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TOPOLOGY OF OXY-ORGANIC COMPOUNDS

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GRAPH theory¹ has, recently, been applied to various branches of theoretical organic chemistry. Several authors have discussed the molecular topology of several types of organic compounds²⁻⁵. The molecular graph¹ is a set of vertices and edges, where the vertices denote the atoms and the edges denote the chemical bonds. In a graph of an organic compound the vertices represent the carbon atoms C and the hetero atoms X, and the edges represent the C-C, carbon-carbon bonds and C-X, the hetero bonds respectively. The hetero atom X may be an O, N, or S atom. In our previous work^{4,5} we have defined the root mean square value of the topological distances W_{rms} of a molecular graph. The index W_{rms} was found to reflect the changes in physical properties of the

organic compounds in a homologous series^{4,5}. In a recent communication⁶ we have defined the edge-weighted graphs and sum of the topological distances⁷ from these graphs of purine and pyrimidine bases. In the present paper we have calculated the W_{rms} values of oxy-organic compounds and correlated them with their boiling points.

The edge-weighted graph⁶ G_{we} is defined as a graph in which, some real numbers known as weights are associated with its edges. In a weighted molecular graph the weights associated with the edges correspond to the k values of the Hückel parameter⁸ for the chemical bonds. The Hückel parameter k is defined by the relationship⁸,

$$\beta_{cx} = k\beta_{cc}, \quad (1)$$

where β_{cc} is the resonance integral of a C-C bond and β_{cx} is that of a hetero bond. The value of k reflects the difference between the resonance integrals of a C-C bond and the C-X hetero bond (X may be O, N, or S).

In the edge-weighted graph the topological distance⁷ d_{ij} between two vertices i and j , is defined as the distance which is associated with a minimum weight⁶. Thus, we can define a distance matrix D associated with the graph⁴. The distance matrix D of a graph is a real $N \times N$ matrix (N is the total number of vertices) the elements of which d_{ij} are the topological distances between the vertices i and j . The root mean square value of the topological distances W_{rms} , is defined by⁴,

$$W_{rms} = \left[\frac{1}{N(N-1)} \sum_{ij} d_{ij}^2 \right]^{1/2}. \quad (2)$$

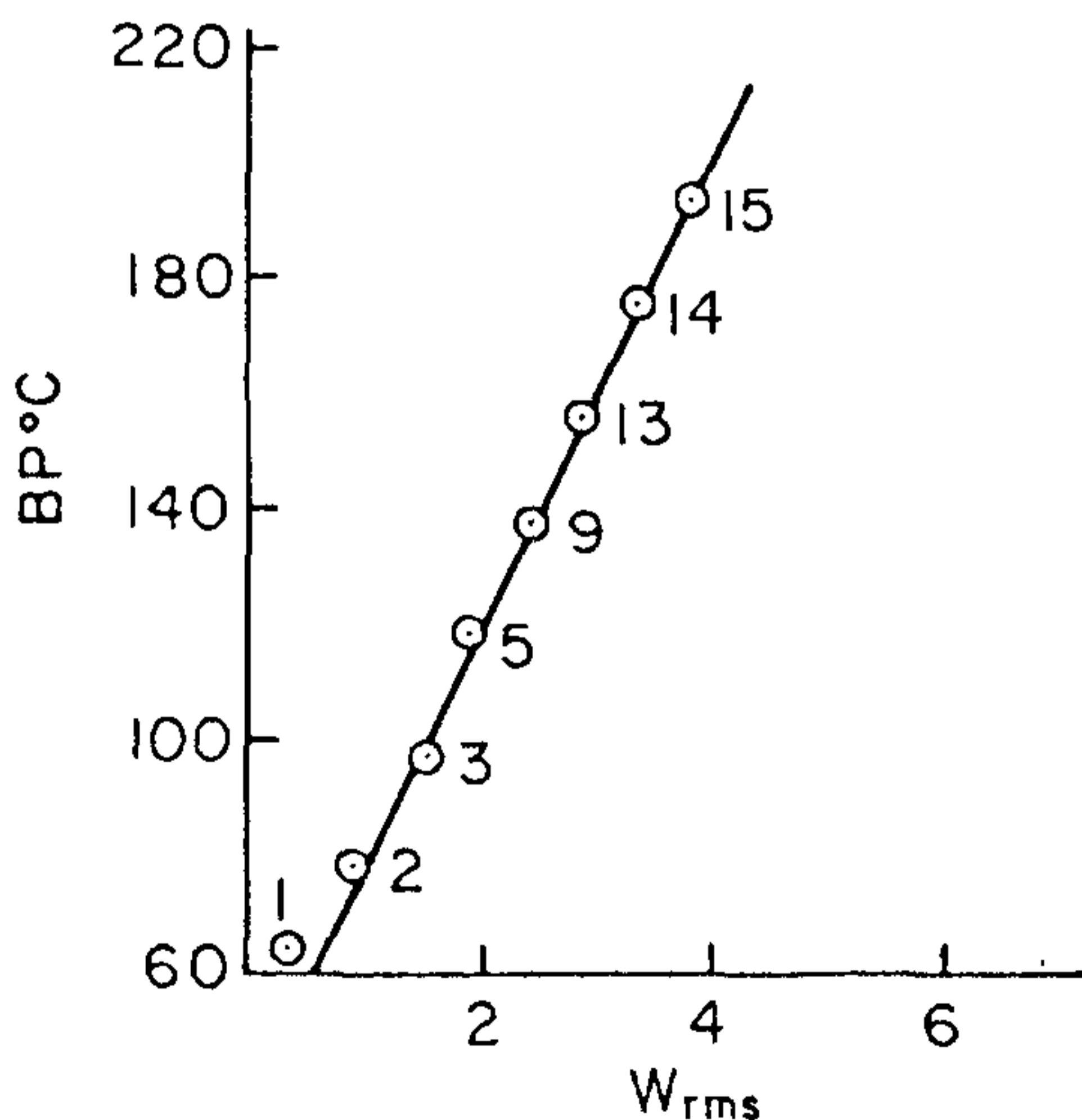
Constructing the edge-weighted graphs and taking appropriate k values for C-C, C-O, and C=O bonds from the well-known results of Hess and Schaad⁹, we have calculated the $W\bar{W}$ and W_{rms} indices⁴ for a series of oxo-organic compounds *e.g.*, alcohols, ethers, aldehydes, ketones and carboxylic acids. The topological indices for oxy-alcohols are reported in table 1. The W_{rms} values for series of compounds in each class are correlated with the experimental boiling points. It has been observed that the boiling points of the oxy-organic compounds containing normal alkyl groups, vary linearly with the index W_{rms} . Table 2 reports the boiling points (BP) of the corresponding homologous series in each class of compound as a function of W_{rms} , along with the standard deviation of the correlation in each case. The linear correlation for normal oxy-alcohols, is shown in figure 1. These correlations show that the physical property of the oxy-organic compound containing a normal alkyl group, depends directly on its topology. There are deviations from linear correlations for the compounds having

