Bounds for the Randić Connectivity Index

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For a saturated hydrocarbon with n carbon atoms and m carbon−carbon bonds and with Randić connectivity index χ, two functions, $L = L(n,m)$ and $U = U(n,m)$, are determined, such that $L \leq \chi \leq U$. These bounds are better than those previously reported; for most chemically relevant values of n and m there exist hydrocarbons for which $\chi = L$ or $\chi = U$.

1. INTRODUCTION

A quarter of a century ago a graph invariant $\chi = \chi(G)$ was put forward by Randić,[1] aimed to be a measure of the branching of the carbon atom skeleton of organic molecules. He called χ *the branching index*, but later it was renamed the *connectivity index*[2,3] or *Randić index*.[4,5] Already Randić[1] noticed that there is a good correlation between χ and several physicochemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. In subsequent studies a great variety of QSPR and QSAR applications of χ have been established, turning the Randić index (and its, later proposed, generalizations) into one of the most popular molecular structure descriptors for predicting physicochemical and, especially, pharmacologic properties of organic compounds.[2,3,6−8] The actual applications of χ are so numerous that only some of the most recent studies along these lines can be mentioned here.[9−20] Among them is particularly interesting the work of Lahana et al.[17] in which a potent immunosuppressive polypeptide was discovered by using (among other structure descriptors) the connectivity index; in this study lower and upper bounds for χ have been utilized.

Throughout this paper we employ the standard graph representation of the carbon atom skeleton of (saturated) organic molecules, the so-called *molecular graph*.[4,21] A molecular graph G is a connected graph in which no vertex has degree (= number of first neighbors) greater than 4. The number of vertices and edges of G is denoted by n and m, respectively. Clearly, n is the number of carbon atoms and m the number of carbon−carbon bonds; if G represents a saturated hydrocarbon, then its formula is C_nH_{4n-2m}. Here $n = 1, 2, 3, ...$, whereas $m = n - 1, n, n + 1, n + 2, ...$ Because the number of independent cycles (the so-called cyclomatic number, corresponding to the number of what chemists call rings) of the molecular graph G is $m - n + 1$, the actual number m of edges is usually significantly smaller than the maximal possible value $2n$. (Recall that the case $m = 2n$ corresponds to pure carbon, e.g., to a fullerene.)

If G is a molecular graph and $\delta(v)$ is the degree of its vertex v, then its connectivity index is defined as[1]

$$\chi = \chi(G) = \sum_{uv} \frac{1}{[\delta(u)\,\delta(v)]^{1/2}} \qquad (1)$$

with the summation embracing all pairs of adjacent vertices, that is, all edges of the graph G.

Recently, the connectivity index was studied by both mathematicians and theoretical chemists, who established a few of its fundamental mathematical properties. Fajtlowicz[22] and, independently, Araujo and de la Peña[23] proved that the n-vertex graphs with maximal χ are the graphs without isolated vertices in which all components are regular graphs; this maximal χ-value is equal to $n/2$. Bollobás and Erdös[24] showed that the connected n-vertex graph with minimal χ is the star; its χ-value is equal to $(n - 1)^{1/2}$. Caporossi, Gutman, and Hansen[25] demonstrated that among n-vertex trees the path graph has maximal χ; if $n \geq 3$, then this maximal value is equal to $(n - 3)/2 + \sqrt{2}$. Eventually, the n-vertex chemical trees (the graph representations of alkanes, for which $m = n - 1$) with minimal and maximal χ were determined for all $n \geq 1$.[26] The n-vertex molecular graphs with minimal χ were determined for all $n \geq 1$ and all m, $n - 1 \geq m \geq 2n$.[27]

All the mentioned results imply lower and upper bounds for the Randić index. Some additional estimates for χ were reported by Araujo and de la Peña.[23,28]

Let, as before, u and v denote two (not necessarily adjacent) vertices of the molecular graph G, and let $\delta(u)$ and $\delta(v)$ be their degrees. Following Chung,[29] associate with G a square matrix $\mathbf{C} = ||C_{ij}||$ of order n, such that

$$C_{ij} = \begin{cases} 1 & \text{if } u = v \text{ and } \delta(u) \neq 0 \\ -1/[\delta(u)\,\delta(v)]^{1/2} & \text{if the vertices } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

Denote the eigenvalues of $\mathbf{C}$ by $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$. In the case of connected graphs, the first $n - 1$ eigenvalues are

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positive, whereas $\lambda_n = 0$.[29] It has been demonstrated that[23]

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

where κ is an auxiliary graph invariant defined as

$$\kappa = (\sum_{i=1}^{n} \sqrt{\delta_i})^2 (\sum_{i=1}^{n} \delta_i)^{-1}$$

Note that $\kappa \le n$.

