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# SOME THEOREMS ABOUT THE RANDIĆ CONNECTIVITY INDEX

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Abstract. We derive some basic facts about the Randić connectivity index. Many corollaries for chemical graphs are then discussed – in particular, we give exact formulae for benzenoids, coronoids, and diamondoids which depend only on the frequency of certain edge types. Many of these results about benzenoids are rediscoveries – but we generalize them to larger families of graphs and shorten and simplify the arguments. One interesting corollary we observe is that the Randić index correlates to branching in cata-condensed benzenoids oppositely as it does for trees – namely, cata-condensed benzenoids with more branched inner duals have higher Randić indices while more branched trees have lower Randić indices.

## 1. Introduction

The Randić connectivity index is a graph invariant introduced to mathematical chemistry by Milan Randić [3], and since has found many applications [2] in correlations to various physico-chemical and bio-chemical properties. Basically, it is a number arrived at by summing the weights of all the edges, with the weight of an edge being the reciprocal of the square root of the product of the degrees of its vertices. That is,

$$\chi = \sum_{vw \in E} \frac{1}{\sqrt{d_v d_w}}, \tag{1}$$

where the sum is over all edges $vw$, from the edge set $E$ of a graph $G = (V, E)$, whose vertices have degrees $d_v$ and $d_w$. Many authors have since proven an assortment of results about the Randić index and generalized Randić indices of the form

$$\chi_p = \sum_{vw \in E} (d_v d_w)^p. \tag{2}$$

In this form, the original Randić index has $p = -\frac{1}{2}$. [4, 7]

In this paper, we derive a simple formula for the traditional Randić index of a graph and pursue consequences first for graphs with maximum degree four (which we here call

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chemical graphs), and then particularly, specialization to benzenoids is considered – where we give $n$-linear best lower and upper bounds for $\chi$. All of the graphs here are assumed to have no isolated vertex.

## 2. Preliminaries

The formula we are interested in deriving comes simply from applying a counting identity which is closely equivalent to the famous handshaking theorem. Namely, given a graph $G = (V, E)$,

$$\sum_{vw \in E} (\frac{1}{d_v} + \frac{1}{d_w}) = n, \tag{3}$$

where $n$ is the number of vertices in $G$. Subtraction of Equation 1 from half of Equation 3 yields

$$\frac{n}{2} - \chi = \frac{1}{2} \sum_{vw \in E} (\frac{1}{d_v} + \frac{1}{d_w} - \frac{2}{\sqrt{d_v d_w}}). \tag{4}$$

Thus we arrive at the following theorem.

**Theorem 1.**

$$\chi = \frac{n}{2} - \frac{1}{2} \sum_{vw \in E} (\frac{1}{\sqrt{d_v}} - \frac{1}{\sqrt{d_w}})^2$$

This formula was already discovered in [5], and was advocated as "justifying" Randić's choice of the $p = -\frac{1}{2}$ exponent in the generalized Randić index.

A few things are immediately apparent from this formulation of the Randić index. First, for edges $vw$ where $d_v = d_w$, there is no contribution to the summation. Hence, it is precisely for graphs which consist only of regular components that the Randić index attains its maximum value of $\frac{n}{2}$. Incidentally, this upper bound of $\frac{n}{2}$ has been noticed before by several authors [8, 9, 10, 11]. It readily comes from applying the Cauchy-Schwarz inequality to a pair of appropriately chosen vectors. Of course, since the terms under the summation in the formula above are always non-negative, we deduce this upper bound quite easily from Theorem 1.

**Corollary 2.** *Let $G$ be a graph with minimum degree at least two and maximum degree at most four. Then*

$$\chi = \frac{n}{2} - \frac{5 - 2\sqrt{6}}{12} m_{23} - \frac{3 - 2\sqrt{2}}{8} m_{24} - \frac{7 - 4\sqrt{3}}{24} m_{34}$$

*where $m_{ij}$ denotes the number of edges with vertices of degree $i$ and $j$.*

This is trivially extended to allow degree one (or degree larger than four) sites, but in the present form this gives the Randić index of diamondoid hydrocarbons, also known as polymantanes, which are three dimensional analogues of benzenoids. Further specialization may be made for benzenoid, coronoid, and multi-coronoid hydrocarbons.

**Corollary 3.** *Let $G$ be a graph with vertices having only degree two or degree three. Then*

$$\chi = \frac{n}{2} - \frac{5-2\sqrt{6}}{12} m_{23}. \tag{5}$$

This shows that for these types of graphs, the number $m_{23}$ of $(2,3)$ edges is all one needs to determine the Randić index. For the special cases of benzenoids and the closely related cata-condensed "phenylenes", this formula was found in [6] by a slightly longer argument.

