8-2011

Randic and Sum Connectivity Indices of Certain Trees

Jennifer L. Feiner
Montclair State University

MONTCLAIR STATE UNIVERSITY

Randić and Sum Connectivity Indices of Certain Trees

by

Jennifer L. Feiner

A Master's Thesis Submitted to the Faculty of

Montclair State University

In Partial Fulfillment of the Requirements

For the Degree of

Master of Science

August 2011

College of Science and Mathematics

Department of Mathematics

[redacted]

Dean of College or School

8/23/11

Date

Thesis Committee:

[redacted]

Thesis Sponsor

[redacted]

Committee Member

[redacted]

Committee Member

[redacted]

Department Chair

Abstract

The focus of this thesis is on new development of the Randić and Sum Connectivity Indices of certain molecular and symmetric trees representing acyclic alkanes, or aliphatic hydrocarbons. The Randić Connectivity Index is one of the most used molecular descriptors in Quantitative Structure-Property and Structure-Activity Relationship modeling because of the relation that the isomers have between their properties and their structure. The structure-boiling point relationship models of aliphatic alcohols have been studied using the Sum Connectivity Index and compared to the Randić Connectivity Index. A specific type of tree $T_{n,a}$, well-known in graph theory as a double star, was studied by Zhou and Trinajstić. In this thesis, $T_{n,a}$ trees are investigated. The tree $T_{n,2}$ which has the third smallest Sum Connectivity Index value among all the trees with n vertices is found to be interesting and thereby is further explored. Some alkane trees are symmetric, which is the concentration of this thesis. The symmetric double star trees are denoted by J_n. The tree J_n has n vertices and is built on the path P_2 with $(n-2)/2$ leaves from each vertex of the path. The Randić and Sum Connectivity Index formulas of the symmetric tree J_n are developed. Also, estimations of the Randić and Sum Connectivity Indices of J_n are given. Relationships and comparisons between the Randić and Sum Connectivity Indices are analyzed in respect to the tree J_n. The ratio and difference of the Randić and Sum Connectivity Indices are further discussed.

The thesis starts with the history of the indices of molecular trees in Chemistry and Biology (Chapter 1). Chapter 2 provides a list of observations of the properties of both connectivity indices of the related trees. The symmetric tree J_n is discussed in Chapter 3, in which formulas and properties of the Randić and Sum Connectivity Indices are given. The main results of the thesis are reported in Chapter 4, where the graphs which have the maximal or minimal Randić and Sum Connectivity values among all $T_{n,a}$ graphs with n vertices are identified. The closeness of the two indices of $T_{n,a}$ trees is also discussed. The paper concludes with a similar tree, denoted $T_{n,a} \times P_m$, extended from the tree $T_{n,a}$ by replacing the middle path P_2 with the path P_m $(m \geq 2)$. The Randić and Sum Connectivity Index formulas are given for this tree (Chapter 5). This topic will be investigated more in future work.

Randić and Sum Connectivity Indices of Certain Trees

A THESIS

Submitted in partial fulfillment of the requirements
for the degree of Masters in Science

by

Jennifer L. Feiner
Montclair State University
Montclair, NJ

2011

Acknowledgments

The author wishes to thank several people. I would like to thank Dr. Li for all the time she put into working with me and for all her help, direction, and patience with the development of this thesis. I would like to thank my husband, Gary, for all his love, support, and patience during the past few years while I've been in graduate school and all his support throughout all of my schooling for the past 8 years. I would also like to thank my children, Gary, Angelica, Gavin, Anthony, and Gabriel, for their understanding when I had homework, studying, and thesis work to do and for being so well behaved when they came to school with me for meetings with Dr. Li. To my parents, Joseph and Lois, I thank you for always supporting me and pushing me to achieve my goals, oh, and letting me use your sunroom for peace and quiet. I want to also thank Stewart Hengeveld, a lot of my LaTeX knowledge and Maple worksheets wouldn't have been possible without you. Thank you to Dick Koch the MacTeX support guru who helped me with converting and inserting graphics for my paper. Last, but certainly not least, I would like to thank my committee members, Dr. Cutler and Dr. Korlie, for their support and time to make my thesis a completed work.

Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Introduction

In this paper, we explore the ideas of molecular trees used in scientific studies, the properties of the Randić connectivity index and the sum connectivity index, and relationships between molecular trees and the corresponding indices. We also analyze relationships between the Randić connectivity index and the sum connectivity index. The connectivity indices of specifically selected trees with biology and chemistry backgrounds, such as double star trees, are examined to provide valuable information about the trees and the underlying data structure. The graphs of these special trees are studied and formulas are developed to compute the indices using Linear Algebra, Discrete Math, Graph Theory, and ideas from Combinatorics.

1.2 History of the Indices of Molecular Trees

Milan Randić, one of the leading experts in the field of Computational Chemistry, first developed the Randić connectivity index (formerly known as branching index [5, 1975]). For simplicity, we call it RCI. Suppose G is a simple graph with vertex-set $V(G)$ and edge-set $E(G)$. In graph theory, the degree d_v of a vertex v is the number of edges connecting to it. Each vertex is assigned an index value of $d_v^{-1/2}$, where d_v is the valency of the considered vertex. In chemistry, valency means vertex degree. For an edge $e = uv$ connecting two vertices u and v, the Randić connectivity index of e is given by $(d_u d_v)^{-1/2}$. The Randić connectivity index, also known as the product connectivity index, of G is defined as $R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}$ (see Definition 3) [5].

The RCI was developed for the purpose of ordering the boiling points of alkane isomers easily. Isomers are two different compounds with the same molecular formula. For example, butane and isobutane are isomers because they have the same number of vertices. The boiling points of isomers decrease with branching because of decreased surface areas [8]. The relative values of the boiling points of smaller alkanes were in fact used in the construction of the connectivity index [7]. The relative magnitudes of the boiling points have a correlation with the RCIs of molecular trees. The remarkable aspect of the Randić paper [6] is that a pure number, encoding alkane skeletal branching, also correlates with a physical property, the boiling point [3]. The RCI is inversely related to the rank order of the boiling points of the corresponding alkane isomer and directly related to the rank order of the corresponding heat of formation of the alkane isomers [3, 11]. All of these facts can be seen in Table B.1 in Appendix B. Burch, Wakefield, and Whitehead [2] have also studied the boiling points of alkanes. They developed single variable models to calculate the boiling points of special families of alkanes and multivariable boiling point models for all alkane isomers up to and including 12 carbon atoms.

The Randić connectivity index is one of the most used molecular descriptors in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) because of the relation of properties to structure. These relationships can represent chemical compositions, connectivities of atoms, and potential energy surface of compounds [5].

Proposed by Bo Zhou and Nenad Trinajstić in 2009 is the sum connectivity index, for simplicity we call it SCI, of a graph G, defined as $S(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}$ (see Definition 3) [12]. The RCI and SCI are highly intercorrelated quantities [12] and are used for molecular graphs (see Definition 2) in Chemistry and Biology. Like the RCI, the SCI has also been studied and applied in QSPR and QSAR modeling. The structure-boiling point models of aliphatic alcohols have been studied using SCI and compared to the RCI. Similarly, the structure-water solubility models of aliphatic alcohols have been studied using SCI and compared to the RCI [14].

1.3 Motivation and Statement of the Problem

Having studied discrete mathematics as an undergraduate, I have always held an interest in trees and graph theory. The relationships among chemistry, biology, and mathematics truly show when dealing with molecular trees and analyzing specific graphs. Not only is it amazing to see from where these trees derive, but it is also interesting to discover what type of information can be gathered and learned from studying these trees.

In this research I will answer the following questions:

1. What type of unknown relationships between the sum and product connectivity indices can we find?

2. Among a special type of graph with the same number of vertices, which one has the maximum RCI/SCI and which one has the minimum?

3. What type of information about the graph structure can be gathered from investigating the maximum and minimum of the RCI and SCI of special trees?
4. What type of estimation of the RCI and SCI values can be found for a specific type of tree, like the double star?
5. Where do the two values of the RCI and SCI meet?
6. Can we use the information we gather from examining the indices of specially selected trees to analyze other trees?

1.4 Useful Definitions, Theorems, and Properties

Throughout the paper, we apply the following commonly used definitions from graph theory, discrete mathematics, linear algebra, chemistry, and biology which come from numerous sources [8–10, 12, 16]. All the graphs are connected and simple. A simple graph is an undirected graph that has no loops and at most one edge connecting any two vertices.

Definition 1 *Denote a simple graph by G=(V,E), where $V = V(G)$ is the vertex-set and $E = E(G)$ is the edge-set. For a vertex v in G, the degree d_v of v is the number of edges connecting to it. A pendant vertex is a vertex of degree one.*

Definition 2 *Let G=(V,E).*

1. *A path P_n is a sequence of vertices such that from each of the vertices there is one edge to the next vertex in the sequence.*
2. *The graph G is called a tree if it is connected and contains no cycle as a subgraph.*
3. *A molecular tree is a tree of maximum degree at most four. It models the skeleton of an acyclic molecule.*

When we talk about simple graphs, we must consider the number of vertices and edges. The following definitions are well known in graph theory.