In a subsequent work[28] the inequalities (2) were simplified as

$$\frac{n}{2}\left[1 - \frac{3}{4}\lambda_1\right] \le \chi(G) \le \frac{1}{2}\left[n - \frac{1}{8n^2}(n - \kappa)\right] \quad (3)$$

Whereas (2) holds for all connected graphs, the bounds (3) are restricted to molecular graphs. The estimates (3) are weaker than (2) because in all cases

$$\frac{n}{2}\left[1 - \frac{3}{4}\lambda_1\right] \le \frac{1}{2}[n - \lambda_1(n - \kappa)]$$

$$\frac{1}{2}\left[n - \frac{1}{8n^2}(n - \kappa)\right] \ge \frac{1}{2}[n - \lambda_{n-1}(n - \kappa)]$$

For molecular graphs with two or more vertices, $1 - 3\lambda_1/4 < 0$, a detail which in ref 28 has been overlooked.

The application of the bounds (2) and (3) is limited by the fact that they require the knowledge of λ_1 and λ_{n-1}, the computation of which requires the use of an appropriate computer software. Besides, the dependence of these eigenvalues on molecular structure is somewhat obscure.

Another known[30] estimate for χ is (23), discussed in more detail in a subsequent section.

THE NEW BOUNDS

In this work we demonstrate the following result.

Let G be a molecular graph with n vertices, m edges, and connectivity index $\chi(G)$. Define the quantities L and U as follows:

$$L = L(n,m) = (4n + m)/12 \quad \text{if } n + m \equiv 0 \pmod 3 \quad (4)$$

$$= (4n + m)/12 + (3\sqrt{3} - 5)/6 \quad \text{if } n + m \equiv 1 \pmod 3 \quad (5)$$

$$= (4n + m)/12 + (3\sqrt{2} - 4)/6 \quad \text{if } n + m \equiv 2 \pmod 3 \quad (6)$$

and

$$U = U(n,m) = (n - 3)/2 + \sqrt{2} \quad \text{if } m = n - 1 \quad (7)$$

$$= n/2 \quad \text{if } m = n \quad (8)$$

$$= 1/3 + (n - 4)/2 + 4/\sqrt{6} \quad \text{if } m = n + 1 \quad (9)$$

$$= (3n - 5)/6 + 2/\sqrt{6} \quad \text{if } m = n + k \quad (10)$$

$$= n/2 \quad \text{if } m = 3n/2 \quad (11)$$

$$= (3n - 7)/6 + 4/\sqrt{12} \quad \text{if } m = (3n + 1)/2 \quad (12)$$

In (10) the parameter k assumes the values 2, 3, ..., $(n - 2)/2$ if n is even, and 2, 3, ..., $(n - 1)/2$ if n is odd. Note that the right-hand-side expression in (10) is independent of k.

For all values of n and m for which $L(n,m)$ and $U(n,m)$ are defined

$$L(n,m) \le \chi(G) \le U(n,m) \quad (13)$$

With the exception of the first few values of n, for all chemically sound choices of the parameters n and m there exist molecular graphs G_* and G^* (the structure of which is specified below), such that $\chi(G_*) = L(n,m)$ and $\chi(G^*) = U(n,m)$. In view of this, L and U may be viewed as the best possible (n,m)-type lower and upper bounds for the Randić connectivity index.

Note that $L(n,m)$ is defined for $n = 3, 4, \ldots$ and for all m, $n - 1 \le m \le 2n$, that is, for all molecular graphs. The quantity $U(n,m)$ is defined for $n = 3, 4, \ldots$ and for m between $n - 1$ and $3n/2$, and thus covers all chemically relevant cases (but not the hypothetical molecular graphs with more than $3n/2$ edges).

