Some Bounds for the Connectivity Index of a Chemical Graph

O. Araujo†

Departamento de Matemáticas, Facultie de Ciencias, Universidad de los Andes, Mérida, Venezuela

J. A. De la Peña*,‡

Instituto de Matemáticas, UNAM, México 04510 D. F., México

Received February 3, 1998

Let G be a simple graph. We say that G is a *chemical graph* if G is connected and the degree $d_i \leq 4$ for every vertex i. We consider the *connectivity index* $^1\chi(G)$ of a chemical graph G. We use some graph theoretic constructions to find bounds for $^1\chi(G)$ which depend only on the number of vertices, the ramification index, and the cyclomatic number of the graph G. The results are related to the problem of graph reconstruction from a collection of graph invariants.

Let G be a simple graph, that is, G does not have loops or multiple edges. Let $\{1, ..., n\}$ be the set of vertices of G and d_i denote the degree of a vertex i. We say that G is a *chemical graph* if G is connected and $d_i \leq 4$ for every $1 \leq i \leq n$.

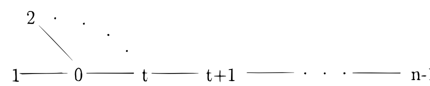
Chemical graphs are pictorical representations of certain organic molecules. Indeed, a saturated hydrocarbon may be represented as a chemical graph whose vertices are the carbon atoms and the edges represent the electronic bonds.[1,2] Many graph invariants have been introduced attempting to find relations between the graph structure and physicochemical properties of organic molecules. In 1975, Randić[3] introduced the *connectivity index* (now called also *Randić index*) as

$$^1\chi(G) = \sum_{i-j} \frac{1}{\sqrt{d_i d_j}}$$

where $i-j$ runs over all the edges of G. This index has been successfully related to chemical properties, namely if G is the molecular graph of an alkane, then $^1\chi(G)$ has a strong correlation with the boiling point and the stability of the compound.[1,4,5]

The purpose of this work is to obtain a priori bounds for $^1\chi(G)$ when G is a chemical graph. Previous results[6] by the authors related $^1\chi(G)$ and the eigenvalues of the corresponding Laplacian matrix. In particular, it is shown that $^1\chi(G) \leq {}^1/_2 n$.

Let T be a tree, that is, T is a graph which has no circuits. We define the *ramification index* of T as $r(T) = \sum_{d_i \geq 3}(d_i - 2)$. For any number $n \in \mathbb{N}$, we denote by A_n the linear graph with n vertices. For $2 \leq t \leq n - 1$, we denote by $T(n, t)$ the following graph which has $r(T(n, t)) = t - 2$ (not necessarily a chemical graph).



Theorem 1. *Let T be a chemical graph which is a tree with n vertices and $r(T) = t - 2$. Then we have*

$$^1\chi(T(n, t)) - c_0(r(T) - 1) \leq {}^1\chi(T) \leq {}^1\chi(A_n) - a_0 r(T)$$

where $a_0 = 1 - \sqrt{3}/3 - \sqrt{6}/6 (\approx 0.01440)$ *and* $c_0 = 0$ *if* $r(T) = 0$ *and otherwise* $c_0 = \sqrt{3}/2 - 3/4 (\approx 0.1160)$.

For a general chemical graph G we obtain bounds in the following way. Let $g(G)$ be the *cyclomatic number* of G, that is, the minimal number of edges that have to be deleted from G to get a connected tree. We have the following.

Theorem 2. Let *G be a chemical graph and T be a maximal subgraph of G which is a tree. Then we have*

$$^1\chi(T) - d_0 g(G) \leq {}^1\chi(G) \leq {}^1\chi(T) + b_0 g(G)$$

where $b_0 = -\sqrt{2}/4 + \sqrt{3}/3 + \sqrt{6}/6 - 1/2 (\approx 0.13204)$ *and* $d_0 = \sqrt{2} + \sqrt{3}/6 - 3/2 (\approx 0.2028)$. *In particular if G has n vertices and $r(T) = t - 2$, then*

$$^1\chi(T(n, t)) - c_0(r(T) - 1) - d_0 g(G) \leq {}^1\chi(G) \leq {}^1\chi(A_n) - a_0 r(T) + b_0 g(G)$$

The proof of the theorems is based on some operations on graphs that we introduce in section 2. The proof of the theorems is given in section 3.