Definition 3 *Let G=(V,E), $u, v \in V(G)$, and $e = uv \in E(G)$.*

1. *The vertex index for v is $d_v^{-1/2}$.*
2. *The end degrees of e are labeled by (d_u, d_v).*
3. *The edge index for $e = uv$ is $(d_u d_v)^{-1/2}$ for the RCI and $(d_u + d_v)^{-1/2}$ for the SCI.*

4. *The Randić Connectivity Index of G is defined as*

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}.$$

5. *The Sum Connectivity Index of G is defined as*

$$S(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}.$$

The structure that the graphs or trees in this paper will mimic is the Lewis structure. The Lewis structures are not meant to imply any three-dimensional arrangement [7]. When drawn out, the Lewis structure looks similar to Figure 1.1. In this paper, we observe the connectivity indices for all alkanes C_n, C being carbons. Here n represents the number of vertices and when we talk about alkanes, n represents atoms. For our example shown in Figure 1.1, we have C_2 where 2 represents the number of carbon atoms or vertices as shown in Table A.1 in Appendix A for the chemical ethane.

```
    H   H
    |   |
H - C - C - H
    |   |
    H   H
```

Figure 1.1: Lewis Structure of Ethane

Definition 4 *The adjacency matrix of G=(V,E), sometimes called the connection matrix, is a matrix with rows and columns labeled by the vertices in G and the (i, j)-entry equals 1 if $v_i v_j \in E$, 0 otherwise.*

Remark: For G, the adjacency matrix must have 0s on the diagonal and is symmetric.

Theorem 1 *Let G=(V,E) be a graph. Then*

1. *The sum of the degrees of all vertices is twice the number of edges:*

$$\sum_{v \in V(G)} d_v = 2 \mid E(G) \mid .$$

2. If G is a tree, then $\mid E(G) \mid = \mid V(G) \mid -1$.

Example 1 *Please refer to the following tree G for detailed description of Definitions 1 - 3 and Theorem 1.*

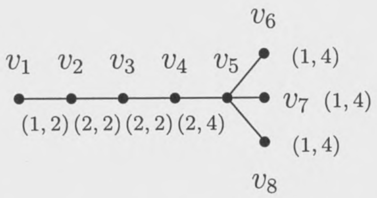


Figure 1.2: Graph G - An Example for Definitions and Theorem

It shows that

- *The tree above can be described as a molecular tree.*
- *A path P_5 can be described as $v_1 \sim v_2 \sim v_3 \sim v_4 \sim v_5$.*
- *The degree of the vertices v_1, v_6, v_7, and v_8 is one. These vertices are called pendant vertices. The degree of the vertices v_2, v_3, and v_4 is two and v_5 is a vertex of degree four.*
- *The vertex index for v_1 is $\frac{1}{\sqrt{1}} = 1$. The vertex index for v_3 is $\frac{1}{\sqrt{2}}$.*
- *The edges of G are labeled as $(1,2), (2,2), (2,4)$, and $(1,4)$. There are two edges labeled as $(2,2)$ and three edges labeled as $(1,4)$.*
- *For $e = v_1v_2$, the RCI edge index is $\frac{1}{\sqrt{2}}$ and the SCI edge index is $\frac{1}{\sqrt{3}}$.*
- *R(G)*$=\frac{1}{\sqrt{2}} + \frac{5}{2} + \frac{1}{\sqrt{8}} = 3.3272$ *and S(G)*$=\frac{1}{\sqrt{3}} + \frac{2}{2} + \frac{1}{\sqrt{6}} + \frac{3}{\sqrt{5}} = 3.5607$.
- *The sum of the degrees of all the vertices, 14, is twice the number of edges, 7.*
- $\mid E(G) \mid = 7 = \mid V(G) \mid -1$.

1.5 Existing Results

The SCI is relatively new. It is known that Zhou and Trinajstić are the first who have studied it [11]. They classified the graphs which have the largest SCI value, the second largest, and the third largest values among all simple graphs of n vertices. They claim that for $n \geq 4$, the path P_n has the maximum SCI value among all trees, which is $\frac{n-3}{2} + \frac{2}{\sqrt{3}}$ (see Figure 1.3). For $n = 4$ the maximum graph P_4 correlates to a Butane tree.

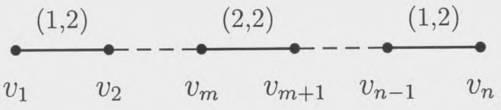


Figure 1.3: Path P_n (maximum)

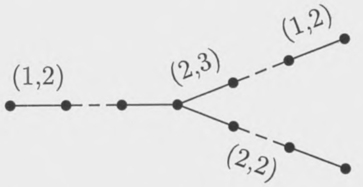


Figure 1.4: Second largest

Figure 1.5: Third largest

Figure 1.4 represents the graph with the second largest SCI which is $\frac{n-7}{2} + \frac{3}{\sqrt{3}} + \frac{3}{\sqrt{5}}$ for $n \geq 7$. When $n = 7$ it is a tree with a single vertex of degree three adjacent to three vertices of degree two. The graph with the third largest SCI, shown by Figure 1.5, is a tree with a single vertex of degree three adjacent to two vertices of degree two and one vertex of degree one. The index is $\frac{n-5}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}}$ $(n \geq 5)$.

The results of the largest, second largest, and third largest SCI values also relate to that of the RCI. Among all the trees with n vertices, the path P_n for $n \geq 4$ has the maximum RCI of $\frac{n-3}{2} + \frac{2}{\sqrt{2}}$. This was observed while examining specific trees. The path P_n has the largest SCI and RCI value because they are highly intercorrelated quantities, as stated before.

Similarly, Zhou and Trinajstić also classified the trees which have the smallest SCI value, the second smallest, and the third smallest values among all molecular trees with n vertices. For $n \geq 5$, the tree with the smallest SCI is the star graph, as shown in Figure 1.6. Bollobás and Erdős [1] studied the star graph and obtained the following result. Among simple connected graphs with a fixed number of vertices, the star has minimal connectivity index.

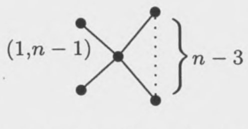


Figure 1.6: Star S_n (minimum)

The SCI index of the star graph can easily be found by using $\frac{n-1}{\sqrt{n}}$ for $n \geq 5$. The second smallest and third smallest are represented by Figures 1.7 and 1.8 below.

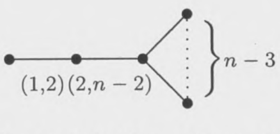


Figure 1.7: Second smallest

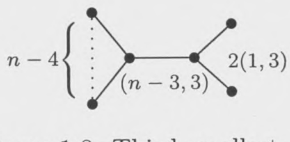


Figure 1.8: Third smallest

The indices for the second and third smallest trees respectfully are $\frac{n-3}{\sqrt{n-1}} + \frac{1}{\sqrt{n}} + \frac{1}{\sqrt{3}}$ for $n \geq 5$ and $\frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}} + 1$ for $n \geq 6$. In Chapter 3 of this paper, we use a variation of the third smallest graph to calculate the SCI and RCI of trees similar to those of the third smallest.

It was shown in [3] that the smallest, second smallest, and third smallest RCI values among all trees with n vertices are, respectively, $\frac{n-1}{\sqrt{n-1}}$ for $n \geq 5$, $\frac{n-3}{\sqrt{n-2}} + \frac{1}{\sqrt{2n-4}} + \frac{1}{\sqrt{2}}$ for $n \geq 5$, and $\frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{3n-9}} + \frac{2}{\sqrt{3}}$ for $n \geq 6$.

Corresponding to the above work, this research investigates the maximum and minimum for double star trees. A specific type of tree $T_{n,a}$, well-known in graph theory as the double star, is the concentration of this thesis. The main results show that the symmetric double star tree J_n, has the maximal SCI and RCI values among all trees on n vertices. The double star tree $T_{n,2}$, which has the minimal SCI and RCI values and the third smallest Sum Connectivity Index value among all the trees with n vertices, is found to be interesting and thereby is further explored. Please note that if the graph is not connected then the indices will have different properties and all the graphs studied in this research are connected.

Chapter 2

Observations and Examples

In Chemistry, the largest RCI and SCI values among isomers belongs to unbranched linear alkanes [5], for example Figure 1.3 (above) or Figure 2.1 (below). Alkanes are aliphatic hydrocarbons having only C − C and C − Hσ bonds [7]. We only observe the connectivity indices for all $C_2 - C_n$ alkanes, C being carbons. For n-alkanes the RCI increases with the number of carbons, the increment being 0.5 per carbon atom [5]. Our n represents the number of vertices, but when we talk about alkanes, we refer to n as atoms. The RCI list of all $C_2 - C_8$ alkanes expressed in terms of contributions from ten kinds of CC bonds can be found in Randić's paper in [5]. At the end of this thesis, in Appendix A, there is a table of RCI and SCI values, along with the graphs of all the alkanes referenced in Randić's paper.

We have examined many simple graphs and found that the decimal parts of these graphs are the same or show specific patterns. The decimal parts in Table 2 of all the figures that correlate with each other are the same. The reason that this happens is because of the long path that can be shortened by taking out some of the (2,2) edges. When n is odd, the decimal part for the SCI value of P_n is 0.1547. When n is even, the decimal part is 0.6547. For example, if we take a look at Figures 2.1 and 2.2, we see that for $n = 4$ the RCI and SCI equal 1.914214 and 1.654701, respectively. Now if we set $n = 5$ the RCI and SCI equal 2.414214 and 2.154701, respectively. It is easily seen that the index increases by 0.5.

