Chinese Chemical Letters Vol. 16, No. 5, pp 709-710, 2005 709
http://www.imm.ac.cn/journal/ccl.html

Studies on the Physical Properties of Alkanes Using Edge-adjacency Information Topological Index

Cai Hua NI[1*], Xian Yu ZENG[2], He HUANG[3]

[1] School of Chemical and Material Engineering, Southern Yangtze University, Wuxi, 214001
[2] College of Materials Science and Engineering, Beijing University of Chemical Technology, Beijing, 100029
[3] School of Chemistry and Materials Science, Hubei University, Wuhan 430062

Abstract: Edge-adjacency index and information topological index for 82 molecules of alkanes have been constructed and calculated. The topological indices were used to correlate with seven physical properties of the alkanes. Some empirical equations were obtained through regression. The regression and calculation results show a good agreement of the topological indices and the properties.

Keywords: Information topological index, physical properties, alkane.

There are numerous reports on QSPR and QSAR studies of organic compounds. In 1995 E.Estrada proposed an edge-adjacency index and studied the molar volume and molar refraction of alkanes using the index[1]. This study proposed an information topological index based on the edge-adjacency index.

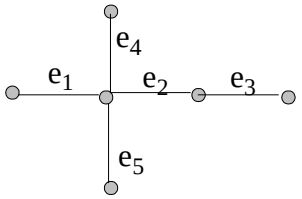
An edge adjacency matrix can be built and expressed: $E=\{g_{ij}\}_{m\times m.}$ Where m is the number of edges in the graph. $g_{ij}=1$ when i is adjacent to j, otherwise $g_{ij} = 0$.

An edge degree $\delta(e_k)$ can be defined as the adjacent number of the edge to other edges[1]: $\delta(e_k) = \sum g_{ij} = \sum g_{kj.}$ The edge adjacency index is defined as:

$$\varepsilon = \sum \varepsilon_i = \sum [\delta(e_i)\,\delta(e_j)]^{-1/2} \qquad (1)$$

Where the sum is over all adjacent edges in the graph.

Scheme 1 The molecular graph and edge adjacency matrix of 2,2-dimethyl butane



$$E = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

* E-mail: caihuani@yahoo.com

The edge degree for 2,2-dimethyl butane: $\delta(e_1)=\delta(e_4)=\delta(e_5)=3$; $\delta(e_2)=4$; $\delta(e_3)=1$. The edge adjacency index: $\varepsilon = 3(3\times4)^{-1/2} + 3(3\times3)^{-1/2} + (4\times1)^{-1/2} = 2.3661$. We proposed an information topological index as follows:

$$I_\varepsilon = -\sum \varepsilon_i/\varepsilon \, LOG(\varepsilon_i/\varepsilon) \qquad (2)$$

According to the definition the information topological index for the above compound: $I_\varepsilon = 2.7798$. The information topological index I_ε and edge-adjacency index ε for alkanes were calculated based on the formula (1) and (2). The topological indices were correlated with seven physical properties such as molar volume M_v (cm^3/mol), evaporating heat H_v(kJ/mol), molar refraction M_R(cm^3/mol), critical volume V_c(cm^3/mol), critical temperature T_c(K), critical pressure P_c(Mpa), and heat capacity C(J/mol.K). Through regression using the experimental data[2,3] and topological indices of 82 alkane molecules, some empiric equations for calculating the physical properties were worked out.

$M_v = 32.97\,\varepsilon - 2.081\,I_\varepsilon + 57.03$ R = 0.9968 (3)

$H_v = 10.23\,\varepsilon - 2.061\,I_\varepsilon + 10.34$ R = 0.9835 (4)

$M_r = 9.027\,\varepsilon + 0.555\,I_\varepsilon + 7.248$ R = 0.9960 (5)

$V_c = 108.5\,\varepsilon - 4.706\,I_\varepsilon + 114.0$ R = 0.9971 (6)

$T_c = 35.86\,\varepsilon + 30.83\,I_\varepsilon + 349.1$ R = 0.9648 (7)

$P_c = -0.3035\,\varepsilon - 0.1648\,I_\varepsilon + 4.169$ R = 0.9555 (8)

$C = 67.00\,\varepsilon - 13.09\,I_\varepsilon + 59.46$ R = 0.9973 (9)

Edge-adjacency index ε is the characterization of molecular size and a way by which atoms are connected. Information topological index I_ε gives information which indicates the weights of the connecting ways of the atoms, and it reflects the environment information around atoms. The R factors indicate that the topological indices are well correlated with the physical properties of the alkanes and the data calculated and experimental are in good agreement.

References

1. E. Estrada, *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 31.
2. H.Lu *et al*,*Handbook of Basic data of prtroleum chemical industry*, Beijing **1982**.
3. P. Ma *et al*, *Handbook of basic data of petroleum chemistry,* Beijing **1993**.

Received 29 July, 2003, Revised 9 May, 2004