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Technical Report No. 53

Novel Application of Randić Molecular Connectivity Index On Data Reduction of Chemical Graphs

by

Sherif El-Basil

Prepared for Publication

in the

Chem. Phys. Letters



University of Georgia Department of Chemistry Athens, Georgia 30602

August 11, 1987

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Novel Applications of Randić Molecular Connectivity Index On data reduction of chemical graphs

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Sherif El-Basil

Department of Chemistry, University of Georgia

Athens, GA 30606 U.S.A.

Benzenoid hydrocarbons are studied in terms of the much simpler <u>caterpillar</u> <u>trees</u>. Using molecular connectivity indices of the latter almost exact linear relations are obtained with natural logarithms of five properties of <u>benzenoid</u> <u>hydrocarbons</u> including all self-avoiding paths, conjugated circuits, number of Kekulé structures, electronic absorption spectra, and heats of atomizations.

Key words: - Graph Theory , - Randie Molecular Connectivity Index - Data Reduction - Caterpillar trees Accesion For NTIS CRA&L Benzenoid Hydrocarbons DHC EAT -[] Unannour cod By Distribution [ Availated y Cutes The differ open of A-1

One of the main goals of every science is the endeavoring to arrange and collate the numerous individual observations and details which present themselves, in order that they become part of one comprehensive picture.<sup>1</sup> Such an objective may be achieved through the use of data reduction which is an essential part of chemical and physical data analysis. In the past the task of data reduction involved mainly curve fitting procedures which have recently become more efficient due to increased availability of computers. Topological approaches which consider additivities of molecular properties have been almost ignored in the past. However some recognition of the role of graph theory became apparent soon after the (important) work of Smolenskii<sup>2</sup> and (to a lesser degree) the work of Gordon and Kennedy<sup>3</sup> who formalized their schemes of general approaches to molecular additivities. Revival of interest in chemical graph theory is probably due to Balaban via his (editing) of a book<sup>4</sup>, which provided a source of problems and numerous other papers. Several counting polynomials were defined which act as descriptors of the connectivity pattern of various types of molecular graphs. The latters are well-defined mathematical objects which describe the bonding relation between atoms in the original molecules. Such counting polynomials are then a combinatorial form of data reduction. Equation 1 describes the general form of a graph-theoretical counting polynomial<sup>5</sup>, F(G;x), for an arbitrary graph G, containing n vertices:

$$F(G;x) = \sum_{k=0}^{M} \Theta(G;k) x^{f(k,n)}$$
(1)

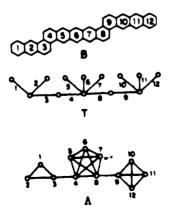
where  $\rho$  is either 1 or  $(-1)^k$ ,  $\theta(G;k)$  enumerates-certain selected <u>graph-invariants</u> in G taken in k independent tuples (i.e. no two of them are adjacent) and M is

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the maximal value of k. For the purpose of this paper we consider three polynomials for all of which  $\rho = 1$  and f(k,n) = n. These are:

- i) The counting polynomial (of Hosoya)<sup>6</sup>, H(G;x) for which  $\theta$ (G;k) = p(G;k) = the number of k-matchings in G.
- ii) The sextet polynomial (of Hosoya and Yamaguchi)<sup>7</sup>, σ(B;x) of which θ(G;k)
   = r(B;k) = the number of selections of k mutually resonant but nonadjacent aromatic sextet in a benzenoid system (= polyhex graph<sup>8</sup>), B.
- iii) The independence polynomial (of Gutman)<sup>9</sup>,  $\omega$  (G;x), for which  $\theta$ (G;k) = 0(G;k) = the number of selections of k independent vertices of G.
- 2. The Caterpillar Tree<sup>10</sup>, the Polyhex Graph<sup>11</sup> and the Clar Graph<sup>9,12</sup>