Another observation that was made is that the integer part of the connectivity index in Figures 2.1 - 2.6 are well related to $\frac{n-2}{2}$. The integer part of the connectivity index in Figures 2.7 and 2.8 are very close to this value, but it is not exact because the graph has many branches. The more branches the graph has, the smaller (less) the connectivity. This concept is examined in more depth in the next section.

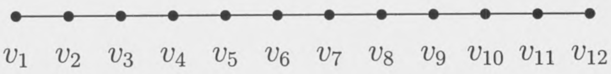


Figure 2.1: Dodecane/P_{12}

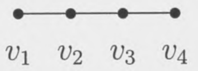


Figure 2.2: Butane/P_4

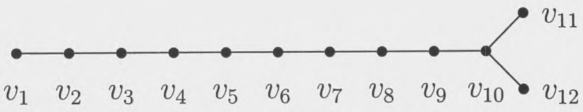


Figure 2.3: 2-Methylundecane

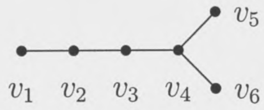


Figure 2.4: 2-Methylpentane

	n	RCI	SCI
Figure 2.1	12	5.914214	5.654701
Figure 2.2	4	1.914214	1.654701
Figure 2.3	12	5.770056	5.524564
Figure 2.4	6	2.770056	2.524564
Figure 2.5	12	5.625900	5.394427
Figure 2.6	8	3.625900	3.394427
Figure 2.7	12	5.207107	4.999778
Figure 2.8	10	4.207107	3.999778

Table 2.1: Connectivity Index

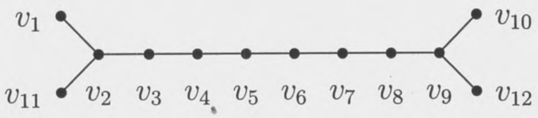


Figure 2.5: 2,9-Dimethyldecane

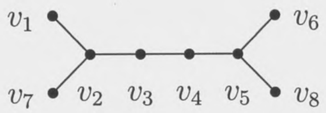


Figure 2.6: 2,5-Dimethylhexane

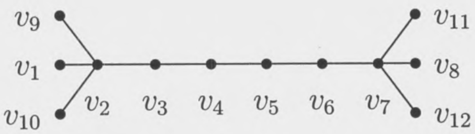


Figure 2.7: 2,2,7,7-Tetramethyloctane

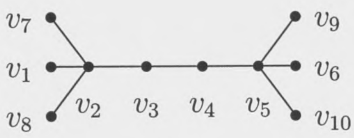


Figure 2.8: 2,2,5,5-Tetramethylhexane

One obvious pattern is that the integer part of the graphs shown above increases as the number of vertices gets larger and more branches get added on.

In the next section, graphs similar to Figure 2.6, Figure 2.8, and the third minimum (Figure 1.8) are analyzed and formulas are developed. If we look at Figure 2.6, we notice that it is a symmetric graph. Our main basis for the next chapter is the symmetric graphs with $a = \frac{n-2}{2}$ branches on each side, where $a \geq 2$.

Chapter 3

Symmetric Double Star Trees

3.1 Introduction to the Double Star Tree $T_{n,a}$ and J_n

In this section, we investigate a specific type of tree $T_{n,a}$, also known as a double star, (see Definition 5) studied by Zhou and Trinajstić in their paper *On a novel connectivity index* [11]. In this paper, the authors analyze the largest and smallest SCI values for molecular trees representing hydrocarbons. The tree that was found to be interesting from this paper, specifically, is the tree $T_{n,2}$ which has the third smallest SCI value among all the trees with n vertices. The motivation to study this type of graph comes from the previous section where we analyzed the graphs of various alkanes.

Definition 5 *For $n \geq 6$ and $2 \leq a \leq \frac{n-2}{2}$, the graph $T_{n,a}$ is a tree with n vertices, $n-2$ leaves, and a center edge with the shape:*

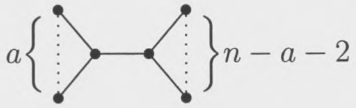


Figure 3.1: Double Star Tree $T_{n,a}$

We say the graph $T_{n,a}$ is symmetric if $a = n - a - 2$, that is, $a = \frac{n-2}{2}$. Denote the corresponding symmetric tree as J_n. In other words, the tree J_n has n vertices and is built on the path P_2 with $(n-2)/2$ leaves from each vertex of the path. Shown in Figure 3.2.

Example 2 *$T_{8,3}$ and $T_{12,5}$ are symmetric trees.*

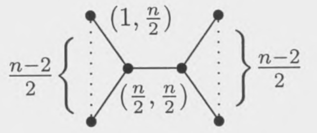


Figure 3.2: Symmetric Double Star Tree J_n

In chemistry, the graph in Figure 3.2 represents (2,3)-Dimethylbutane ($T_{6,2}$) when $n = 6$ and (2,2,3,3)-Tetramethylbutane ($T_{8,3}$) when $n = 8$, where both of these trees are symmetric. These trees can be found in the table in Appendix A.

In the following two sections, the SCI and RCI of the symmetric tree J_n are investigated. We analyze how close the SCI value $S(J_n)$ and $\sqrt{2n+4}$ are, and similarly, how close the RCI value $R(J_n)$ and $\sqrt{2n}$ are. To do this, the derivative is taken and the critical point is found. A lower bound is given for both $S(J_n)$ and $R(J_n)$.

3.1.1 Estimating the SCI of J_n

Theorem 2 *Let J_n be a symmetric tree with $n \geq 6$, defined in Definition 5. Then the SCI value $S(J_n)$ satisfies the following properties:*

1. $S(J_n) = \frac{\sqrt{2}(n-2)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}} = \sqrt{2n+4} - \frac{4\sqrt{2}}{\sqrt{n+2}} + \frac{1}{\sqrt{n}}$.
2. *For every fixed real number $M \geq 1$ and all $n \geq M$,* $0 \leq \sqrt{2n+4} - S(J_n) \leq \frac{4\sqrt{2}}{\sqrt{M+2}} - \frac{1}{\sqrt{M}}$.
3. *Given $\epsilon > 0$, there exists $M_\epsilon > 0$ such that $|\sqrt{2n+4} - S(J_n)| < \epsilon$ provided $n > M_\epsilon$.*

PROOF:

1. The graph J_n has $n-2$ leaves labeled by $(1, n/2)$ and one edge labeled by $(n/2, n/2)$, as shown in Figure 3.2. By the definition of SCI,

$$\begin{aligned} S(J_n) &= \frac{n-2}{\sqrt{\frac{n}{2}+1}} + \frac{1}{\sqrt{n}} = \frac{\sqrt{2}(n-2)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}} = \frac{\sqrt{2}(n+2-4)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}} \\ &= \sqrt{2n+4} - \frac{4\sqrt{2}}{\sqrt{n+2}} + \frac{1}{\sqrt{n}}. \end{aligned}$$

2. To determine how close $S(J_n)$ and $\sqrt{2n+4}$ are, we define a real function $f(x)$ as follows:

$$f(x) = \frac{4\sqrt{2}}{\sqrt{x+2}} - \frac{1}{\sqrt{x}}.$$

Then $f(x) \geq 0$ for $x > 0$, $f(n) = \sqrt{2n+4} - S(J_n)$ for positive integers n, and

$$f'(x) = -\frac{1}{2}\Big(\frac{4\sqrt{2}x^{3/2} - (x+2)^{3/2}}{x^{3/2}(x+2)^{3/2}}\Big).$$

It follows that $f'(x) = 0$ only at $x = \frac{2}{2\sqrt[3]{4}-1}$ or more simply $x \approx 0.9196239$. Furthermore, $f(0.9196239)$ is the absolute maximum of $f(x)$ on $(0, \infty)$ and $f(x)$ is decreasing on $(0.9196239, \infty)$. See Figures 3.3 and 3.4. Thus, for every real number $M \geq 1$, $f(M)$ is the maximum value of $f(x)$ on the interval $[M, \infty)$. Therefore, for all integers $n \geq M$,

$$0 \leq \sqrt{2n+4} - S(J_n) \leq f(M) = \frac{4\sqrt{2}}{\sqrt{M+2}} - \frac{1}{\sqrt{M}}. \qquad (1)$$

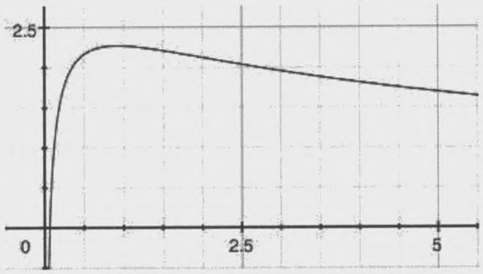


Figure 3.3: Graph of $f(x)$

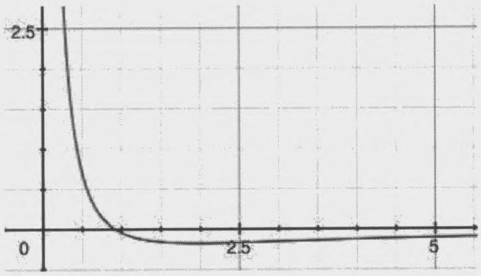


Figure 3.4: Graph of $f'(x)$

3. Given a small positive integer ϵ, we want to find a lower bound M_ϵ such that when $n \geq M_\epsilon$,

$$\sqrt{2n+4} - S(J_n) < \epsilon.$$

From expression (1), it is sufficient to solve the inequality $f(M) < \epsilon$. However,

$$f(M) = \frac{4\sqrt{2}}{\sqrt{M+2}} - \frac{1}{\sqrt{M}} < \frac{4\sqrt{2}}{\sqrt{M}} - \frac{1}{\sqrt{M}} = \frac{4\sqrt{2}-1}{\sqrt{M}}.$$

Thus, we take

$$M_\epsilon = \frac{33 - 8\sqrt{2}}{\epsilon^2}.$$

If $n > M_\epsilon$, then $\sqrt{2n+4} - S(J_n) \leq f(M_\epsilon) < \epsilon$. QED

Theorem 2 provides an explicit formula for $S(J_n)$, an estimation of it by $\sqrt{2n+4}$, and error bounds of the estimation.