ESTIMATING THE CONNECTIVITY INDEX

Denote by x_{ij} the number of edges uv of G, for which $\delta(u) = i$ and $\delta(v) = j$. Then (1) is readily transformed into

$$\chi(G) = \sum_{1 \le i \le j \le 4} x_{ij}/(ij)^{1/2} \quad (14)$$

Note that $x_{11} = 0$ whenever $n \ge 3$, and therefore the case $i = j = 1$ need not be considered any further. Consequently, the right-hand side of (14) is a linear function of the following nine variables:

$$x_{12}, x_{13}, x_{14}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}, x_{44}$$

Let the graph G possess n_i vertices of degree i. Then

$$n_1 + n_2 + n_3 + n_4 = n \quad (15)$$

Counting the edges terminating at vertices of degree i, we obtain for $i = 1, 2, 3, 4$

$$x_{12} + x_{13} + x_{14} = n_1 \quad (16)$$

$$x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2 \quad (17)$$

$$x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \quad (18)$$

$$x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4 \quad (19)$$

Another linearly independent relation of this kind is

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m \quad (20)$$

Its left-hand side is just the sum of the vertex degrees, known[4,21] to be equal to twice the number of edges.

Assuming that the parameters n and m are fixed, (15)−(20) may be understood as a system of six linear equations in thirteen unknowns: n_1, n_2, n_3, n_4, x_{12}, x_{13}, x_{14}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}, and x_{44}. Solving it in the unknowns n_1, n_2, n_3, n_4, x_{14}, and x_{44} (for details see elsewhere[25,26,30]), one obtains

$$\chi(G) = \frac{4n + m}{12} + c_{12}x_{12} + c_{13}x_{13} + c_{22}x_{22} + c_{23}x_{23} + c_{24}x_{24} + c_{33}x_{33} + c_{34}x_{34} \quad (21)$$

where

$$c_{12} = 1/\sqrt{2} - 7/12 \approx 0.123\ 77$$
$$c_{13} = 1/\sqrt{3} - 19/36 \approx 0.049\ 57$$
$$c_{22} = 1/12 \approx 0.083\ 33$$
$$c_{23} = 1/\sqrt{6} - 13/36 \approx 0.047\ 14$$
$$c_{24} = 1/(2\sqrt{2}) - 1/3 \approx 0.020\ 22$$
$$c_{33} = 1/36 \approx 0.027\ 78$$
$$c_{34} = 1/(2\sqrt{3}) - 5/18 \approx 0.010\ 90$$

Because all coefficients c_{ij} on the right-hand side of (21) are positive-valued, this expression is convenient for deducing the lower bound for χ.

If, in turn, we solve (15)−(20) in the unknowns n_1, n_2, n_3, n_4, x_{12}, and x_{22} (for details see elsewhere[25,26,30]), we arrive at

$$\chi(G) = \frac{(2\sqrt{2}-2)n + (3-2\sqrt{2})m}{2} + c'_{13}x_{13} + c'_{14}x_{14} + c'_{23}x_{23} + c'_{24}x_{24} + c'_{33}x_{33} + c'_{34}x_{34} + c'_{44}x_{44} \quad (22)$$

where

$$c'_{13} = -(1 + 2\sqrt{2} - 2\sqrt{3})/6 \approx -0.060\ 72$$
$$c'_{14} = -(\sqrt{2} - 1)/4 \approx -0.103\ 55$$
$$c'_{23} = -(4 - \sqrt{6} - \sqrt{2})/6 \approx -0.022\ 72$$
$$c'_{24} = -(3 - 2\sqrt{2})/4 \approx -0.042\ 89$$
$$c'_{33} = -(3 - 2\sqrt{2})/6 \approx -0.028\ 60$$
$$c'_{34} = -(11 - 5\sqrt{2} - 2\sqrt{3})/12 \approx -0.038\ 74$$
$$c'_{44} = -(3 - 2\sqrt{2})/4 \approx -0.042\ 89$$

All coefficients c'_{ij} on the right-hand side of (22) are negative-valued, a feature convenient for designing upper bounds for the connectivity index.

From (21) we immediately see that $\chi(G)$ cannot be less than $(4n + m)/12$. From (22) it follows that $\chi(G)$ cannot be greater than $[(2\sqrt{2} - 2)n + (3 - 2\sqrt{2})m]/2$. Hence, we obtain the, earlier reported,[30] (n,m)-type estimates

$$\frac{4n+m}{12} \le \chi(G) \le \frac{(2\sqrt{2}-2)n + (3-2\sqrt{2})m}{2} \quad (23)$$

A more advertent consideration of relations (22) and (23) makes it possible to deduce (n,m)-type bounds for the Randić index, better than (23).

PROVING $L(n,m) \le \chi(G)$

In what follows we assume that the parameters n and m, pertaining to the molecular graph G, have some fixed (constant) values.