The bounds given in the above theorems should be considered in the context of the "inverse" problems in chemistry. These problems consider the construction of structures (molecules) which possess a given set of physical properties (graph invariants). This kind of problem has been addressed by Kier and Hall[7] and Kvasnička,[8] among others. We refer to the work of Milne[9] for a more complete account.

† E-mail: araujo@ciens.ula.ve.
‡ E-mail: jap@penelope.matem.unam.mx.

S0095-2338(98)00012-2 CCC: $15.00
Published on Web 08/19/1998

In our case, given a value for the connectivity index κ, the bounds in theorems 1 and 2 show that only certain chemical graphs G with number of vertices n, ramification index $r(T)$ for a maximal subgraph T of G which is a tree, and cyclomatic number $g(G)$ may have ${}^1\chi(G) = \kappa$. The invariants n, $r(T)$, and $g(G)$ associated to G yield valuable information on the structure of the graph G.

1. EXAMPLES AND PRELIMINARY CALCULATIONS

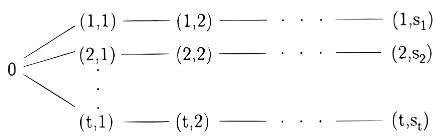
1.1. Consider the linear graph A_n:

$$1 - 2 - \cdots - n - 1 - n$$

Then ${}^1\chi(A_n) = {}^1\!/_2 n - ({}^3\!/_2 - \sqrt{2})$.

Given numbers $2 \le t \le n - 1$, we consider the tree $T(n, t)$ as in the introduction. Then ${}^1\chi(T(n, t)) = \sqrt{t} + ({}^1\!/_{\sqrt{2}} - 1)\ {}^1\!/_{\sqrt{t}} + (n-t-2)/2 + {}^{\sqrt{2}}\!/_2$ in case $t < n - 1$ and ${}^1\chi(T(n, n - 1)) = \sqrt{n-1}$.

Given numbers $s_1 \ge s_2 \ge \cdots \ge s_t \ge 1$, we consider the tree graph $T(s_1, s_2, ..., s_t)$ defined in the following graphic.



Observe that $T(n, t)$ is short for $T(n - t, 1, ..., 1)$. The following result will be useful.

Lemma. *Let $t \ge 2$ and $s_1 \ge s_2 \ge \cdots \ge s_t \ge 1$ be a sequence of numbers with $n = 1 + \sum_{i=1}^t s_i$. Then ${}^1\chi(T(s_1, s_2, ..., s_t)) \ge {}^1\chi(T(n, t))$.*

Proof: Let $1 \le m \le t$ be such that $s_1 \ge s_2 \ge \cdots s_m \ge 2$ and $s_{m+1} = \cdots = s_t = 1$. Then we have

$$
\begin{aligned}
{}^1\chi(T(s_1, ..., s_t)) &= \sum_{i=1}^{m}\frac{(s_i - 2)}{2} + \frac{m}{\sqrt{2}} + \frac{m}{\sqrt{2t}} + \frac{(t-m)}{\sqrt{t}} \\
&= \frac{n}{2} - \frac{t}{2} + \sqrt{t} - \frac{1}{2} + \\
&\qquad m\left[\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{t}} - \frac{1}{2}\right]
\end{aligned}
$$

The number in the last parentheses is non-negative for $t \ge 2$. Hence

$$
{}^1\chi(T(s_1, ..., s_t)) \ge \frac{n}{2} - \frac{t}{2} + \sqrt{t} - \frac{1}{2} + \left[\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2t}} - \frac{1}{\sqrt{t}} - \frac{1}{2}\right] = {}^1\chi(T(n, t))
$$

1.2. In our calculations in the next section we shall repeatedly encounter functions of the form h_A: $[2, \infty) \to \mathrm{R}$ with

$$h_A(x) = \sqrt{x - 1} - \sqrt{x} + \frac{A}{\sqrt{x}}$$

where A is a constant.

Lemma. For $-4 \le A < {}^1\!/_2$, *the function $h_A(x)$ is monotonically increasing on* $[2, \infty)$.