Example 3 *Let $\epsilon = 0.001$.*

$$\frac{33 - 8\sqrt{2}}{0.001^2} = 21,686,291 = M_\epsilon.$$

By Theorem 2, if $n > M_\epsilon$, then $\sqrt{2n+4} - S(J_n) < 0.001$. It is easy to check that if we take $n = 22,000,000 > M_\epsilon$, then

$$\frac{4\sqrt{2}}{\sqrt{n+2}} - \frac{1}{\sqrt{n}} \approx 0.0009928 < 0.001,$$

which confirms the theorem.

3.1.2 Estimating the RCI of J_n

Similarly, as was done above for the SCI values of J_n, we give corresponding results for the RCI of J_n.

Theorem 3 *Let J_n be as above. Then*

1. $R(J_n) = \frac{\sqrt{2}(n-2)}{\sqrt{n}} + \frac{2}{n} = \sqrt{2n} - \frac{2\sqrt{2}}{\sqrt{n}} + \frac{2}{n}$.
2. *For every fixed real number $M \geq 1$ and all $n \geq M$, $0 \leq \sqrt{2n} - R(J_n) \leq \frac{2\sqrt{2M}-2}{M}$.*
3. *Given $\epsilon > 0$, there exists $M_\epsilon > 0$ such that $|\sqrt{2n} - R(J_n)| < \epsilon$ provided $n > M_\epsilon$.*

PROOF:

1. Similarly as in the proof of Theorem 2(1),

$$R(J_n) = \frac{n-2}{\sqrt{\frac{n}{2}}} + \frac{2}{n} = \frac{\sqrt{2}(n-2)}{\sqrt{n}} + \frac{2}{n} = \sqrt{2n} - \frac{2\sqrt{2}}{\sqrt{n}} + \frac{2}{n}.$$

2. How close are $R(J_n)$ and $\sqrt{2n}$? To answer this question, we define $g(x)$ as:

$$g(x) = \frac{2\sqrt{2x} - 2}{x}.$$

One can check that $g(x) > 0$ when $x \geq 1$. Further,

$$g'(x) = 2\Big(\frac{1}{x^2} - \frac{\sqrt{2}}{2x^{3/2}}\Big) = 2\Big(\frac{\sqrt{x} - \sqrt{2}}{\sqrt{2}x^2}\Big),$$

with a unique root of $n = 2$. Also, $g(2)$ equals the absolute maximum of $g(x)$ on the interval $(1, \infty)$ and $g(x)$ is decreasing on $(2, \infty)$. Thus, on $[M, \infty)$ with $M \geq 2$

$$0 \leq \sqrt{2n} - R(J_n) \leq g(M). \qquad (2)$$

See Figures 3.5 and 3.6.

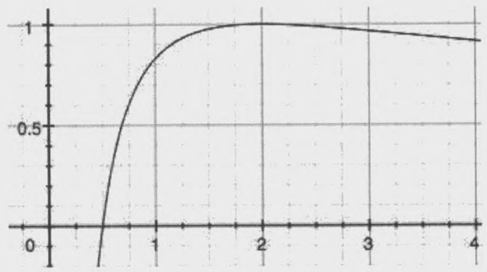


Figure 3.5: Graph of $g(x)$

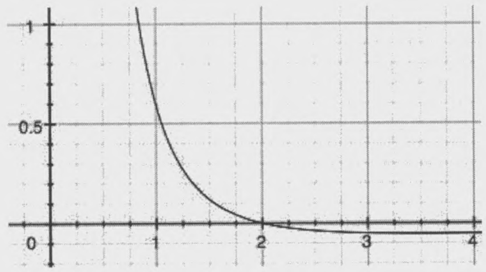


Figure 3.6: Graph of $g'(x)$

3. Given a small positive integer ϵ, we want to find a lower bound M_ϵ such that when $n \geq M_\epsilon$,

$$\sqrt{2n} - R(J_n) < \epsilon.$$

From equation (2), it is sufficient to solve the inequality $g(M) < \epsilon$. While,

$$g(M) = \frac{2\sqrt{2M} - 2}{M} < \epsilon \iff \epsilon^2 n^2 + (4\epsilon - 8)n + 4 > 0.$$

There are two solution intervals, but we are only interested in the one that is reasonable for our problem, when

$$n > \frac{-2\epsilon + 4 + 4\sqrt{1 - \epsilon}}{\epsilon^2} = M_\epsilon.$$

Since $g(M_\epsilon)$ is the absolute maximum on $[M_\epsilon, \infty)$, then for every $n > M_\epsilon$, it is true that $\sqrt{2n} - R(J_n) < \epsilon$. QED

Example 4 *Let* $\epsilon = 0.001$. *Take*

$$M_\epsilon = \frac{-2(0.001) + 4 + 4\sqrt{1 - 0.001}}{0.001^2} = 7995999.$$

If $n > M_\epsilon$, *then* $\sqrt{2n} - R(J_n) < 0.001$. *For example, if we take* $n = 8,000,000$, *which is greater than* M_ϵ, *then*

$$\frac{2\sqrt{2n} - 2}{n} \approx 0.0009997 < 0.001.$$

3.2 Comparison of $S(J_n)$ and $R(J_n)$

In this section we examine how close the two values $S(J_n)$ and $R(J_n)$ are by considering the limit situation of the ratio of the values and by estimating the difference. The result is very similar to those referenced by Zhou and Trinajstić in their papers about the correlation coefficient of the alkane trees that they examined [11–15]. As mentioned before, the SCI and RCI are highly intercorrelated quantities or highly intercorrelated molecular descriptors. The correlation coefficient between the product-connectivity index and the sum-connectivity index for 137 alkane-trees is 0.9996 [15]. In [11], Zhou and Trinajstić claim that the value of the correlation coefficient being 0.991 for trees representing lower alkanes. Both numbers are close to 1.

Theorem 4 *As $n \to \infty$ the ratio $S(J_n)/R(J_n)$ approaches* 1.

PROOF:

$$\lim_{n\to\infty} \frac{S(J_n)}{R(J_n)} = \lim_{n\to\infty} \frac{\sqrt{2n+4} - \frac{4\sqrt{2}}{\sqrt{n+2}} + \frac{1}{\sqrt{n}}}{\sqrt{2n} - \frac{2\sqrt{2}}{\sqrt{n}} + \frac{2}{n}} = \lim_{n\to\infty} \sqrt{1 + \frac{2}{n}} = 1.$$

QED

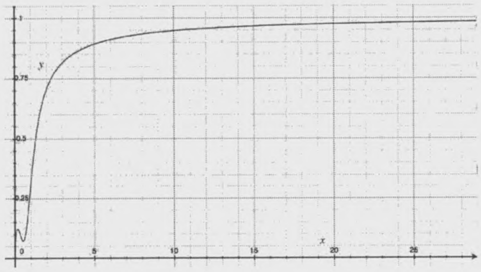


Figure 3.7: Limit of the ratio of $S(J_n)/R(J_n)$

For all the alkanes and special trees that have been looked at, the RCI values are always larger than those of SCI and the differences are always greater than zero. Table 2 and Table A given in Appendix A show that all the RCI values are greater than the SCI values. The following theorem assures the truth of this fact.

Theorem 5 *Let J_n be a symmetric tree as above, with $n \geq 6$. Then,*

1. $R(J_n) > S(J_n)$.
2. *For every $\epsilon > 0$, $R(J_n) - S(J_n) < \epsilon$ provided $n > 2/\epsilon^2 - 2$.*
3. $\lim_{n\to\infty} \Big[R(J_n) - S(J_n)\Big] = 0$.