Table 1. Smallest Number of Vertices of (n,m)-Molecular Graphs for Which There Is a Graph with a Randić Connectivity Index Equal to $L(n,m)$

		$n+m \equiv 0$	$n+m \equiv 1$	$n+m \equiv 2$
acyclic	$m = n-1$	5	13	9
unicyclic	$m = n$	9	11	7
bicyclic	$m = n+1$	10	9	8
tricyclic	$m = n+2$	8	7	9

Table 2. Smallest Number of Vertices of (n,m)-Molecular Graphs for Which There Is a Graph with Randić Connectivity Index Equal to $U(n,m)$

acyclic	$m = n-1$	3
unicyclic	$m = n$	3
bicyclic	$m = n+1$	4
tricyclic	$m = n+2$	4
tetracyclic	$m = n+3$	5
pentacyclic	$m = n+4$	7
hexacyclic	$m = n+5$	9

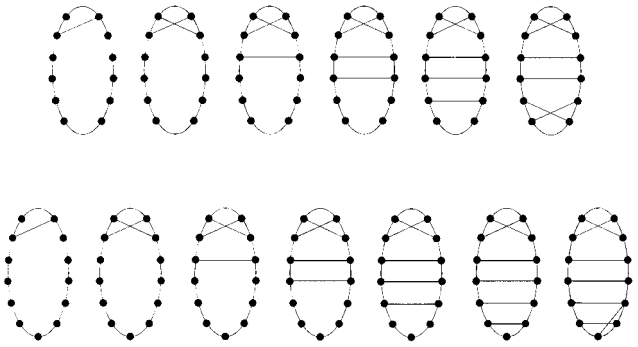

Figure 1. Molecular graphs with maximal Randić connectivity indices for $n = 12$, $m = 13-18$ and $n = 13$, $m = 14-20$. Their construction is performed so as to maximize the number of pairs of adjacent vertices of degree 3.

In view of (21), $\chi(G)$ will attain its smallest value if all the x_{ij} values occurring on the right-hand side of (21) are equal to zero or are as close to zero as possible. Because x_{14} and x_{44} do not appear in (21), molecular graphs with minimal χ should have as many as possible edges connecting vertices of degrees 1 and 4, and edges connecting two vertices of degree 4.

In summary, to minimize $\chi(G)$, the values of n_2 and n_3 need to be chosen equal to zero or as close to zero as possible.

Now, by means of (15) and (20), the choice $n_2 = n_3 = 0$ implies $n_1 = (4n - 2m)/3$ and $n_4 = (2m - n)/3$. Because n_1 and n_4 must be integers, the conditions $n_2 = n_3 = 0$ can be satisfied only if both $4n - 2m$ and $2m - n$ are divisible by 3

$$4n - 2m \equiv 2m - n \equiv 0 \pmod 3$$

However, the above is tantamount to

$$n + m \equiv 0 \pmod 3 \quad (24)$$

and we see that if (24) holds, then the molecular graphs with minimal connectivity indices have $n_2 = n_3 = 0$ and $\chi = (4n + m)/12$. This yields (4) for $L(n,m)$.

It remains to examine the cases when $n + m$ is not divisible by 3. Then it must be either $n_2 > 0$ or $n_3 > 0$ or both.

Table 3. Lower Bound L, (4)−(6), and the Upper Bound U, (7)−(12) for the Randić Connectivity Index of Acyclic ($m = n - 1$), Unicyclic ($m = n$), Bicyclic ($m = n + 1$), Tricyclic ($m = n + 2$), Tetracyclic ($m = n + 3$), Pentacyclic ($m = n + 4$), and Hexacyclic ($m = n + 5$) Saturated Hydrocarbons with n Carbon Atoms, $5 \leq n \leq 20$

