On the basis of foregoing discussion, the structure of Fe(II) and Ni(II) complexes may be octahedral, Co(II) complex tetrahedral while that of Cu(II) complex square pyramidal.

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TOPOLOGY AND PHYSICAL PROPERTIES OF ALICYCLIC COMPOUNDS

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ABSTRACT

A correlation between the topological indices and the physical properties of the saturated alicyclic hydrocarbons is reported. Boiling points, refractive indices, specific gravities and the bond energies vary linearly with the mean and root mean square values of the Wiener number while the heat of formation varies linearly with the reciprocal of W_{rms}.

INTRODUCTION

RECENTLY the molecular graph theory[1,2] has been applied to various systems of conjugated hydrocarbons[3–6] in the framework of Hückel molecular orbital theory. The topological characterization of cyclic systems was developed by Trinajstić and others[7,8]. The Wiener number[9] was found to be most useful in characterizing the monocycles. In monocyclic structures the toplogical index was found to be sensitive to the change in ring size and also to their physical and chemical properties[10]. Various other topological indices were also introduced, *e.g.*, Rouvray's index[11], Randić index[12], Platt index[13] and Hosoya index[14]. Trinajstic interrelated these indices and developed a relationship for monocyclic systems[7].

In our previous work[15] we have defined the root mean square value of the Wiener number (W_{rms}) and derived a relationship between some physical properties of *n*-alkanes and the mean value of the Wiener number ($\bar{W}$). In the present work we have developed a relationship between the mean and the root mean square values of the Wiener number and some physical properties of the saturated alicyclic hydrocarbons.

THEORY

The molecular graph G of a hydrocarbon system is a set of edges representing the C–C bonds and vertices representing the carbon atoms. The distance matrix[16] $D(G)$, associated with G, is defined as a $N \times N$ matrix where N is the number of vertices in the graph G.

The elements of the matrix $D(G)$ are integers (0, 1, 2,..) *e.g.*, the element D_{ij} for i, j neighbours, will be equal to 1 if $i \neq j$, or it will be equal to zero if $i = j$. The Wiener number is equal to half the sum of the off-diagonal elements of the distance matrix. As defined earlier[15] we can easily calculate the Wiener number (W), and the indices $\bar{W}$ and W_{rms}. For example the values of the topological indices for the cyclobutane graph are,

$$W = 8, \quad \bar{W} = 1{\cdot}33 \text{ and } W_{rms} = 1{\cdot}414.$$

Table I reports the values of W, $\bar{W}$ and W_{rms} for a series of alicyclic systems. The values of W and $\bar{W}$ can be obtained easily by the equations derived by Bonchev and Trinajstić[17]. We have plotted some of the physical properties like heat of formation (ΔH_f), bond energy, boiling points, refractive indices (η_D^{20}) and the specific gravities against the mean and rms values of the Wiener number. Table II reports some of the physical properties of cycloalkanes.

TABLE I

Values of the topological indices W, $\bar{W}$, W_{rms}

Cycloalkane	Ring size	W	$\bar{W}$	W_{rms}
Cyclopropane	3	3	1·00	1·00
Cyclobutane	4	8	1·33	1·414
Cyclopentane	5	15	1·50	1·563
Cyclohexane	6	27	1·80	1·947
Cycloheptane	7	42	2·00	2·160
Cyclooctane	8	64	2·29	2·500
Cyclononane	9	90	2·50	2·738
Cyclodecane	10	125	2·78	3·073

Results and Discussion

Physical properties of alicyclic hydrocarbons have been discussed by Raphael[20]. The melting points and densities first increase with the ring size and then decrease for the higher rings. Heat of combustion of the cyclic paraffins per CH_2 group also shows fluctuations as the ring size increases. The maximum and minimum in the curve of the physical property of the ring systems lies in the region between the eight- and twelve-membered rings. The higher rings behave or tend to behave like linear paraffins. The strain in the alicyclic systems also oscillates with the ring size[21].