PROOF: We first examine the following difference:

$$\begin{aligned} R(J_n) - S(J_n) &= \frac{\sqrt{2}(n-2)}{\sqrt{n}} + \frac{2}{n} - \left(\frac{\sqrt{2}(n-2)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}}\right) \\ &= \sqrt{2}(n-2)\left(\frac{1}{\sqrt{n}} - \frac{1}{\sqrt{n+2}}\right) + \frac{2}{n} - \frac{1}{\sqrt{n}}. \end{aligned}$$

By Mean Value Theorem, $\sqrt{n+2} - \sqrt{n} = \frac{1}{\sqrt{c}}$ for some $c \in (n, n+2)$, thus $\sqrt{n+2} - \sqrt{n} = \frac{1}{\sqrt{c}} > \frac{1}{\sqrt{n+2}}$.

$$\frac{1}{\sqrt{n}} - \frac{1}{\sqrt{n+2}} = \frac{\sqrt{n+2} - \sqrt{n}}{\sqrt{n(n+2)}} > \frac{\frac{1}{\sqrt{n+2}}}{\sqrt{n(n+2)}} = \frac{1}{\sqrt{n}(n+2)}.$$

Thus

$$\begin{aligned} R(J_n) - S(J_n) &> \frac{\sqrt{2}(n-2)}{\sqrt{n}(n+2)} + \frac{2}{n} - \frac{1}{\sqrt{n}} = \frac{\sqrt{2}(n-2)\sqrt{n} + 2(n+2) - \sqrt{n}(n+2)}{n(n+2)} \\ &= \frac{1}{n^2+2n}\left[n\sqrt{n}(\underbrace{\sqrt{2}-1}_{>0}) + 2\Big(n+2-(\sqrt{2}+1)\sqrt{n}\Big)\right]. \end{aligned}$$

1. To show $R(J_n) > S(J_n)$ for all positive integers n, we need to find conditions for n so that $n+2-(\sqrt{2}+1)\sqrt{n} > 0$. By examining the minimal value of the quadratic function $x^2 - (\sqrt{2}+1)x + 2$, we find that the curve of the parabola is completely above the x-axis since the x-coordinate of the vertex is $x = \frac{\sqrt{2}+1}{2} > 0$ and the parabola opens up. Thus $n+2-(\sqrt{2}+1)\sqrt{n} > 0$ for all positive integers n and $R(J_n)$ is always greater than $S(J_n)$. The graph of $R(J_n) - S(J_n)$ can also be seen in Figure 3.8.

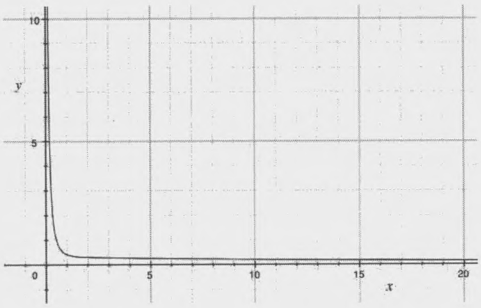


Figure 3.8: $RCI - SCI > 0$

2. Next we give some upper bounds for the difference $R(J_n) - S(J_n)$. Let ϵ be any positive real number.

Same as the above, by Mean Value Theorem, $\sqrt{n} - \sqrt{n+2} = \frac{1}{\sqrt{c}}$ for some $c \in (n, n+2) \Longrightarrow \sqrt{n} - \sqrt{n+2} < \frac{1}{\sqrt{n}}$. Thus

$$\frac{1}{\sqrt{n}} - \frac{1}{\sqrt{n+2}} = \frac{\sqrt{n+2} - \sqrt{n}}{\sqrt{n(n+2)}} < \frac{\frac{1}{\sqrt{n}}}{\sqrt{n(n+2)}} = \frac{1}{n\sqrt{n+2}},$$

which implies

$$R(J_n) - S(J_n) = \frac{\sqrt{2}(n-2)}{n\sqrt{n+2}} + \frac{2}{n} - \frac{1}{\sqrt{n}} < \frac{\sqrt{2}}{\sqrt{n+2}} < \epsilon$$

for all $n > \frac{2}{\epsilon^2} - 2$.

For 3, it is straightforward from 2. QED

Chapter 4

General Double Star Trees

4.1 Double Star Trees with the Maximum and Minimum SCI and RCI

In this section, we investigate the general double star tree $T_{n,x}$. The definitions, theorems, lemmas, and propositions shown hereafter are developed from Definition 5 shown in Section 3.1. Note that $T_{n,a}$ was used in the previous section.

Consider the set $\Gamma = \{T_{n,x} | n \geq 6, 2 \leq x \leq n-4\}$. We are interested in knowing which tree in this set has the maximum or minimum SCI/RCI value. The maximum, discussed a little later, corresponds to the symmetric case, the tree J_n, as shown in the previous chapter. This result is true for both SCI and RCI. We begin first with the formulas of the SCI and RCI of the tree $T_{n,x}$. For convenience we make the following definition.

Definition 6 *Define* $S_n(x) = S(T_{n,x})$ *and* $R_n(x) = R(T_{n,x})$.

Proposition 1 *Let* $T_{n,x}$, $S_n(x)$, *and* $R_n(x)$ *be as above. Then*

$$\begin{aligned}
S_n(x) &= \frac{x}{\sqrt{x+2}} + \frac{n-x-2}{\sqrt{n-x}} + \frac{1}{\sqrt{n}} \\
R_n(x) &= \frac{x}{\sqrt{x+1}} + \frac{n-x-2}{\sqrt{n-x-1}} + \frac{1}{\sqrt{(x+1)(n-x-1)}}.
\end{aligned}$$

PROOF: The SCI and RCI formulas are clearly developed from the tree graph of $T_{n,x}$ in Figure 4.1 below. There are x edges labeled by $(1, x+1)$, $n-x-2$ edges labeled by $(n-x-1, 1)$, and 1 edge labeled by $(x+1, n-x-1)$.

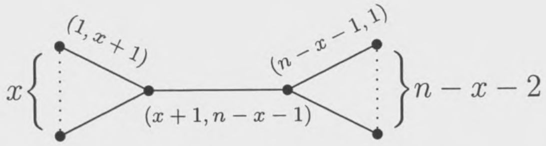


Figure 4.1: General Double Star Tree $T_{n,x}$

QED

One can refer to the tree in Figure 4.1 and clearly see that the branches on the left and right can be switched and still obtain the same value for the appropriate index. The following lemma shows the graphs of $S_n(x)$ and $R_n(x)$ are symmetric with respect to the vertical line $x = \frac{n-2}{2}$.

Lemma 1 *The following is true:*

1. $S_n(x) = S_n(n-x-2)$
2. $S_n'(x) = -S_n'(n-x-2)$
3. $R_n(x) = R_n(n-x-2)$
4. $R_n'(x) = -R_n'(n-x-2)$.

PROOF: For 1, by definition of $S_n(x)$,

$$\begin{aligned} S_n(n-x-2) &= \frac{n-x-2}{\sqrt{(n-x-2)+2}} + \frac{n-(n-x-2)-2}{\sqrt{n-(n-x-2)}} + \frac{1}{\sqrt{n}} \\ &= \frac{n-x-2}{\sqrt{n-x}} + \frac{x}{\sqrt{x+2}} + \frac{1}{\sqrt{n}} = S_n(x). \end{aligned}$$

Therefore

$$S_n(x) = S_n(n-x-2).$$

For 2, by 1,

$$\frac{d}{dx}S_n(x) = \frac{d}{dx}S_n(n-x-2) = S_n'(n-x-2)(-1) = -\frac{d}{dx}S_n(n-x-2).$$

Therefore

$$S_n'(x) = -S_n'(n-x-2).$$

For 3, by definition of $R_n(x)$,

$$\begin{aligned} R_n(n-x-2) &= \frac{n-x-2}{\sqrt{(n-x-2)+1}} + \frac{n-(n-x-2)-2}{\sqrt{n-(n-x-2)-1}} \\ &+ \frac{1}{\sqrt{((n-x-2)+1)\,(n-(n-x-2)-1)}} \\ &= \frac{n-x-2}{\sqrt{n-x-1}} + \frac{x}{\sqrt{x+1}} + \frac{1}{\sqrt{(n-x-1)(x+1)}} = R_n(x). \end{aligned}$$

Therefore

$$R_n(x) = R_n(n-x-2).$$

For 4, by 3,

$$\frac{d}{dx}R_n(x) = \frac{d}{dx}R_n(n-x-2) = R_n'(n-x-2)(-1) = -\frac{d}{dx}R_n(n-x-2).$$

Therefore

$$R_n'(x) = -R_n'(n-x-2).$$

QED

4.2 Maximum and Minimum of the SCI

Now we investigate the behavior of the graph $T_{n,x}$. It is interesting to see that the symmetric tree $J_n = T_{n,(n-2)/2}$ has the maximum RCI and SCI values.

Theorem 6 *Consider the set $\Gamma = \{T_{n,x} | n \geq 6, 2 \leq x \leq n-4\}$. Then*

1. *J_n has the maximum SCI among all the graphs in Γ with*

$$\max_{G\in\Gamma}\{S(G)\} = S_n\Big(\frac{n-2}{2}\Big) = \frac{\sqrt{2}(n-2)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}}.$$

2. *$T_{n,2}$ has the minimum SCI among all the graphs in Γ with*

$$\min_{G\in\Gamma}\{S(G)\} = S_n(2) = 1 + \frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}}.$$

PROOF: We observe that the graph of $S_n(x)$ has the maximum in the middle of the interval and decide to look at the derivative. Below we show that the derivative has a unique real root. The derivative of $S_n(x)$ is

$$S_n'(x) = \frac{x+4}{2(x+2)^{3/2}} + \frac{x-2-n}{2(n-x)^{3/2}}.$$

By factorization

$$\begin{aligned}
S_n'(x) = 0 \iff & \frac{x+4}{(x+2)^{3/2}} + \frac{n+2-x}{(n-x)^{3/2}} = 0 \\
\iff & (x+4)^2(n-x)^3 - (x+2)^3(n+2-x)^2 = 0 \\
\iff & (n-2x-2)[(x+2)^2(n-x)^2 + 4(x+2)(n-x)(n+2) \\
& +4(n-x)^2 + 4(n-x)(x+2) + 4(x+2)^2] = 0 \\
\iff & n - 2x - 2 = 0 \iff x = \frac{n-2}{2},
\end{aligned}$$

since

$$\begin{aligned}
(x+2)^2(n-x)^2 &+ 4(x+2)(n-x)(n+2) \\
&+ 4[(n-x)^2 + (n-x)(x+2) + (x+2)^2] > 0.
\end{aligned}$$

Thus $x_0 = \frac{n-2}{2}$ is a unique real root of $S_n'(x)$.