In a given Kekulé structure an (aromatic) sextet is defined as a set of three double bonds circularly conjugated so that no two sextets can have a common bond. When two rings (hexagons) can have aromatic sextets so that all other carbon atoms are spanned by a sextet or by double bond, such two rings are called <u>resonant.<sup>9,12</sup></u> The individual hexagons of a given benzenoid system may or may not be resonant<sup>7</sup>. Information on such resonance relations (among the individual hexagons) are best "<u>reduced</u>" (i.e. described) using either a caterpillar tree<sup>10</sup> or a Clar graph.<sup>9</sup> To illustrate this <u>fundamental</u> relation<sup>13</sup> we consider the three graphs shown below:



The <u>hexagons</u> of B may be grouped into three subsets, viz.,  $\{1,2,3\}$ ;  $\{4,5,6,7,8\}$ ;  $\{9,10,11,12\}$ . One observes that <u>no two hexagons are resonant if they belong</u> <u>to one subset</u>. Similarly the edges of T may be subdivided into analgous three subsets observing that no two <u>edges</u> of the same subset can be adjacent. A similar description obtains for the <u>vertices</u> of graph A. In fact bijective (i.e. one-to-one, onto)<sup>14</sup> mapping might be defined between the hexagons of B, the edges of T and the vertices of A: the latter is called <u>the Clar graph</u><sup>9,12</sup> <u>of B</u>. It is easy to verify the following identity:

$$\sigma (B;x) = H(T;x) = \omega(\Lambda;x) = 1 + 12X + 45X^2 + 53X^3$$
(2)

A caterpillar tree such as T whose counting polynomial is identical to the sextet polynomial of a benzenoid hydrocarbon B will be called an equivalent caterpillar to the benzenoid hydrocarbon. the set of graphs { B,T,A} shown above will be called <u>a set of equivalent graphs</u>. Gutman<sup>15</sup> demonstrated that for every nonbranched<sup>16</sup> benzenoid hydrocarbon there is an "equivalent" caterpillar tree.

#### 3. Conjecture

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The physical properties of a benzenoid hydrocarbon which depend on its topological structure may be predicted from graph-theoretical properties of its equivalent graphs.

# 4. Results and tests of Conjectures

Fig. 1 shows benzenoid hydrocarbons and their equivalent caterpillar trees studied in this work. <u>4.a</u> Graph theoretical (combinatorial) properties

Three <u>graph-theoretical properties</u> of benzenoid hydrocarbons, viz., self-avoiding paths<sup>19</sup>, conjugated circuits<sup>20</sup> and the number of Kekulé structures (i.e. number of perfect matchings) are correlated with the molecular connectivity indices,<sup>21</sup> x 's of the equivalent caterpillar (or pseudocaterpillar) trees. Fig. 2 shows the types of linear correlations obtained. In all cases correlation coefficients  $\geq$  0.999 were obtained.

## 4b. Physical properties

Two <u>physical properties</u> viz., electronic absorption spectra<sup>22</sup>, and heats of atomizations<sup>23</sup> of several homologous series of benzenoid hydrocarbons are linearly correlated with X (T)'s; the molecular connectivity indices<sup>21</sup> of the corresponding equivalent trees. Details of data are available of request<sup>17</sup> but as an illustraton Table 1 is included which contains  $\beta$  and p bands of the electronic spectra of two families of hydrocarbons of Fig. 3. A separate manuscript is submitted elsewhere<sup>24</sup> dealing with electronic absorption spectra of 27 arene systems all linearly correlated with  $\chi$ (T) values. The same type of <u>data reduction</u> is obtainable<sup>17</sup> when molecular properties (topological or physical) of benzenoid hydrocarbons are studied in terms of connectivity functions of their equivalent Clar graphs.<sup>25</sup> Fig. 4 is a plot of heats of atomizations of some benzenoid hydrocarbons versus connectivity indices of the corresponding caterpillar trees.