In this work we have performed a systematic study of the variation of various physical properties with the mean and root mean square values of the Wiener number. Linear plots were obtained in case of bond energy, boiling point, refractive index and specific gravity. The heat of formation varies linearly with the reciprocal of W_{rms}. This shows the direct dependence of the physical properties on the topology of the structures. The slopes of the linear plots between the boiling points, refractive indices, densities and bond energy curves are given by the following equations:

$$\text{boiling point B.P.} = 148\,\bar{W} - 176 \ (^\circ\text{C})$$

$$\text{refractive index } \eta_D^{20} = 0{\cdot}06\,\bar{W} + 1{\cdot}335$$

$$\text{density (liq.) } \rho = 0{\cdot}12\,\bar{W} + 0{\cdot}565$$

$$\text{bond energy } E_b = -24{\cdot}0\,\bar{W} + 6{\cdot}50 \text{ k.cal/mole.}$$

The plot of ΔH_f heat of formation at 25°C against W_{rms}^{-1} is a straight line for the systems of the ring size 5 to 10. Figure 1 shows the ΔH_f curve. The deviations of cyclobutane and cyclohexane from the linear curve is attributed to the various conformational structures in these compounds. The steric energy of cycloalkanes is also plotted with W_{rms}

TABLE II

Physical properties of alicyclic hydrocarbons

Ring size	Heat of formation[a] k. cal/mole	Steric energy[a] k.cal/mole	Bond energy[a] k.cal/mole	Boiling point[b] °C	Density[c] liq.	Refractive index[d] η_D^{20}
3	..	..	..	−33	0·688	..
4	6·38	27·17	−23·88	13	0·704	..
5	−18·46	7·53	−29·85	49	0·746	1·4090
6	−29·43	1·75	−35·82	81	0·778	1·4268
7	−28·34	8·04	−41·79	118	0·810	1·4449
8	−30·06	11·04	−47·76	149	0·830	1·4581
9	−31·80	14·97	−53·73	..	0·853	1·4328
10	−36·29	..	−59·70	..	0·857	1·7414

a. Ref. 18; *b.* Ref. 19; *c.* Ref. 19 and Ref. 20, p. 768; *d.* Ref. 20, pp. 249, 258 and 268.

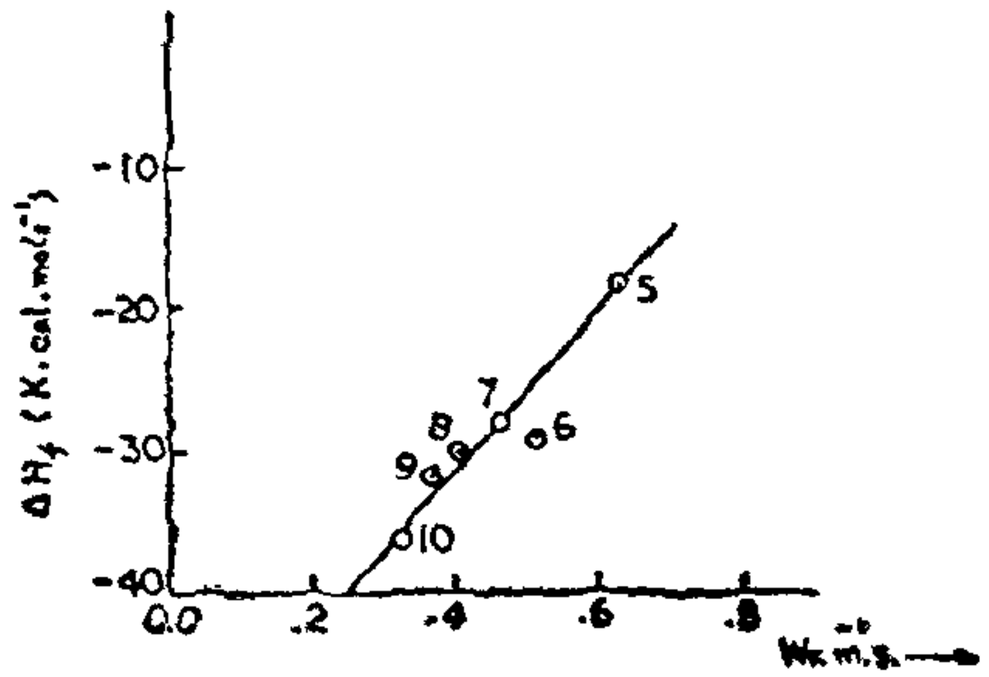

FIG. 1. Variation of the heat of formation with W_{rms}^{-1}.