Now we check the signs of $S_n'(x)$ at each side of $x_0 = \frac{n-2}{2}$. We pick two points $x_1 = x_0 - 1 = \frac{n}{2} - 2$ and $x_2 = x_0 + 1 = \frac{n}{2}$. Then

$$S_n'\Big(\frac{n}{2} - 2\Big) > 0 \quad \text{and} \quad S_n'\Big(\frac{n}{2}\Big) < 0.$$

Thus the function is increasing from 2 to x_0 and decreasing from x_0 to $n-4$. $S_n(x)$ reaches its maximum value at x_0 and its minimum value at 2 and $n-4$.

$$\begin{aligned}
\max_{G\in\Gamma}\{S(G)\} &= S_n\Big(\frac{n-2}{2}\Big) = \frac{\sqrt{2}(n-2)}{\sqrt{n+2}} + \frac{1}{\sqrt{n}} \\
\min_{G\in\Gamma}\{S(G)\} &= S_n(2) = 1 + \frac{n-4}{\sqrt{n-2}} + \frac{1}{\sqrt{n}} = S_n(n-4).
\end{aligned}$$

QED

The two corresponding graphs are isomorphic as shown below.

Figure 4.2: $S_n(2)$

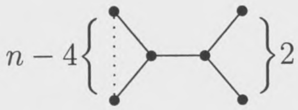


Figure 4.3: $S_n(n-4)$

Figure 4.4 and Figure 4.5 are an example when $n = 8$. The maximum value of $S_8(x)$ occurs at x=3, as shown in Figure 4.4.

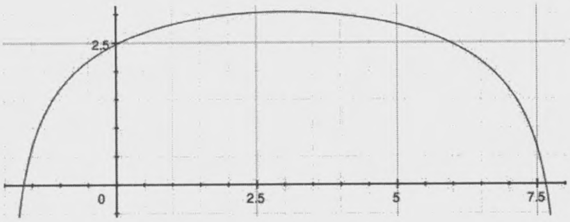


Figure 4.4: Graph of $S_8(x)$

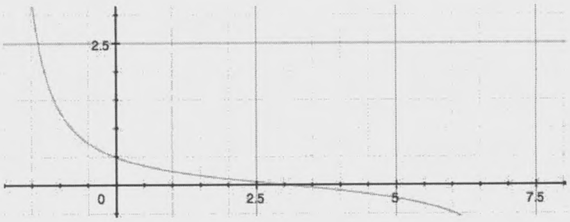


Figure 4.5: Graph of $S_8'(x)$

4.3 Maximum and Minimum of the RCI

Now that the SCI has been proven, we look at the RCI which has similar results.

Theorem 7 *Consider the set* $\Gamma = \{T_{n,x} | n \geq 6, 2 \leq x \leq n-4\}$. *Then*

1. J_n *has the maximum RCI among all the graphs in* Γ *with*

$$\max_{G \in \Gamma}\{R(G)\} = R_n\Big(\frac{n-2}{2}\Big) = \frac{\sqrt{2}(n-2)}{\sqrt{n}} + \frac{2}{n}.$$

2. $T_{n,2}$ *has the minimum RCI among all the graphs in* Γ *with*

$$\min_{G \in \Gamma}\{R(G)\} = R_n(2) = \frac{2}{\sqrt{3}} + \frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{3(n-3)}}.$$

PROOF:

$$R_n(x) = \frac{x}{\sqrt{x+1}} + \frac{n-x-2}{\sqrt{n-x-1}} + \frac{1}{\sqrt{(x+1)(n-x-1)}}$$

$$\begin{aligned} R_n'(x) &= \frac{x+2}{2(x+1)^{3/2}} + \frac{x-n}{2(n-x-1)^{3/2}} + \frac{2x-n+2}{2\Big[(x+1)(n-x-1)\Big]^{3/2}} \\ &= \frac{(x+2)(n-x-1)^{3/2} + (x-n)(x+1)^{3/2} + 2x - n + 2}{2\Big[(x+1)(n-x-1)\Big]^{3/2}}. \end{aligned}$$

Similar as for $S_n(x)$, we want to show that the graph of $R_n(x)$ is increasing on the interval $[2, (n-2)/2)$ and decreasing on the interval $[(n-2)/2, n-4]$. We first show that $x_0 = (n-2)/2$ is the only zero of $R_n'(x)$, that is, $x_0 = (n-2)/2$ is the only critical number for $R_n(x)$ on $[2, n-4]$. Obviously, $R_n'(x) = 0$ if and only if the numerator of the last expression above is zero. Because of the complexity of the function involved, we introduce the following notations:

$$\Delta = (x+2)(n-x-1)^{3/2} + (x-n)(x+1)^{3/2} + 2x - n + 2$$

$$a = \sqrt{x+1} \quad \text{and} \quad b = \sqrt{n-x-1}.$$

The following relationships are useful later:

on the interval $[2, n-4]$,

$$\begin{array}{llll} a^2 = x+1 \geq 3, & b^2 = n-1-x \geq 3, & ab \geq 3, & a+b < a^2+b^2 \\ a^2+b^2 = n, & a^2-b^2 = 2x-n+2. & & \end{array}$$

Thus

$$\begin{aligned} \Delta &= (x+2)(n-x-1)^{3/2} + (x-n)(x+1)^{3/2} + 2x - n + 2 \\ &= [(x+1)+1]b^3 + [(x-n+1)-1]a^3 + (2x-n+2) \\ &= a^2b^3 + b^3 - b^2a^3 - a^3 + a^2 - b^2 = (a^2b^3 - b^2a^3) + (b^3 - a^3) + (a^2 - b^2) \\ &= (b-a)[a^2b^2 + (b^2 + a^2 + ab) - (b+a)]. \end{aligned}$$

It implies that $a = b$ gives a solution to $\Delta = 0$ or $R_n'(x) = 0$. By definition of a, b, $a = b \Longleftrightarrow x = (n-2)/2 = x_0$. So $R_n'(x_0) = 0$. Next we claim that x_0 is the only zero of $R_n'(x)$ on the interval $[2, n-4]$. It is equivalent to show that $\Delta \neq 0$ for all x where $2 \leq x \leq n-4$ and $x \neq x_0$. Note that

$$a^2b^2 + (b^2 + a^2 + ab) - (b+a)] > a^2b^2 + ab \geq 12 > 0.$$

Thus x_0 is the only zero of Δ, thus the only zero of $R_n'(x)$.

Now we check the signs of $R_n'(x)$ at each side of $x_0 = \frac{n-2}{2}$. Similarly we use the two points $x_1 = x_0 - 1 = \frac{n}{2} - 2$ and $x_2 = x_0 + 1 = \frac{n}{2}$. Then

$$R_n'\left(\frac{n}{2} - 2\right) > 0 \quad \text{and} \quad R_n'\left(\frac{n}{2}\right) < 0.$$

Thus it is easily seen that the function is increasing from 2 to x_0 and decreasing from x_0 to $n-4$. $R_n(x)$ reaches its maximum value at x_0 and its minimum value at 2 and $n-4$.

$$\begin{aligned} \max_{G\in\Gamma}\{R(G)\} &= R_n\left(\frac{n-2}{2}\right) = \frac{\sqrt{2}(n-2)}{\sqrt{n}} + \frac{2}{n} \\ \min_{G\in\Gamma}\{R(G)\} &= R_n(2) = \frac{2}{\sqrt{3}} + \frac{n-4}{\sqrt{n-3}} + \frac{1}{\sqrt{3(n-3)}} = R_n(n-4). \end{aligned}$$

QED

Similarly, Figure 4.6 and Figure 4.7 are an example when $n = 8$. The maximum value of $R_8(x)$ occurs at 3, as shown in Figure 4.6.