n		ac	unic	bic	tric	tetrac	pentac	hexac
5	L	2.000	2.116	2.207	2.250	2.366	2.457	2.500
	U	2.414	2.500	2.466	2.483	2.488		
6	L	2.457	2.500	2.616	2.707	2.750	2.866	2.957
	U	2.914	3.000	2.966	2.983	3.000		
7	L	2.866	2.957	3.000	3.116	3.207	3.250	3.366
	U	3.414	3.500	3.466	3.483	3.483	3.488	
8	L	3.250	3.366	3.457	3.500	3.616	3.707	3.750
	U	3.914	4.000	3.966	3.983	3.983	4.000	
9	L	3.707	3.750	3.866	3.957	4.000	4.116	4.207
	U	4.414	4.500	4.466	4.483	4.483	4.483	4.488
10	L	4.116	4.207	4.250	4.366	4.457	4.500	4.616
	U	4.914	5.000	4.966	4.983	4.983	4.983	5.000
11	L	4.500	4.616	4.707	4.750	4.866	4.957	5.000
	U	5.414	5.500	5.466	5.483	5.483	5.483	5.483
12	L	4.957	5.000	5.116	5.207	5.250	5.366	5.457
	U	5.914	6.000	5.966	5.983	5.983	5.983	5.983
13	L	5.366	5.457	5.500	5.616	5.707	5.750	5.866
	U	6.414	6.500	6.466	6.483	6.483	6.483	6.483
14	L	5.750	5.866	5.957	6.000	6.116	6.207	6.250
	U	6.914	7.000	6.966	6.983	6.983	6.983	6.983
15	L	6.207	6.250	6.366	6.457	6.500	6.616	6.707
	U	7.414	7.500	7.466	7.483	7.483	7.483	7.483
16	L	6.616	6.707	6.750	6.866	6.957	7.000	7.116
	U	7.914	8.000	7.966	7.983	7.983	7.983	7.983
17	L	7.000	7.116	7.207	7.250	7.366	7.457	7.500
	U	8.414	8.500	8.466	8.483	8.483	8.483	8.483
18	L	7.457	7.500	7.616	7.707	7.750	7.866	7.957
	U	8.914	9.000	8.966	8.983	8.983	8.983	8.983
19	L	7.866	7.957	8.000	8.116	8.207	8.250	8.366
	U	9.414	9.500	9.466	9.483	9.483	9.483	9.483
20	L	8.250	8.366	8.457	8.500	8.616	8.707	8.750
	U	9.914	10.000	9.966	9.983	9.983	9.983	9.983

Table 4. Randić Connectivity Index (χ) of Some Saturated Hydrocarbons and Its Estimates (13)[a]

hydrocarbon	χ		(13)	(23)	(2)
hexane, C_6H_{14}	2.914	lower	2.457	2.42	2.86
		upper	2.914	2.91	2.99
cycloheptane, C_7H_{14}	3.500	lower	2.957	2.92	3.50
		upper	3.500	3.50	3.50
bicyclo[2.2.2]octane, C_8H_{14}	3.949	lower	3.457	3.42	3.93
		upper	3.966	4.09	3.98
cubane, C_8H_8	4.000	lower	3.707	3.67	4.00
		upper	4.000	4.34	4.00
2-methyloctane, C_9H_{20}	4.270	lower	3.707	3.67	4.21
		upper	4.414	4.41	4.49
3-methyloctane, C_9H_{20}	4.308	lower	3.707	3.67	4.21
		upper	4.414	4.41	4.49
spiro[4.4]nonane, C_9H_{16}	4.414	lower	3.866	3.83	4.38
		upper	4.466	4.59	4.49
decane, $C_{10}H_{22}$	4.914	lower	4.116	4.08	4.85
		upper	4.914	4.91	5.00
menthane, $C_{10}H_{20}$	4.698	lower	4.207	4.17	4.60
		upper	5.000	5.00	4.97
pinane, $C_{10}H_{18}$	4.621	lower	4.250	4.25	4.48
		upper	4.966	5.09	4.94
hexamethylpentane, $C_{11}H_{24}$	4.500	lower	4.500	4.50	4.30
		upper	5.414	5.41	5.42
1,1,2,2,4,4-hexamethylcyclopentane, $C_{11}H_{22}$	4.664	lower	4.616	4.58	4.53
		upper	5.500	5.50	5.39
2,2,4,4-tetramethyl-3,3-diethylpentane, $C_{13}H_{28}$	5.621	lower	5.366	5.33	5.30
		upper	6.414	6.41	6.42
perhydropyrene, $C_{16}H_{26}$	7.933	lower	6.957	6.92	7.84
		upper	7.983	8.26	7.99
octamethylcubane, $C_{16}H_{24}$	7.000	lower	7.000	7.00	6.40
		upper	7.983	8.34	7.71
1,4-dicyclohexylpentane, $C_{17}H_{32}$	8.360	lower	7.207	7.17	8.28
		upper	8.466	8.59	8.50

[a] For comparative purposes we also give the earlier reported bounds (2)[23,28] and (23).[30]

An inspection of (21) and the numerical values of the coefficients c_{ij} indicates that the choice $n_2 = 0$ and $n_3 = 1$ (with $x_{34} = 3$) is the optimal one. For such molecular graphs, $n_1 = (4n - 2m - 1)/3$ and $n_4 = (2m - n - 2)/3$ which is integer-valued only if

$$n + m \equiv 1 \pmod 3 \tag{25}$$

If (25) is obeyed, then the molecular graphs with minimal connectivity indices have $n_2 = 0$, $n_3 = 1$, $x_{34} = 3$, and $\chi = (4n + m)/12 + 3c_{34}$. This latter expression for χ is just (5) for $L(n,m)$.