Proof: The points x such that $h'_A(x) = 0$ satisfy the equation $(2A - 1)x^2 + (A^2 - 2A)x - A^2 = 0$ with roots $[(2A - A^2) \pm A\sqrt{A^2+4A}]/(4A - 2)$ which are either imaginary or smaller that 2 for $-4 \le A < {}^1\!/_2$.

Using Taylor expansion, we get that $h_A(x) = (A - {}^1\!/_2)\, x^{-1/2} + {}^1\!/_8 x^{-3/2} + ...$ where the dots stand for terms of smaller order. Hence $h_A(x) < 0$ for $x \gg 0$ if $A < {}^1\!/_2$. Moreover, $\lim_{x\to\infty} h_A(x) = 0$. The statement follows.

1.3. For the sake of completeness we recall the bounds[6] for ${}^1\chi(G)$. If G is a graph without loops or multiple edges and vertices 1, ..., n, *the Laplacian* L of G is the $n \times n$ matrix with entries

$$
\mathsf{L}(i, j) = \begin{cases} 1, & \text{if } i = j \text{ and } d_i \ne 0 \\ -\dfrac{1}{\sqrt{d_i d_j}}, & \text{if } i - j \\ 0, & \text{else} \end{cases}
$$

As shown by Chung,[10] L has eigenvalues $0 = \lambda_1 \le \cdots \le \lambda_{n-1}$.

Theorem.[6] *The following inequalities hold:*

$$\frac{1}{2}[n - \lambda_{n-1}(n - \kappa)] \le {}^1\chi(G) \le \frac{1}{2}[n - \lambda_1(n - \kappa)]$$

where κ is a graph invariant defined as $\kappa = (\sum_{i=1}^n \sqrt{d_1})^2/(\sum_{i=1}^n d_i)(\le n)$. Moreover, ${}^1\chi(G) = {}^1\!/_2 n$ (and $\kappa = n$) if and only if G is regular.

Corollary. *Let G be a chemical graph, then the following inequalities hold:*

$$\frac{1}{2}n\left[1 - \frac{3}{2}\lambda_{n-1}\right] \le {}^1\chi(G) \le \frac{1}{2}\left[n - \frac{1}{8n^2}(n - \kappa)\right]$$

Proof: Since G is chemical, we have

$$\mathrm{vol}\ G = \sum_{i=1}^{n} d_i \le 4n$$

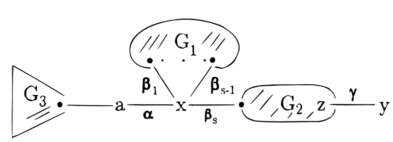
Hence $0 \le n - \kappa \le {}^3\!/_4 n$ and the first inequality follows. On the other hand, by Cheeger's inequality[10] we have

$$\lambda_1 \ge \frac{2}{(\mathrm{vol}\ G)^2} \ge \frac{1}{8n^2}$$

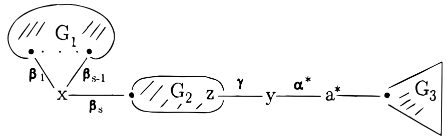
which implies the second inequality.

2. TWO OPERATIONS ON GRAPHS

2.1. Let G be a connected simple graph with vertices 1 ..., n. Let x, y be vertices of G with $d_x \ge 3$ and $d_y = 1$ such that G has the following structure



where each of the graphs G_1 and G_2 consists of at least one vertex and G_3 may be empty (and then $d_a = 1$). Observe that $d_a \le 2 \le d_z$ and $s = d_x - 1$. We define a new graph $G^{(x,y)}$ as follows:



Observe that $G^{(x,y)}$ is a connected simple graph; if G is chemical, then $G^{(x,y)}$ is chemical. Moreover, $r(G^{(x,y)}) = r(G) - 1$.