## 3. Best Linear Bounds on the Randić Index of Benzenoids

It is a quite natural to seek out the best possible bounds on the Randić index for a given family of graphs. In particular, we seek here the best lower and upper bounds on this invariant as linear functions of the number of vertices for benzenoids. There is a partial ordering of the bounds of the form $\alpha n + \beta$, for constants $\alpha$ and $\beta$, such that one upper bound is better than a second if and only if, for any of the graphs under consideration, i.e. benzenoids, the first never exceeds in value the second and has a strictly smaller value for at least one graph. Similarly, one lower bound is better than a second if and only if, for any of the graphs under consideration, the first is never smaller in value than the second and has a strictly larger value for at least one graph. There are non-comparable linear bounds for benzenoids, such as the two upper bounds, $\frac{3}{5}n$ and $\frac{5}{7}n - 1$. In the case that both $n$-linear upper and lower bounds are unique bests for a given class of graphs, we say that this invariant is **best-bounded** for the class.

**Theorem 4.** *For the class of benzenoids, the Randić connectivity index is $n$-linearly best-bounded as*

$$\frac{1+2\sqrt{6}}{12} n + \frac{5-2\sqrt{6}}{2} \leq \chi \leq \frac{n}{2}.$$

*Both of these bounds are tight, with equality holding from above for and only for benzene, and equality holding from below for and only for polyacene chains.*

Before proceeding to the proof of this theorem, it might be noted how close these bounds are to each other, differing by less than one hundredth. Namely,

$$\frac{49}{100} n = .49n < \frac{1+2\sqrt{6}}{12} n + \frac{5-2\sqrt{6}}{2} \leq \chi \leq .5n = \frac{50}{100} n.$$

This shows that, at least for benzenoids, the dominant dependence of $\chi$ seems to be, up to proportionality, just the carbon atom count $n$. Thence it becomes natural to ask about the difference between these invariants, say by defining

$$r = c(\frac{n}{2} - \chi),$$

where $c = \frac{6}{5-2\sqrt{6}} \approx 59.394$. This is an invariant with non-negative values and indeed for benzenoids, is just half the number of $(2,3)$ edges, to which has been given a further

interpretation in [6]. In that paper, $r$ is called the number of inlets of a benzenoid and is equal to the sum of the number of bays, coves, fjords, lagoons, and fissures (interested readers are referred to [6]). One can also think of $r$ in the following informative way. Starting at a vertex of degree three, every walk around the boundary of a benzenoid has disjoint sequences of degree two vertices, each of which contributes two $(2,3)$ edges. Hence $r$ is the number of these disjoint sets, which we can call ring exposures.

*Proof.* (Theorem 4) From Theorem 1 and Equation 5, the upper bound is obvious. Consider whether $B_1 = \alpha_1 n + \beta_1$ might be a better upper bound on $\chi$ than $\frac{n}{2}$. First, it cannot be the case that $\alpha_1 < \frac{1}{2}$, since the Randić index of some benzenoids can be made arbitrarily close to $\frac{n}{2}$ so that $B_1$ could not have been an upper bound after all regardless of how large $\beta_1$ is (repeatedly circumscribing benzene with hexagons will suffice as an example). Next, suppose that $\alpha_1 = \frac{1}{2} + \epsilon$ for some $\epsilon \geq 0$. Since, in particular, $B_1$ must be satisfied for benzene with $n = 6$ and $\chi = 3$,

$$(\frac{1}{2} + \epsilon)6 + \beta_1 \geq 3$$

so that $\beta_1 \geq -6\epsilon$. But now,

$$B_1 = (\frac{1}{2} + \epsilon)n + \beta_1 \geq (\frac{1}{2} + \epsilon)n - 6\epsilon = \frac{n}{2} + \epsilon(n-6) \geq \frac{n}{2}.$$

So that $\frac{n}{2}$ is a better upper bound than $B_1$ when $\alpha_1 \geq \frac{1}{2}$. Thus, the upper bound in the theorem is the best possible. Also, it is clear from Theorem 1 (and is well known) that $\chi = \frac{n}{2}$ only for regular graphs (or graphs where each component is regular) [5, 7, 11] so benzene is clearly the only case of equality for the upper bound among benzenoids.