The analysis of the third case

$$n + m \equiv 2 \pmod 3 \tag{26}$$

is analogous: This time the choice must be $n_2 = 1$, $n_3 = 0$, and $x_{24} = 2$, and the respective molecular graphs have then the smallest possible connectivity indices. This minimal value is $(4n + m)/12 + 2c_{24}$ which directly leads to (6).

By this we demonstrated the validity of the left inequality (13).

The graphs G_* for which the equality $\chi(G_*) = L(n,m)$ is obeyed exist if the number of vertices is sufficiently large. What "sufficiently large" is depends on the value of m and the congruence class of $n + m$. In Table 1 are given the smallest values of n for which at least one acyclic, unicyclic, bicyclic, and tricyclic molecular graph G_* exists; the acyclic case has been reported previously.[26]

PROVING $\chi(G) \leq U(n,m)$

To find an upper bound for the Randić index, one should consider (22). Because this equation does not contain the terms x_{12} and x_{22}, the graphs with maximal χ have to be constructed so as to have as many as possible edges connecting two vertices of degree 2, or connecting a vertex of degree 1 with a vertex of degree 2. The other x_{ij} values should be either zero or as close to zero as possible.

In summary, to maximize $\chi(G)$, the values of n_3 and n_4 need to be chosen equal to zero or as close to zero as possible.

In the case of acyclic ($m = n - 1$) and unicyclic ($m = n$) molecular graphs the situation is simple: there exist such graphs with $n_3 = n_4 = 0$, namely, the path and the cycle; the respective χ-values are just what has been chosen for $U(n,n-1)$ and $U(n,n)$, (7) and (8).

Starting with the bicyclic case, the molecular graphs must possess vertices of degree 3 and/or 4. An inspection of (22) and the numerical values of the coefficients c'_{ij} reveals that vertices of degree 3 are preferred over vertices of degree 4. Furthermore, among molecular graphs possessing several (fixed number) vertices of degree 3, the maximal connectivity index will be attained if as many as possible such vertices are mutually adjacent. This reasoning leads to the construction of the (n,m)-graphs G^* with maximal connectivity indices, illustrated in Figure 1. The right-hand sides of (9)−(12) are just expressions[31] for the connectivity indices of the graphs G^*. The right inequality (13) follows now straightforwardly.

Similarly as in the case of the lower bound, the graphs G^* satisfying the equality $\chi(G^*) = U(n,m)$ exist only if the number of vertices is sufficiently large. However, in the case of the upper bound the critical values of n are rather low, as seen from the data given in Table 2. Thus, in the case of practically all saturated hydrocarbons the upper bound (13) is the best possible.

DISCUSSION

By means of (4)−(12) the new lower and upper bounds for $\chi(G)$ can easily be computed. In Table 3 these bounds are given for values of n and m which cover practically all chemically relevant cases.

In Table 4 we show a few examples, and compare the new bounds (13) with those previously reported. It is seen that (13) is better than the earlier (n,m)-type estimate (23).[30] This is no surprise whatsoever, because (13) happen to be the best possible bounds depending solely on the parameters n and m. On the other hand, the bounds (13) are sometimes better and sometimes weaker than the estimates (2),[23,28] which are anyway much more difficult to compute.

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(31) For instance, (10) is obtained as follows. The graph G^* with $n + k$ edges, $2 \le k \le \lfloor (n-1)/2 \rfloor$, has $n_3 = 2k$ vertices of degree 3 and $n_2 = n - 2k$ vertices of degree 2. It is easy to see (cf. Figure 1) that $x_{23} = 2$, $x_{22} = n_2 - 1 = n - 2k - 1$ and $x_{33} = n + k - x_{23} - x_{22} = 3k - 1$. Therefore

$$\chi(G^*) = \frac{2}{\sqrt{6}} + \frac{n-2k-1}{2} + \frac{3k-1}{3}$$

On the right-hand side of the above formula the terms containing the parameter k cancel out, resulting in (10).

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