Lemma. *If G is a chemical graph, then ${}^1\chi(G^{(x,y)}) \geq {}^1\chi(G) + a_0$.*

Proof: Observing that $x \neq z$ in the above pictures, we get

$$^1\chi(G^{(x,y)}) - {}^1\chi(G) = \sum_{\alpha\neq\beta:x-b} \frac{1}{\sqrt{d_b}}\left(\frac{1}{\sqrt{d_x-1}} - \frac{1}{\sqrt{d_x}}\right) + \frac{1}{\sqrt{d_z}}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{1}{\sqrt{2d_a}}\left(1 - \frac{\sqrt{2}}{\sqrt{d_x}}\right)$$

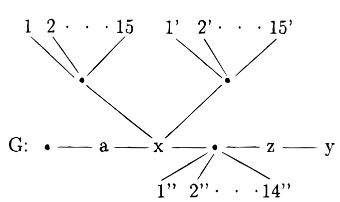
The first summand is positive and has minimal value when $d_b = 4$; the second and third summands reach minimal values when $d_z = 2 = d_a$. Hence,

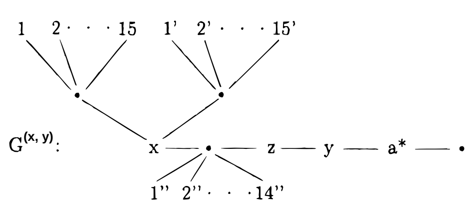
$$^1\chi(G^{(x,y)}) - {}^1\chi(G) \geq \frac{1}{2}(d_x - 1)\left(\frac{1}{\sqrt{d_x-1}} - \frac{1}{\sqrt{d_x}}\right) + \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2d_x}} = \frac{1}{2}h_A(d_x) + \left(1 - \frac{1}{\sqrt{2}}\right)$$

where $A = 1 - \sqrt{2}$ and $h_A(t)$ is the function defined in (1.2). Therefore,

$$^1\chi(G^{(x,y)}) - {}^1\chi(G) \geq \frac{1}{2}h_A(3) + \left(1 - \frac{1}{\sqrt{2}}\right) = a_0$$

2.2. We want to remark that if G is not chemical, then ${}^1\chi(G^{(x,y)}) \geq {}^1\chi(G)$ may fail. Consider the following *example*:

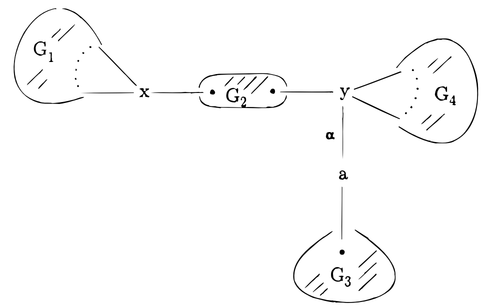




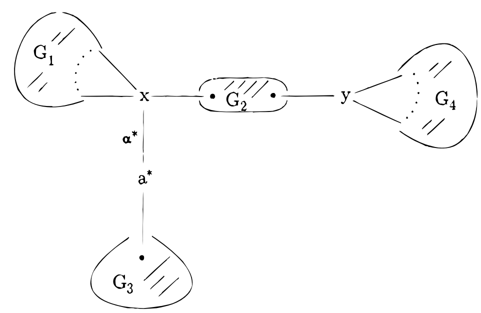
Then,

$$^1\chi(G) = \frac{1}{8}(91 + 11\sqrt{2}) \sim 15.26 \text{ and } {}^1\chi(G^{(x,y)}) = 12 + \frac{3}{8}\sqrt{2} + \frac{1}{4}\sqrt{3} \sim 15.06.$$

2.3. We shall introduce now a second operation on graphs. Let G be a connected simple graph and x, y be two vertices with $d_x \geq d_y \geq 3$. Assume that G has the following structure



where G_1 (respectively, G_4) has at least two (respectively, one) vertices and G_2, G_3 may be empty (if G_2 is empty, then x and y are neighbors; if G_3 is empty, then $d_a = 1$). Then we define a new graph $G_{(x,y)}$ as follows:



Observe that $r(G_{(x,y)}) = r(G)$.

Lemma. *Let G and $G_{(x,y)}$ be as above. Suppose that $d_i \leq 4$ for every vertex $i \neq x$ in G. Then ${}^1\chi(G_{(x,y)}) - (\sqrt{3}/2 - 3/4) \leq {}^1\chi(G)$.*

Proof: We distinguish two situations.

