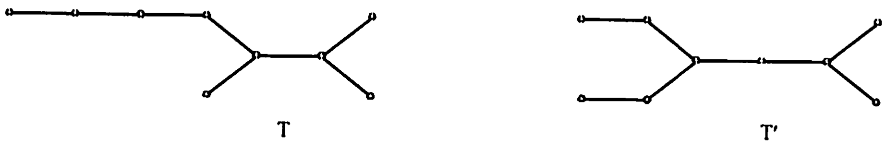

Figure 4

It is clear that $e_{13} - e'_{13} = e_{33} - e'_{33} = 1$ hence, by theorem 3.3, $c_6(T) = c_6(T')$. However, by corollary 2.5, ${}^1\chi(T) \neq {}^1\chi(T')$. □

In ([2]) we analyze the problem whether the Randić index is monotone increasing over the linear ordered set of all cospectral classes of trees with a fixed number of vertices. As we pointed out in [2, Thm 3.4], it is true over Ω_n, the set of all cospectral classes of trees with n vertices and unique vertex of degree greater than 2. We can use our previous results to define new sets over which the Randić index is monotone increasing:

Corollary 3.8. *Let T and T' be chemical trees with n vertices, $\Delta(T) \leq 3$, $\Delta(T') \leq 3$, $k_3 = k'_3$ and $e_{33} = e'_{33}$. Then*

$$c_6(T) = c_6(T') \Leftrightarrow e_{13} = e'_{13} \Leftrightarrow {}^1\chi(T) = {}^1\chi(T')$$
$$c_6(T) < c_6(T') \Leftrightarrow e_{13} < e'_{13} \Leftrightarrow {}^1\chi(T) > {}^1\chi(T')$$

In particular, ${}^1\chi$ is monotone increasing over the set of all cospectral classes of trees of maximal degree 3, with a fixed number of vertices n, k_3 and e_{33}.

Proof: First of all, $c_2(T) = c_2(T')$ since T and T' have the same number of vertices and $k_3 = k_3'$ implies, by corollaries 2.2 and 3.4, that $c_4(T) = c_4(T')$. Now, by theorem 3.3, bearing in mind that $e_{33} = e_{33}'$ we deduce that $-6\,[c_6(T) - c_6(T')] = -6(e_{13} - e_{13}')$. On the other hand, by theorem 2.3, $24\cdot[{}^1\chi(T) - {}^1\chi(T')] = \eta(e_{13} - e_{13}')$. It follows easily from here the first part of the result. To see that ${}^1\chi$ is monotone increasing assume that $T \leq T'$. Then, $|c_6(T)| \leq |c_6(T')|$ or, equivalently, $c_6(T) \geq c_6(T')$. Hence, by the first part of this result, ${}^1\chi(T) \leq {}^1\chi(T')$. □

Example:3.9 *In tables 1 and 2 we list all trees with* $n = 10$, $k_3 = 2$ *and* $e_{33} = 0$ *and* $n = 10$, $k_3 = 2$ *and* $e_{33} = 1$, *respectively, ordered lexicographically.*

As we can see, in tables 1 and 2 the Randić index ${}^1\chi$ is monotone increasing as we should expect from corollary 3.8. □

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