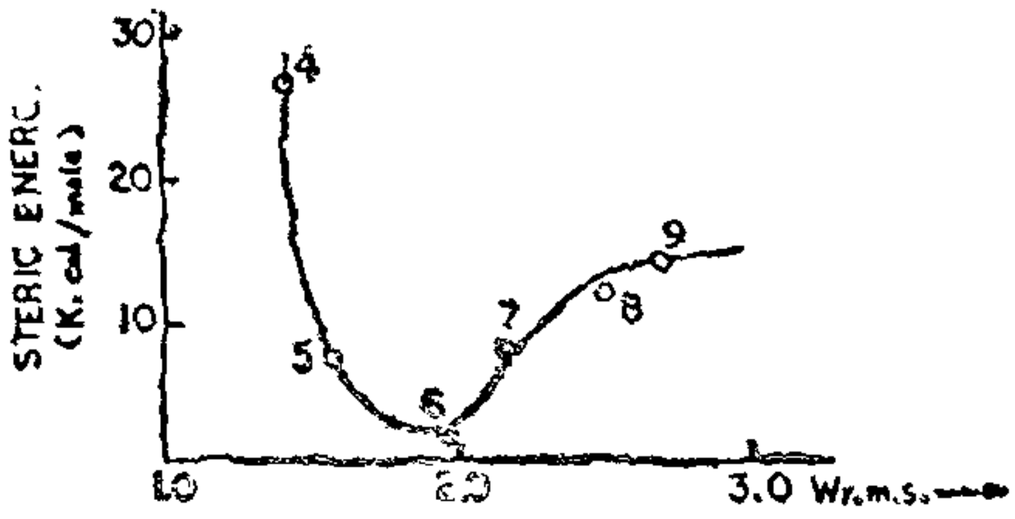

FIG. 2. Variation of the steric energy with W_{rms}.

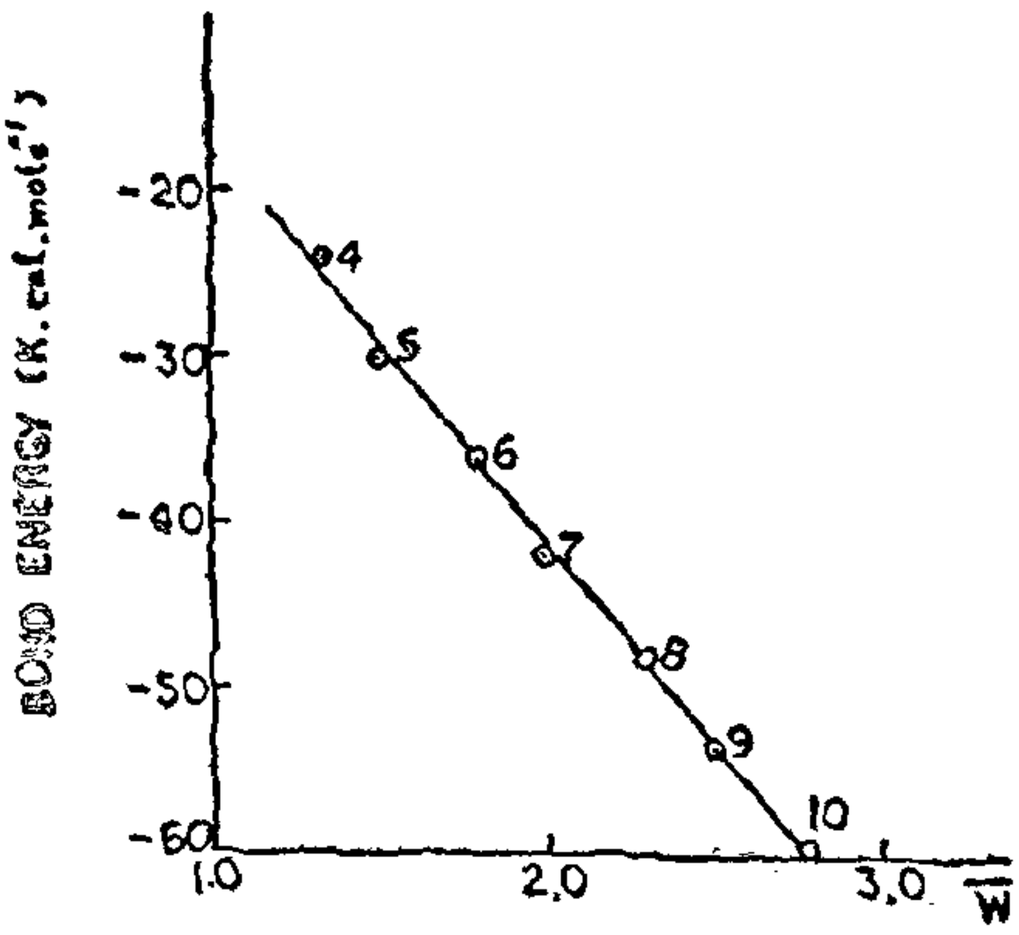

FIG. 3. Variation of bond energy with $\bar{W}$.