Assume that $G_2 \neq \varnothing$, that is, x and y are not neighbors. Then

$$^1\chi(G_{(x,y)}) - {}^1\chi(G) = \sum_{x-b\neq a^*} \frac{1}{\sqrt{d_b}}\left[\frac{1}{\sqrt{d_x+1}} - \frac{1}{\sqrt{d_x}}\right] + \sum_{y-c\neq a} \frac{1}{\sqrt{d_c}}\left[\frac{1}{\sqrt{d_y-1}} - \frac{1}{\sqrt{d_y}}\right] + \frac{1}{\sqrt{d_a}}\left[\frac{1}{\sqrt{d_x+1}} - \frac{1}{\sqrt{d_y}}\right]$$

The first summand is negative and takes its maximal value when $d_b = 4$ for all $x{-}b \neq a^*$ (since $d_i \leq 4$ for all $i \neq x$); the second summand is positive and reaches its maximal value when $d_c = 1$ for all $y{-}c \neq a$; finally, the third summand has maximal value when $d_a = 2$. Therefore,

$$^1\chi(G_{(x,y)}) - {}^1\chi(G) \leq \frac{1}{2}d_x\left[\frac{1}{\sqrt{d_x+1}} - \frac{1}{\sqrt{d_x}}\right] + (d_y - 1)\left[\frac{1}{\sqrt{d_y-1}} - \frac{1}{\sqrt{d_y}}\right] + \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{d_x+1}} - \frac{1}{\sqrt{d_y}}\right] = -\frac{1}{2}h_A(d_x+1) + h_B(d_y)$$

with $A = 1 - \sqrt{2}$ and $B = 1 - {}^{1}/_{\sqrt{2}}$. By (1.2) and $3 \le d_y \le 4$, we get

$$-\frac{1}{2}h_A(d_x + 1) + h_B(d_y) \le -\frac{1}{2}h_A(4) + h_B(4) = \frac{\sqrt{3}}{2} - \frac{3}{4} =:\ c_0$$

In case x—y in G, then

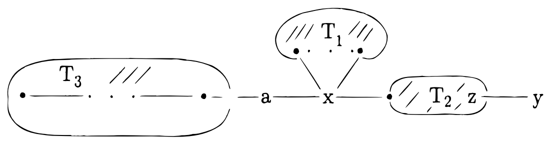
$$ {}^1\chi(G_{(x,y)}) - {}^1\chi(G) \le \frac{1}{2}(d_x - 1)\left[\frac{1}{\sqrt{d_x + 1}} - \frac{1}{\sqrt{d_x}}\right] + (d_y - 2)\left[\frac{1}{\sqrt{d_y - 1}} - \frac{1}{\sqrt{d_y}}\right] + \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{d_x + 1}} - \frac{1}{\sqrt{d_y}}\right] + \left[\frac{1}{\sqrt{(d_x + 1)(d_y - 1)}} - \frac{1}{\sqrt{d_x d_y}}\right] \le c_0 + \frac{1}{\sqrt{d_x}}\left[\frac{1}{2} - \frac{1}{\sqrt{d_y}}\right] + \frac{1}{\sqrt{d_x + 1}}\left[\frac{1}{\sqrt{d_y + 1}} - \frac{1}{2}\right] + \left[\frac{1}{\sqrt{d_y}} - \frac{1}{\sqrt{d_y - 1}}\right] < c_0$$

for $3 \le d_x$ and $3 \le d_y \le 4$. The proof is complete.

3. PROOF OF THE THEOREMS

3.1. *Proof of Theorem 1.* Let T be a chemical tree with vertices 1, ..., n. We show first that ${}^1\chi(T) \le {}^1\chi(A_n) - a_0 r(T)$.

If $r(T) = 0$, then $T = A_n$ and there is nothing to prove. Assume that $r(T) > 0$. Since T is a tree we may find vertices x and y in T with $d_x \ge 3$ and $d_y = 1$ in such a way that T has the following structure



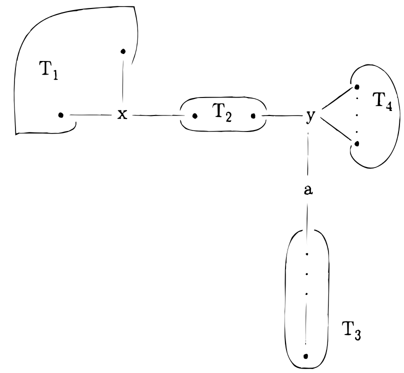
that is, T_3 is linear and possibly $z = x$. If for every choice of x, y, z we have $x = z$, then clearly $T = T(1, ..., 1)$ in the notation of (1.1). In that case, $n \in \{4, 5\}$ and $r(T) = n - 3$. Hence, trivially ${}^1\chi(T) < {}^1\chi(A_n) - a_0(n - 3)$.

