Wiener Index and Vibrational Energy

Ivan Gutman and Igor G. Zenkevich[a]

Faculty of Science, University of Kragujevac, P. O. Box 60, YU-34000 Kragujevac, Yugoslavia
[a] Chemical Research Institute, St. Petersburg State University,
  Universitetsky pr. 26, St. Petersburg 198504, Russia

Reprint requests to Prof. I. G.; Fax: +381 34 335040, E-mail: gutman@knez.uis.kg.ac.yu

The Wiener index (W) is known to represent a rough measure of the surface area of molecules, which is used to explain why W is correlated with numerous physico-chemical properties of organic compounds. We now point out another aspect of W, unrelated to surface area, namely the relation between W and the internal (mainly vibrational) energy of organic molecules. For isomeric alkanes a theoretical justification of this result is offered. Another example – the dithioderivatives $C_3H_8S_2$ – indicates that this regularity may be applicable also to other groups of isomeric acyclic organic compounds.

Key words: Wiener Index; Intramolecular Energy; Vibrational Energy;
        Acyclic Organic Compounds; Alkanes.