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### 6. Discussion

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Caterpillar trees and Clar graphs seem to be quite promising "storage devices" which preserve many properties of (the much larger) equivalent polyhex graphs. In contrast to the Balaban-Harary dualist graphs<sup>26</sup> they do not have a geometric element and as such, connectivity alone best describes them. It is amazing that some of the studied properties such as the total number of paths<sup>19</sup> in a polyhex graph (Fig. 2) take nearly 30 minutes on a Corona computer, $2^7$ yet can be retrieved by very simple hand calculation of the connectivity index of a much simpler graph! Table 2 lists percent retrievals of the total number of self-avoiding paths for a series of nonbranched benzenoid hydrocarbons shown in Fig. 1. All the above mentioned correlations imply classification of molecules into families (i.e. homologous series). The concept of classification is well-known in science: the periodic table of the elements and recently table of alkanes introduced by Randić and Wilkins<sup>28</sup> and more recently table of benzenoid hydrocarbons of Dias<sup>29</sup> are all non-mathematical forms of set theory. However in constrast to the latter two tables, which result from graph theoretical considerations, the "old" periodic table is a result of group theory as it follows from symmetry properties of atoms.

#### Acknowledgments

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Electron absorption spectra of the  $\beta$  bands,  $\lambda_{\beta}$ , of the homologous series of benzenoid hydrocarbons shown in Fig. 3. X (TYs are molecular connectivity indices of the equivalent pseudocaterpillar trees.

| Hydrocarbon* | <u>X(T)</u> | λ <u>β (Å)</u> | $\frac{\lambda_{p}(A)}{\lambda_{p}(A)}$ |
|--------------|-------------|----------------|---|
| A            | 3.914       | 2570           |   |
| В            | 4.684       | 2870           |   |
| С            | 5.293       | 3130           |   |
| D            | 5.812       | 3430           |   |
|              |             |                |   |
| 1            | 1.000       |                | 2068                                    |
| 2            | 1.414       |                | 2850                                    |
| 3            | 1.732       |                | 3745                                    |
| 4            | 2.000       |                | <b>47 1</b> 0                           |
| 5            | 2.236       |                | 5755                                    |
| 6            | 2.449       |                | <b>693</b> 0                            |

\*c.f. Fig. 3

Table 2

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Percent retrieval of the total number of self-avoiding paths for the series of nonbranched benzenoid hydrocarbons shown in Fig. 2. The regression line is Y = 4.374 + 0.484X with a correlation coefficient = 1.0000.

| Hydrocarbon* | Calcd. <u>Spi(B)</u> * | Actuals pi(B)* | Difference | <u>% Retrieval</u> a) |
|--------------|------------------------|----------------|------------|-----------------------|
| E            | 3254                   | 3277           | 23         | 99.298                |
| F            | 7391                   | 7413           | 22         | 99.704                |
| C            | 16055                  | 16055          | 0          | 100.000               |
| н            | 33827                  | 33879          | 52         | 99.846                |
| 1            | 69675                  | 69857          | 182        | 99.740                |
| J            | 141060                 | 142645         | 1585       | 98.889                |

\*c.f. Fig. 2

a) = 100 - 100 | Calcd-Actual | /Actual

## Fig. 1

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Polyhex graphs of benzenoid hydrocarbons studied in this work together with the molecular graphs of their corresponding caterpillar trees.

# Fig. 2

Combinatorial properties of benzenoid hydrocarbons studied: K(B),  $\Sigma p(B)$  and  $\Sigma R_{tot}(B)$  respectively indicate number of Kekulé structures, total number of self-avoiding paths and total number of conjugated circuits of a benzenoid system, B, plotted versus the connectivity index of the corresponding caterpillar tree, X(T) raised to various powers. (The hydrocarbons and their caterpillars are shown in Fig. 1).

#### Fig. 3

Electronic absorption spectra of benzenoid hydrocarbons: Points 1-6 indicate benzene, naphthalene, anthracene, tetracene, pentacene and hexacene; the line passing through these points is a plot of their absorption para band (in ln units) vs. the connectivity index of the corresponding caterpillar trees, X(T). The line passing through points A-D is a plot of the beta band vs. X(T) where the hydrocarbons and their trees are shown in Fig. 1.

#### Fig. 4

A plot of the natural logarithms of the heats of atomizations of some benzenoid hydrocarbons, In Ht At(B), against the connectivity indices,  $\chi(T)$ 's, of the corresponding caterpillar trees shown in Fig. 1.