We may therefore assume that $x \ne z$ and construct the graph $T^{(x,y)}$. By (2.1), ${}^1\chi(T^{(x,y)}) \ge {}^1\chi(T) + a_0$ and $T^{(x,y)}$ is a chemical graph with $r(T^{(x,y)}) = r(T) - 1$. By induction hypothesis, ${}^1\chi(T) \le {}^1\chi(A_n) - a_0(r(T) - 1)$ and the desired inequality follows.

Now we shall show that ${}^1\chi(T(n, t)) - c_0(r(T) - 1) \le {}^1\chi(T)$, where $t = r(T) - 2$ and $c_0 = 0$ if $r(T) = 2$ and $c_0 = {}^{\sqrt{3}}/_2 - {}^3/_4$, otherwise.

If $r(T) = 0$, then $T = A_n = T(n, t)$ and the equality holds. Assume that $r(T) > 0$, then we may choose a vertex x with d_x maximal (in particular, $d_x \ge 3$). If x is the unique ramification vertex of T, then $T = T(s_1, s_2, ..., s_t)$ for some $s_1 \ge s_2 \ge \cdots \ge s_t$ as in (1.1). Hence ${}^1\chi(T) \ge {}^1\chi(T(n, t))$ and the desired inequality holds.

Assume that T has at least two ramification vertices. We may then choose $y \ne x$ such that T has the following structure



where T_3 is linear. Since T is a chemical tree, then the degrees d_i' in $T_{(x,y)}$ satisfy $d_i' \le 4$ for $i \ne x$. We may apply (2.3) to get ${}^1\chi(T_{(x,y)}) - c_0 \le {}^1\chi(T)$. Applying inductively the procedure (choosing always x as the first ramification vertex), we get the desired inequality.

3.2. Corollary. *Let T be a chemical tree with n vertices, then*

$${}^1\chi(T) \le \frac{n}{2} - \left(\frac{3}{2} - \sqrt{2}\right) - a_0 r(T)$$

Proof. Clearly, ${}^1\chi(A_n) = {}^n/_2 - ({}^3/_2 - \sqrt{2})$.

3.3. For the proof of theorem 2 we require the following construction. Let G be a simple graph and $x \overset{\alpha}{—} y$ an edge in G. Then $G(\alpha)$ is the graph obtained from G by deleting α.

Proposition. *Let G be a chemical graph and $x \overset{\alpha}{—} y$ be an edge in G with d_x, $d_y \ge 2$. Then*

$${}^1\chi(G(\alpha)) - d_0 \le {}^1\chi(G) \le {}^1\chi(G(\alpha)) + b_0$$

Proof: Clearly,

$${}^1\chi(G) - {}^1\chi(G(\alpha)) = \sum_{x—b\ne y} \frac{1}{\sqrt{d_b}}\left[\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right] + \sum_{y—c\ne x} \frac{1}{\sqrt{d_c}}\left[\frac{1}{\sqrt{d_y}} - \frac{1}{\sqrt{d_y - 1}}\right] + \frac{1}{\sqrt{d_x d_y}}$$

The minimal value is reached when $d_b = 1$ (x—$b \ne y$) and $d_c = 1$ (y—$c \ne x$), the maximal when $d_b = 4$ (x—$b \ne y$) and $d_c = 4$ (y—$c \ne x$). Hence

$$(d_x - 1)\left[\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right] + (d_y - 1)\left[\frac{1}{\sqrt{d_y}} - \frac{1}{\sqrt{d_y - 1}}\right] + \frac{1}{\sqrt{d_x d_y}} \le {}^1\chi(G) - {}^1\chi(G(\alpha)) \le \frac{1}{2}(d_x - 1)\left[\frac{1}{\sqrt{d_x}} - \frac{1}{\sqrt{d_x - 1}}\right] + \frac{1}{2}(d_y - 1)\left[\frac{1}{\sqrt{d_y}} - \frac{1}{\sqrt{d_y - 1}}\right] + \frac{1}{\sqrt{d_x d_y}}$$

that is,

$$-h_A(d_x) - h_1(d_y) \le {}^1\chi(G) - {}^1\chi(G(\alpha)) \le -\frac{1}{2}h_B(d_x) - \frac{1}{2}h_1(d_x)$$