Figure 2 shows the variation of the steric energy of the rings with W_{rms}. The curve is approximately a parabola for ring size 4 to 8 and after that the steric energy increases smoothly and then again decreases. The steric energy change is attributed to bond angles and bond lengths changes in the most favourable conformations[22]. Figure 3 shows the variation of bond energies with $\bar{W}$. The effect of these changes in energetics on chemical properties has already been studied[23]. The topological structures of the cyclic systems thus provide a new basis for the study of these observed facts.

The variation of the physical properties with the number of carbon atoms does not behave in a simple manner and shows a zig-zag curve, but the variation with the topological indices is smooth and therefore it is possible to derive a relationship between the topological structure and physical properties.

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DEVELOPMENTAL CHANGES IN THE PATTERN OF GLUCOSE-6 PHOSPHATASE ACTIVITY IN THE TESTIS OF *PTEROPUS GIGANTEUS GIGANTEUS* BRUNNICH (MEGACHIROPTERA : MAMMALIA)

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ABSTRACT

Histochemical comparison of the site and pattern of distribution of glucose-6-phosphatase (G-6-Pase) in the spermatogenic and androgenic cells of the testis of impuberal and sexually active males of *Pteropus giganteus giganteus* revealed considerable differences. The developmental pattern of this enzyme from impuberal to sexually active state was marked by varying intensities of G-6-Pase activity in the spermatogonia, leptotene and pachytene spermatocytes, spermatids in various phases of spermiogenesis, dimorphic spermatozoa, Sertoli and Leydig cells. It is proposed that this may be linked with the differential turnover of glucose—a readily metabolizable substrate commensurate with cellular dynamics of various germ cell types and Leydig cells.

INTRODUCTION

LIKE mammals, the chiropteran testes represents a heterogeneous assemblage of cells which are compartmentalised in the seminiferous tubules and in the interstitium. In impuberal males, the seminiferous tubules consist of spermatogonia, spermatocytes and Sertoli cells ; while the interstitium is occupied by Leydig cells. However, in sexually active males, the seminiferous epithelium exhibits germ cells in various phases of growth, meiotic division and differentiation culminating in the formation of spermatozoa[1–5].

A variety of metabolic enzymes has been histochemically localised, biochemically estimated and electrophoretically assayed in the bat testis[6–8]. However, very little comparative information is available on the site and pattern of distribution of enzymes in the histological constituents of the impuberal testes and the changes they undergo during the spermatogenesis in sexually active males.

The present report deals with the developmental changes in the histochemical site and paradigm of glucose-6-phosphatase (G-6-Pase) in the seminiferous epithelium and Leydig cells of the testes from impuberal to a sexually mature state ; in the case of giant fruit bat—*Pteropus giganteus giganteus*.

MATERIAL AND METHODS

Males of *P. g. giganteus* were trapped/shot locally from their roosting sites throughout the year. Bats were sacrificed by cervical dislocation. Surgical procedures, recovery of tissues and the parameter for determining impuberal and sexually active state of the testis were as described in earlier report.

Fresh frozen sections (10 μM) of impuberal and spermatogenically active testes were similarly incubated in the substrate medium (pH 6·0) at 37° C for 40 min, prepared according to Wachstein and Meisel's method[9] and post-fixed in neutral formalin. Brownish black deposits of lead sulphide was taken as the index for ascertaining the site and distribution of G-6-Pase acivity in the various cell types of the seminiferous epithelium and Leydig cells. Controls were incubated similarly but in a substrate deficient medium.

Enzyme activity in the testicular elements was visually appraised and graded as described earlier.

RESULTS AND DISCUSSION

G-6-Pase activity in the seminiferous epithelium and Leydig cells of the testis of impuberal males