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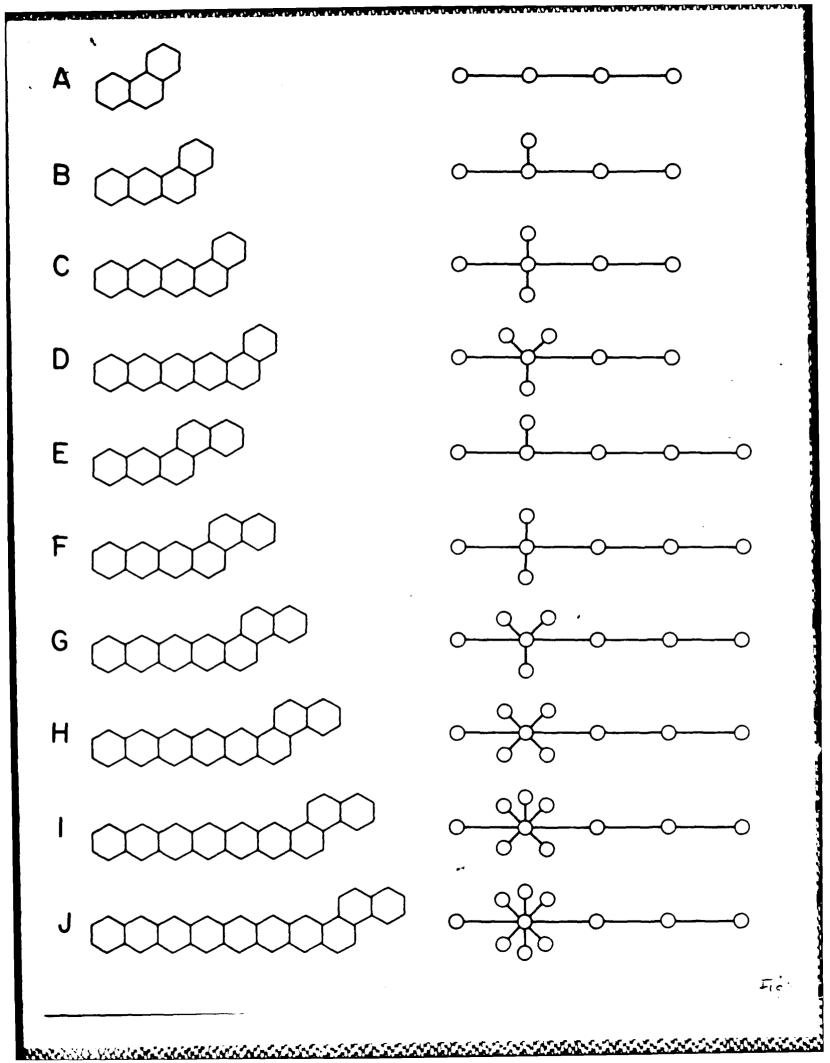
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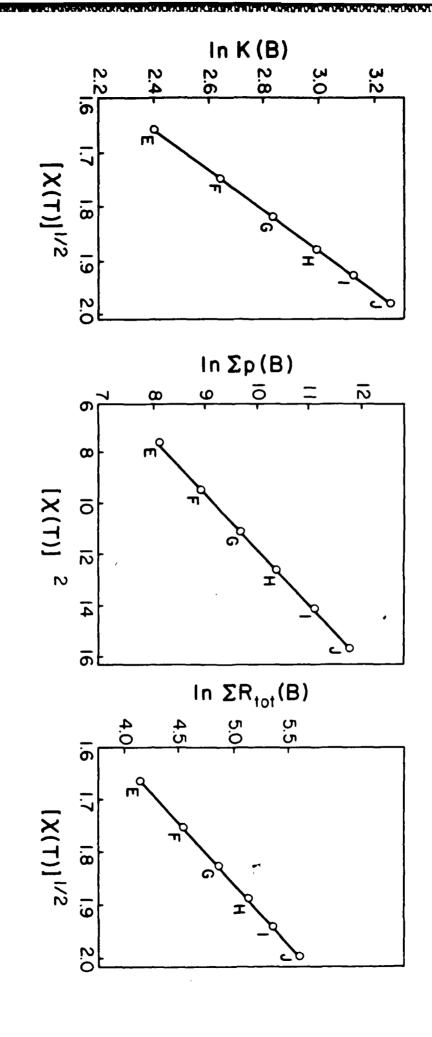