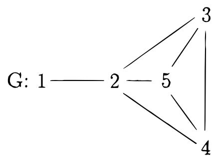
where $A = 1 - {}^{1}/_{\sqrt{d_y}} \in [{}^{1}/_{2}, 1 - {}^{1}/_{\sqrt{2}}]$ and $B = 1 - 2/\sqrt{d_y} < {}^{1}/_{2}$. An easy inspection of the possible cases (d_x, $d_y \in \{2, 3, 4\}$) shows the result.

3.4. Proof of Theorem 2. Let G be a chemical graph and T be a maximal subgraph of G which is a tree. Then T may be obtained from G by deleting exactly $g(G)$ edges. By (3.2) and induction we get that

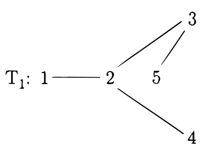
$$^{1}\chi(T) - d_0 g(G) \leq {}^{1}\chi(G) \leq {}^{1}\chi(T) + b_0 g(G)$$

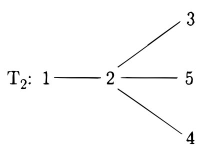
Theorem 1 implies the last statement of the result.

3.5. Example. Consider the following chemical graph



We shall consider the following two maximal subtrees of G





We have $g(G) = 3$; $r(T_1) = 1$ and $^{1}\chi(T_1) = {}^{1}/_{\sqrt{2}} + {}^{2}/_{\sqrt{3}} + {}^{1}/_{\sqrt{6}}$; $r(T_2) = 2$ and $^{1}\chi(T_2) = 2$. The bounds given by theorem 2 are as follows:

$$1.6614 \approx {}^{1}\chi(T_1) - 3d_0 \leq {}^{1}\chi(G) \leq {}^{1}\chi(T_2) + 3b_0 \approx 2.396$$

The value of $^{1}\chi(G)$ is ${}^{3}/_{2} + {}^{3}/_{\sqrt{12}} \approx 2.366$. The bounds obtained are better than those given by Corollary (1.3).

ACKNOWLEDGMENT

This work was done during a sabatical stay of the first named author at the Instituto de Matemáticas, UNAM. Both authors gratefully acknowledge support from their institutions and from DGAPA, UNAM, and CONACyT, México.

REFERENCES AND NOTES

(1) Mihalić, Z.; Trinajstić, N.: A graph theoretical approach to structure-properties Relationships. *J. Chem. Educ.* **1992**, *9*, 701−712.
(2) Trinajstić, N.: Chemical graph theory. Vol. I and II. *CRC Press*. Florida, 1983.
(3) Randić, M.: On characterization of molecular branching. *J. Am. Chem. Soc.* **1975**, *97*, 6609−6615.
(4) Morales, D.; Araujo, O.: On the search of the best correlation between graph theoretical invariants and physicochemical properties. *J. Math. Chem.* **1993**, *13*, 95−106.
(5) Randić, M.; Hansen, P. J.; Jurs, P. C.: Search for useful graph theoretical invariants of molecular structure. *J. Chem. Inf. Comput. Sci.* **1988**, *28*, 60−68.
(6) Araujo, O.; de la Peña, J. A.: The connectivity index of a weighted graph. To appear *Linear Alg. Appl.*
(7) Kier, L. B.; Hall, L. H.: The generation of molecular structures from a graph based QSAR equation. *Quant. Struct.-Act. Relat.* **1993**, *12*, 383−388.
(8) Krasnička, V.; Pospichal, J.: Simulated Annealing construction of molecular graphs with required properties. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 516−526.
(9) Milne, G. W. A.: Mathematics as a basis for chemistry. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 639−644.
(10) Chung, F.: Spectral graph Theory. *Conference Board on Math. Sc.* 92 AMS, 1996.

CI980012S