For the lower bound, note that the total number of boundary edges $m_b$ equals the total number of boundary vertices $n_b$ – which is smaller than the total number of vertices. Then with the realization (widely recognized as in [13]) that at least 6 boundary edges are of the type $(2,2)$, we have

$$m_{23} + 6 \leq m_b = n_b \leq n$$

whence $m_{23} \leq n - 6$. Substituting this into Equation 5 we find,

$$\chi = \frac{n}{2} - \frac{5-2\sqrt{6}}{12} m_{23} \geq \frac{n}{2} - \frac{5-2\sqrt{6}}{12}(n-6) = \frac{1+2\sqrt{6}}{12} n + \frac{5-2\sqrt{6}}{2}, \tag{6}$$

proving the lower bound.

To characterize equality, suppose first that the benzenoid is a polyacene chain with $h \geq 2$ hexagons (note that for benzene with $h = 1$, equality is satisfied). Let us call hexagons with four degree two vertices pendants. Note that each non-pendant hexagon has four $(2,3)$ edges and each of the two pendant hexagons has two $(2,3)$ edges. Together this yields, $m_{23} = 4(h-1) = n - 6$, since $n = 4h + 2$. As can be seen from Equation 6 above, this indicates that polyacenes satisfy Theorem 4 with equality.

Conversely, suppose that

$$\chi = \frac{1+2\sqrt{6}}{12}n + \frac{5-2\sqrt{6}}{2} = \frac{n}{2} - \frac{5-2\sqrt{6}}{12}m_{23},$$

implying that $m_{23} = n - 6$. Again with $m_{22} \geq 6$ and $n \geq n_b \geq m_{22} + m_{23}$ we deduce that $m_{22} = 6$ and that all the vertices are on the boundary cycle, whence the benzenoid is cata-condensed. We also deduce from this that the benzenoid has no branches or kinks, for any branch would imply at least three pendant hexagons and at least nine $(2,2)$ edges while any kink would imply at least seven $(2,2)$ edges (six for the two pendant hexagons and another for each kink), both of which are contrary to the fact that $m_{22} = 6$. To conclude we note that the only cata-condensed benzenoids with no branches and no kinks are the polyacenes.

To see that this lower bound is best possible, let $B_2 = \alpha_2 n + \beta_2$ be a lower bound which is no worse than the one in the theorem. Since polyacenes satisfy the lower bound from the theorem with equality, it cannot be the case that $\alpha_2 > \frac{1+2\sqrt{6}}{12}$. Otherwise, regardless of how small $\beta_2$ was, there would be a large enough polyacene chain whose Randić index would be less than $B_2$ – contradicting the fact that $B_2$ was a lower bound. So suppose, for $\epsilon \geq 0$, that $\alpha_2 = \frac{1+2\sqrt{6}}{12} - \epsilon \leq \frac{1+2\sqrt{6}}{12}$. We know that the lower bound $B_2$ must be satisfied for benzene, the smallest benzenoid with $n = 6$ and $\chi = 3$, so

$$B_2 = (\frac{1+2\sqrt{6}}{12} - \epsilon)6 + \beta_2 \leq 3$$

$$\beta_2 \leq 3 - \frac{1+2\sqrt{6}}{2} + 6\epsilon = \frac{5-2\sqrt{6}}{2} + 6\epsilon.$$

Thus for all other benzenoids,

$$\begin{aligned} B_2 &= (\frac{1+2\sqrt{6}}{12} - \epsilon)n + \beta_2 \\ &\leq (\frac{1+2\sqrt{6}}{12} - \epsilon)n + \frac{5-2\sqrt{6}}{2} + 6\epsilon \\ &= \frac{1+2\sqrt{6}}{12}n + \frac{5-2\sqrt{6}}{2} - \epsilon(n-6) \\ &\leq \frac{1+2\sqrt{6}}{12}n + \frac{5-2\sqrt{6}}{2}. \end{aligned}$$

Thence $B_2$, being less than or equal to the lower bound of the theorem, we conclude that the stated lower bound is best possible. □

This theorem illuminates an interesting observation. First, from Theorem 1 we see that for alkanes, the Randić index decreases as the amount of branching increases (we use the word branching in an intuitive but reasonable sense). Thus, as reported in [12], paths have largest indices while chemical graphs amalgamated out of stars have smallest indices. This trend is reversed in the class of cata-condensed benzenoids, which resemble trees with

maximum degree three in that this is what their inner duals are. Here, as illustrated by the last theorem, the polyacenes have the smallest Randić indices by attaining equality with their lower bound, while branches and kinks (in the inner dual) increase the value of this invariant. Roughly speaking, branches and kinks increase the number of $(2, 2)$ edges and, as a consequence, for a fixed number of hexagons, decrease the relative ratio of $(2, 3)$ edges thereby increasing the Randić index. Thus it may be said that benzenoids, rather than alkanes, have their branching extent correlated positively to the Randić index.

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