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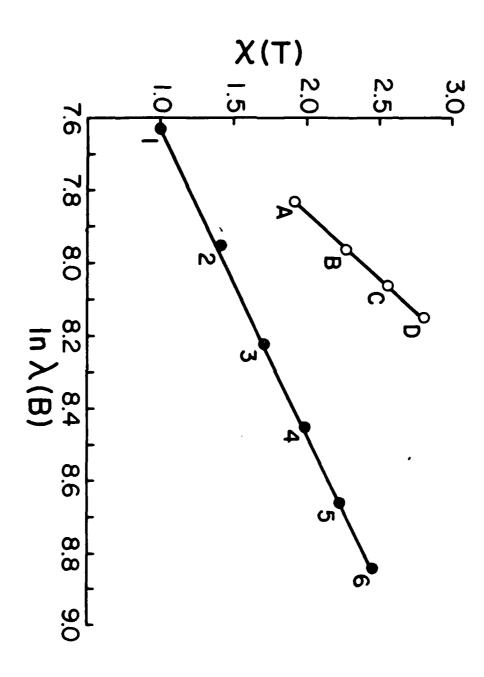
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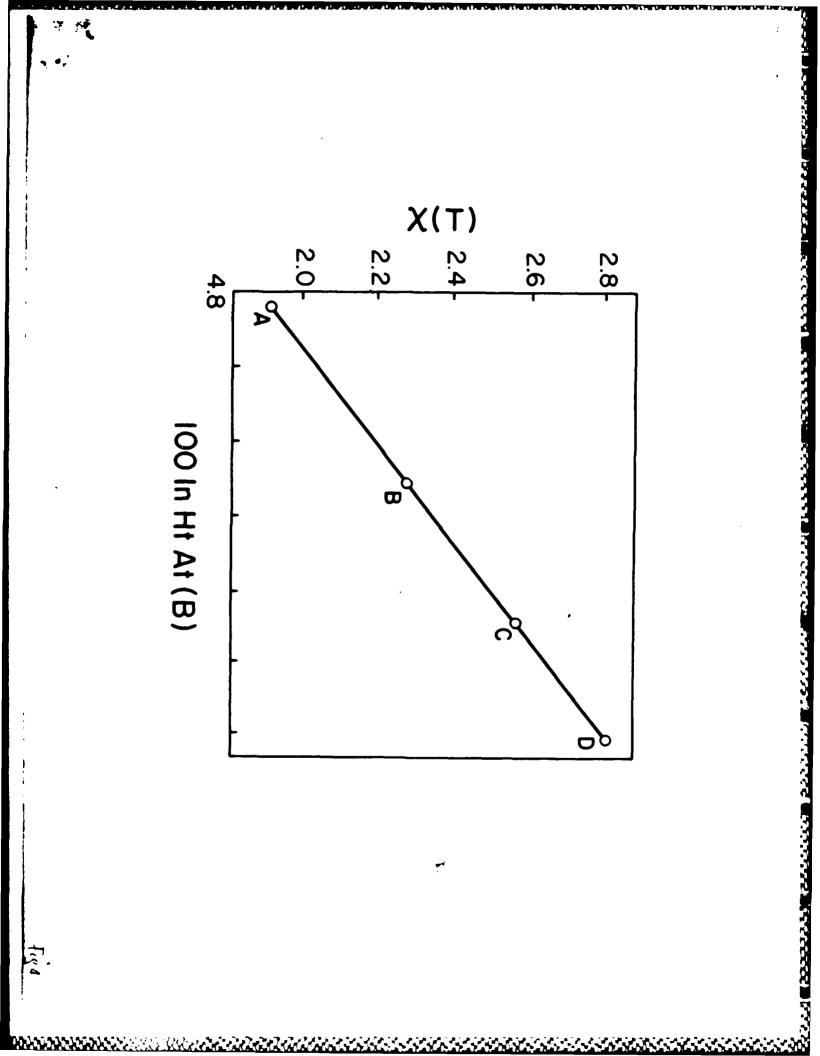
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