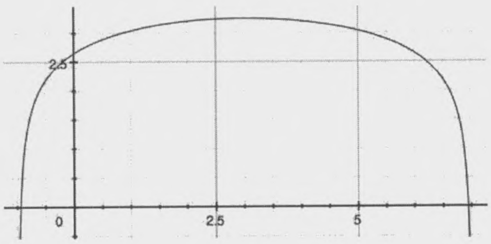


Figure 4.6: Graph of $R_8(x)$

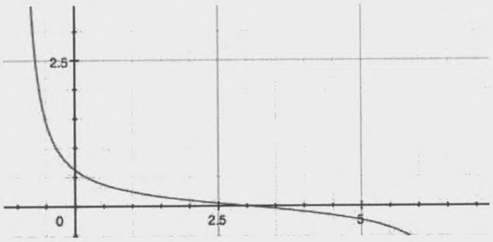


Figure 4.7: Graph of $R'_8(x)$

4.4 Intersection of the $S_n(x)$ and $R_n(x)$

Theorem 8 *The graphs $R_n(x)$ and $S_n(x)$ have exactly one intersection point when $x > 0$. The intersection point occurs when $n - 2 \leq x < n - 1$.*

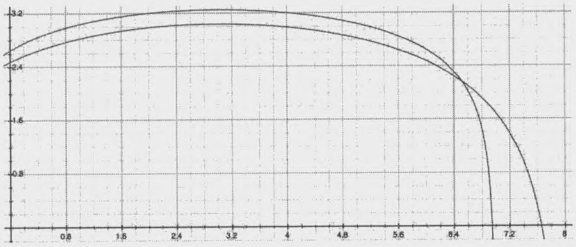


Figure 4.8: Intersection of SCI and RCI

PROOF: Notice that the graphs of $R_n(x)$ and $S_n(x)$ are symmetric with respect to the vertical line $x = \frac{n-2}{2}$. It is sufficient to consider $x > \frac{n-2}{2}$. In this case the graphs $R_n(x)$ and $S_n(x)$ are both decreasing. Thus, $R_n(x)$ and $S_n(x)$ can have at most one intersection point. Set $x = n - 2 + \epsilon$, where $0 \leq \epsilon < 1$.

$$\begin{aligned} R_n(x) - S_n(x) &= \frac{n-2+\epsilon}{\sqrt{n-1+\epsilon}} - \frac{n-2+\epsilon}{\sqrt{n+\epsilon}} + \frac{\epsilon}{\sqrt{2-\epsilon}} - \frac{\epsilon}{\sqrt{1-\epsilon}} \\ &+ \frac{1}{\sqrt{(n-1+\epsilon)(1-\epsilon)}} - \frac{1}{\sqrt{n}}. \end{aligned}$$

When $x = n - 2$, $\epsilon = 0$ and

$$R_n(n-2) - S_n(n-2) = \frac{n-2}{\sqrt{n-1}} - \frac{n-2}{\sqrt{n}} + \frac{1}{\sqrt{n-1}} - \frac{1}{\sqrt{n}} > 0.$$

As $\epsilon \to 1^-$,

$$\lim_{\epsilon \to 1^-} R_n(n-2) - S_n(n-2) = \frac{n-1}{\sqrt{n}} - \frac{n-1}{\sqrt{n+1}} + 1 - \frac{1}{\sqrt{n}}$$

$$+ \lim_{\epsilon \to 1^-} \frac{1}{\sqrt{1-\epsilon}} \left(\frac{1}{\sqrt{n}} - 1 \right) = -\infty.$$

Thus, $R_n(x) - S_n(x) < 0$ when x is close to $n-1$. There exists $x_0 \in (n-2, n-1)$ such that $R_n(x_0) = S_n(x_0)$. QED

Chapter 5

$T_{n,a} \times P_m$ Trees

5.1 Introduction to the tree $T_{n,a} \times P_m$

If we look at the tree $T_{n,a}$ and extend the length of the middle to a path P_m of length m, we derive the following definition.

Definition 7 *The tree $T_{n,a} \times P_m$ with $n \geq 6$ and $2 \leq a \leq n-m-3$, is a tree with n vertices, $n-m-1$ leaves, and a path of length m in the middle with the shape:*

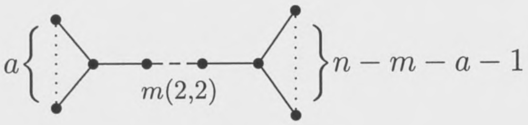


Figure 5.1: Tree $T_{n,a} \times P_m$

We say the graph $T_{n,a} \times P_m$ is symmetric if $a = n-m-a-1$, that is, $a = \frac{n-m-1}{2}$. Denote the corresponding symmetric tree as $J_{n,m}$. In other words, the tree $J_{n,m}$ has n vertices and is built on the path P_m with $(n-m-1)/2$ leaves from each end vertex of the path. Shown in Figure 5.2.

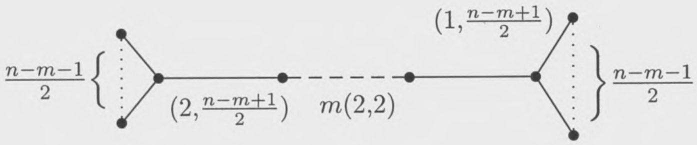


Figure 5.2: Tree $J_{n,m}$

Example 5 *$T_{8,2} \times P_3$ is a symmetric tree and in Chemistry it is known as $2,5-$ Dimethylhexane.*

5.2 The SCI and RCI of $J_{n,m}$ and Comparison Study

Theorem 9 *For $n \geq 6$ and $2 \leq m \leq n-5$, let $T_{n,a} \times P_m = J_{n,m}$ be a symmetric tree where $a = \frac{n-m-1}{2}$. Then*

$$\begin{aligned} S(J_{n,m}) &= \frac{\sqrt{2}(n-m-1)}{\sqrt{n-m+3}} + \frac{2\sqrt{2}}{\sqrt{n-m+5}} + \frac{m-2}{2} \\ R(J_{n,m}) &= \frac{\sqrt{2}(n-m-1)+2}{\sqrt{n-m+1}} + \frac{m-2}{2}. \end{aligned}$$

PROOF:

The graph $J_{n,m}$ has $n-m-1$ leaves labeled by $(1, \frac{n-m+1}{2})$, two edges labeled by $(2, \frac{n-m+1}{2})$, and the path in the middle, separating the two stars, labeled by $(\frac{m-2}{2})$ as shown in Figure 5.2. By the definition of SCI,

$$\begin{aligned} S(J_{n,m}) &= \frac{n-m-1}{\sqrt{\frac{n-m+1}{2}+1}} + \frac{2}{\sqrt{\frac{n-m+1}{2}+2}} + \frac{m-2}{2} \\ &= \frac{\sqrt{2}(n-m-1)}{\sqrt{n-m+3}} + \frac{2\sqrt{2}}{\sqrt{n-m+5}} + \frac{m-2}{2} \end{aligned}$$

and by the definition of RCI,

$$\begin{aligned} R(J_{n,m}) &= \frac{n-m-1}{\sqrt{\frac{n-m+1}{2}}} + \frac{2}{\sqrt{2(\frac{n-m+1}{2})}} + \frac{m-2}{2} \\ &= \frac{\sqrt{2}(n-m-1)+2}{\sqrt{n-m+1}} + \frac{m-2}{2}. \end{aligned}$$

QED

Theorem 10 *Let $J_{n,m}$ be a symmetric tree as above, with $n \geq 6$. Then for every fixed m with $2 \leq m \leq n-5$,*

1. $\lim_{n\to\infty} R(J_{n,m}) - S(J_{n,m}) = 0.$
2. $\lim_{n\to\infty} \frac{S(J_{n,m})}{R(J_{n,m})} = 1$

PROOF:

$$\begin{aligned} \lim_{n\to\infty} R(J_{n,m}) - S(J_{n,m}) &= \lim_{n\to\infty} \sqrt{2(n-m-1)}\left(\frac{1}{\sqrt{n-m+1}} - \frac{1}{\sqrt{n-m+3}}\right) \\ &+ \frac{2}{\sqrt{n-m+1}} - \frac{2\sqrt{2}}{\sqrt{n-m+5}} = 0. \end{aligned}$$

$$\lim_{n\to\infty} \frac{S(J_{n,m})}{R(J_{n,m})} = \lim_{n\to\infty} \frac{\sqrt{2(n-m+3)} + \frac{m-2}{2}}{\sqrt{2(n-m+1)} + \frac{m-2}{2}} = 1.$$

QED

Chapter 6

Future Directions

In the future, I hope to continue working on Chapter 5 and work to get results for the symmetric case of the RCI. I would like to get similar results to Chapter 4 and compare the indices of the tree $T_{n,a}$ with a path of length 2 and the tree $T_{n,a} \times P_m$ with a path of length m.

I also would like to find different applications in which the indices can be used and how they can relate outside of Chemistry and Biology.

Lastly, I hope to answer the following open questions:

1. Do trees with long branches show special characteristics in reference to their index values?
2. What special properties does a tree have if it has many copies of the same subtree?
3. In practice, what do the indices mean, for example, what can the indices tell about tetramethyl- trees in Chemistry?
4. For a given positive integer α, what graph can have RCI and SCI equal to α or very close to α?
5. For a given graph with RCI α and given a positive integer ϵ, can we find another graph whose RCI is within $(\alpha - \epsilon, \alpha + \epsilon)$?

Bibliography

[1] Béla Bollobás and Paul Erdős. Graphs of extremal weights. *Ars Combinatoria*, 50:225–233, 1998.

[2] Kimberly J. Burch, Diane K. Wakefield, and Earl G. Whitehead. Boiling point models of alkanes. *MATCH-Communications in Mathematical and in Computer Chemistry*, 47:25–52, 2003.

[3] Lowell H. Hall and Lemont B. Kier. Issues in representation of molecular structure: The developement of molecular connectivity. *Journal of Molecular Graphics and Modelling*, 20:4–18, February 2001.

[4] P. Hansen and H. Mélot. Variable neighborhood search for extremal graphs. 6. analyzing bounds for the connectivity index. *Journal of Chemical Information and Computer Sciences*, 43:1–14, 2003.

[5] Mati Karelson. *Molecular Descriptors in QSAR/QSPR*. John Wiley and Sons, Inc., 2000.

[6] Milan Randić. On characterization of molecular branching. *Journal of the American Chemical Society*, 97(23):6609–6615, November 1975.