Table 1 Topological distances of oxy-alcohols

Compound	W	\bar{W}	W_{rms}
Methyl alcohol	0.34	0.34	0.34
Ethyl alcohol	2.68	0.9933	0.9850
<i>n</i> -Propyl alcohol	8.02	1.3366	1.4936
Iso-propyl alcohol	7.02	1.1700	1.2719
<i>n</i> -Butyl alcohol	17.36	1.7360	1.9632
Iso-butyl alcohol	15.36	1.5360	1.6692
Sec-butyl alcohol	15.36	1.5360	1.7082
<i>t</i> -Butyl alcohol	13.36	1.3360	1.4318
<i>n</i> -Amyl alcohol	31.70	2.1133	2.4135
<i>t</i> -Amyl alcohol	24.70	1.6466	1.8069
Iso-amyl alcohol	28.70	1.9133	2.1244
Neo-pentyl alcohol	24.70	1.6466	1.7576
1-Hexanol	52.04	2.4780	2.8526
1-Heptanol	79.38	2.8350	3.2846
1-Octanol	114.78	3.1866	3.7117
1-Decanol	159.06	3.5346	4.1352

Table 2 Correlation equations for normal oxy-organic compounds boiling points vs W_{rms}

Compounds	Boiling point (°C)	Standard deviation
Alcohols	$40 W_{rms} + 36$	2.803
Ethers	$60 W_{rms} - 48$	1.776
Aldehydes	$65 W_{rms} - 70$	0.2636
Ketones	$55 W_{rms} - 26$	1.757
Carboxylic acids (mono)	$48 W_{rms} + 58$	1.343

**Figure 1.** Variation of boiling points of normal oxy-alcohols with topological index W_{rms} (data of experimental BP from ref. 13)

branched alkyl groups. The correlation of the physical properties with the number of carbon atoms and the molecular formula weight has been reported by some authors^{10, 11}. The topological studies of the compounds in a homologous series are much more interesting, as the topological index provides a fundamental basis for all types of compounds. The topological studies from edge-weighted graphs are more applicable in biological compounds^{6, 12}.

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FURTHER EVIDENCE TO THE STRUCTURE OF SEMECARPUFLAVANONE*

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FROM the defatted nut shells of *Semecarpus anacardium* Linn., two new compounds^{1, 2} jeediflavanone(IV) and semecarpuf flavanone(V) besides the three known biflavanones³ A(I), B(II) and C(III) have been recently

*Part IV in the series partial conversions in biflavanoids for Part III see ref 6.