[7] Milan Randić. The connectivity index 25 years after. *Journal of Molecular Graphics and Modelling*, 20:19–35, 2001.

[8] Janice Smith. *Organic Chemistry*. McGraw-Hill Companies, 3rd edition, 2010.

[9] Alan Tucker. *Applied Combinatorics*. John Wiley and Sons, Inc., 5th edition, 2007.

[10] K. Vesztergombi and L. Lovasz. *Discrete Mathematics*. Yale University. Tankonyvkiado, Budapest 1972, lecture notes edition, 1999.

[11] Lian-Zhu Zhang, Mei Lu, and Feng Tian. Maximum randić index on trees with k-pendant vertices. *Journal of Mathematical Chemistry*, 41(2):161–171, February 2007.

[12] Bo Zhou and Nenad Trinajstić. On a novel connectivity index. *Journal of Mathematical Chemistry*, 46(4):1252–1270, 2009.

[13] Bo Zhou and Nenad Trinajstić. On general sum-connectivity index. *Journal of Mathematical Chemistry*, 47(1):210–218, 2010.

[14] Bo Zhou, Nenad Trinajstić, and Zhibin Du. Minimum general sum-connectivity index of unicyclic graphs. *Journal of Mathematical Chemistry*, 48(3):697–703, 2010.

[15] Bo Zhou, Nenad Trinajstić, and Zhibin Du. Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number. *Journal of Mathematical Chemistry*, 47(2):842–855, 2010.

[16] Bo Zhou, Nenad Trinajstić, and Rundan Xing. Sum-connectivity index of molecular trees. *Journal of Mathematical Chemistry*, 48(3):583–591, 2010.

Appendix A

Alkane Tree Connectivity Indices

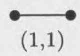
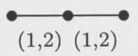
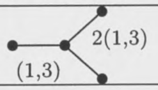
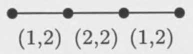
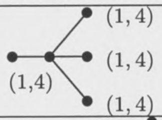
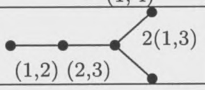
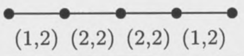
Molecule	Graph	SCI	RCI
Ethane		0.7071	1
Propane		1.1547	1.4142
Isobutane		1.5000	1.7321
n-Butane		1.6547	1.9142
2,2-Dimethylpropane		1.7889	2
2-Methylbutane		2.0246	2.2701
n-Pentane		2.1547	2.4142

Table A.1: Connectivity Indices of Alkane Trees with $2-5$ vertices

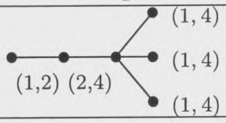
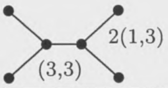
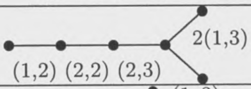
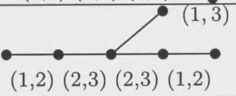
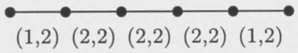
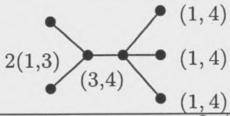
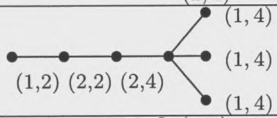
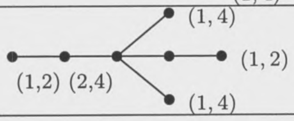
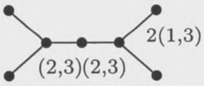
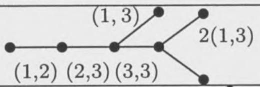
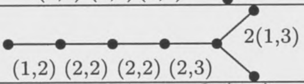
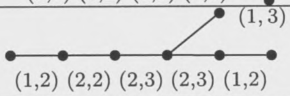
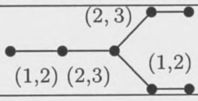
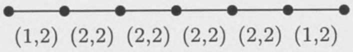
Molecule	Graph	SCI	RCI
2,2-Dimethylbutane		2.3272	2.5607
2,3-Dimethylbutane		2.4082	2.6427
2-Methylpentane		2.5246	2.7701
3-Methylpentane		2.5491	2.8081
n-Hexane		2.6547	2.9142
2,2,3-Trimethylbutane		2.7200	2.9434
2,2-Dimethylpentane		2.8272	3.0607
3,3-Dimethylpentane		2.8656	3.1213
2,4-Dimethylpentane		2.8944	3.1259
2,3-Dimethylpentane		2.9328	3.1807
2-Methylhexane		3.0246	3.2701
3-Methylhexane		3.0491	3.3081
3-Ethylpentane		3.0737	3.3461
n-Heptane		3.1547	3.4142

Table A.2: Connectivity Indices of Alkane Trees with 6 or 7 vertices

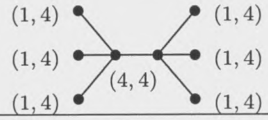
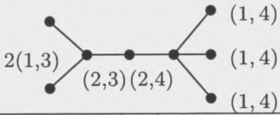
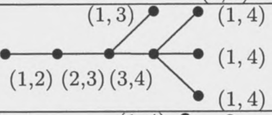
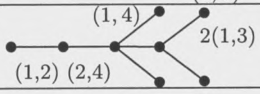
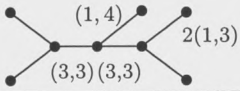
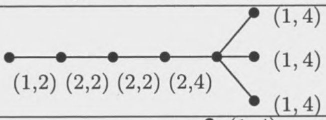
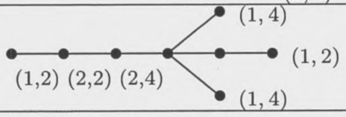
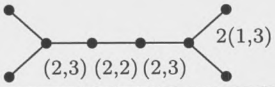
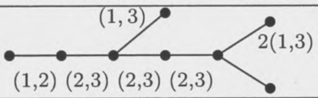
Molecule	Graph	SCI	RCI
2,2,3,3-Tetramethylbutane		3.0368	3.2500
2,2,4-Trimethylpentane		3.1971	3.4165
2,2,3-Trimethylpentane		3.2442	3.4814
2,3,3-Trimethylpentane		3.2580	3.5040
2,3,4-Trimethylpentane		3.3165	3.5534
2,2-Dimethylhexane		3.3272	3.5607
3,3-Dimethylhexane		3.3656	3.6213
2,5-Dimethylhexane		3.3944	3.6259
2,4-Dimethylhexane		3.4190	3.6639

Table A.3: Connectivity Indices of Alkane Trees with 8 vertices

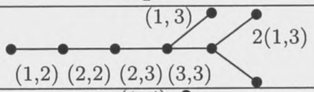
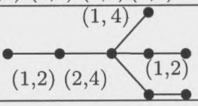
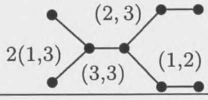
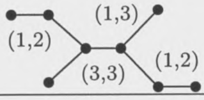
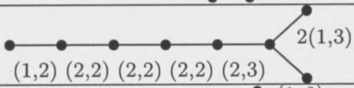
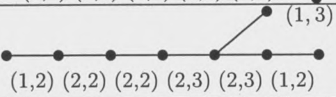
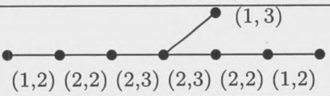
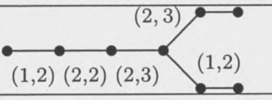
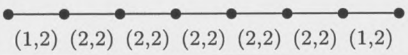
Molecule	Graph	SCI	RCI
2,3-Dimethylhexane		3.4328	3.6807
3,3-Methylethylpentane		3.4040*	3.6819
2-Methyl-3-ethylpentane		3.4574	3.7187
3,4-Dimethylhexane		3.4574	3.7187
2-Methylheptane		3.5246	3.7701
3-Methylheptane		3.5491	3.8081
4-Methylheptane		3.5491	3.8081
3-Ethylhexane		3.5737	3.8461
n-Octane		3.6547	3.9142

Table A.4: Connectivity Indices of Alkane Trees with 8 vertices (cont.)

Appendix B

Relation of RCI/SCI Values to the Structure Properties of Hexane Isomers

The number in the parenthesis is the rank order of the property values. The abbreviations in the table BP is Boiling Point and HF is Heat of Formation. When the RCI and SCI values increase, the boiling point increases and the heat of formation decreases. Part of this table was taken from [2].

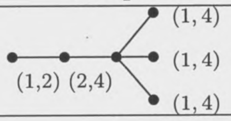
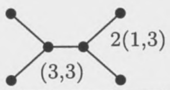
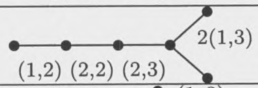
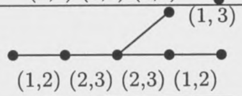
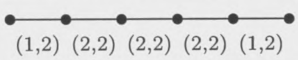
Molecule	Graph	SCI	RCI	BP	HF
2,2-Dimethylbutane		2.3272	2.5607	49.7 (5)	44.35 (1)
2,3-Dimethylbutane		2.4082	2.6427	58.0 (4)	42.49 (2)
2-Methylpentane		2.5246	2.7701	60.3 (3)	41.66 (3)
3-Methylpentane		2.5491	2.8081	63.2 (2)	41.02 (4)
n-Hexane		2.6547	2.9142	68.7 (1)	39.96 (5)

Table B.1: Relation of RCI/SCI Values to the Structure Properties of Hexane Isomers