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BOOK REVIEW

The Harary Index of a Graph

by

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This is a book written by graph–theoretical mathematicians interested in topological indices of graphs. It is addressed mainly to other mathematicians with the same interests.

Chemical graphs (or molecular graphs) symbolize chemical compounds whose atoms are represented by graph vertices, and whose covalent bonds are represented by graph edges. In most cases undirected connected simple graphs are involved (devoid of loops or multiple edges). For finding quantitative relationships between discrete molecular structure (topology of the graph) and physical/chemical properties, or biological activities of substances (QSPR and QSAR, respectively) measured by a continuum of real numbers, one has to associate with each graph a number (integer, rational, or real). Such numbers (molecular descriptors) are currently called topological indices (TIs). The first TIs were described in 1947 (H. Wiener, J. R. Platt), 1971 (H. Hosoya), and 1972 (I. Gutman and N. Trinajstić). The Wiener index decreases with increasing compactness of the graph because the largest contributions are due to topological distances between vertex pairs which are remote from each other. However, chemists know that nearest neighbor interactions are the most important in molecules, and the introduction of the Harary index is due to this axiom.

The Harary indices (HIs) are integer, rational, or real numbers associated with graphs, and they were independently proposed in by two research groups in Zagreb (D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić) and Bucharest (O. Ivanciuc, T. S. Balaban, A. T. Balaban) and published in the same 1991 issue of the *Journal of Mathematical Chemistry*. In the following, these two papers will be designated as PNTM and IBB, respectively. The Wiener index is the half–sum of all distances in the distance matrix, whose elements are the topological distances (number of edges along the shortest path between two vertices). By contrast, the Harary index is the half–sum of the reciprocal–distance matrix, whose elements are the reciprocals of the topological distances between vertex pairs. In both cases (Wiener and Harary indices) the diagonal elements are equal to zero. The Zagreb mathematical chemists enriched knowledge about properties and applications of HI considerable after publishing the PNTM paper, and many mathematical studies of the HI were published by the Chinese and Korean co-authors of this book.

The six chapters of the book reflect the interests of the three authors (two mathematicians and one mathematical–theoretical chemist). After introducing in the first chapter the Harary index and its modified form, mH, the next (2nd) chapter is about extreme graphs – a beloved ground for mathematicians, who like to explore upper or lower bounds of vertex numbers for various classes of graphs. In this and subsequent chapters, a series of theorems are presented without proofs, but with the corresponding references to published articles. Little attention is paid to chemically relevant graphs (organic molecules correspond to hydrogen–depleted graphs with vertex degrees 4 or less).

Chapter 3 discusses relationships with related TIs, but only a few from the numerous candidates have been selected, and one feels that there are many other TIs that one would be tempted to explore. For chemists such as the parents of the HI, the 4th chapter discussing properties and applications of HI offers a few useful pieces of information. This is the longest chapter of the book (20 pages), whilst the other five chapters have between 5 and 14 pages. The Harary indices of dendrimers and polyhex nanotori are presented by two theorems. Seven physical properties (normal boiling point, molar volume, molar refraction, heat of vaporization, critical tempera-

ture, critical pressure, and surface tension) for 74 lower alkanes are presented. One has to note that the statistical parameters for the mono– and bi-parametric QSPR correlations involving the number N of carbon atoms, HI or mH are erroneously swapped on page 52 between Tables 4.9 and 4.10.

Finally, like chapters 2 and 3, the 5th chapter discusses via theorems several variants of HI, whereas chapter 6 presents open problems. Both these chapters are totally mathematical and without degree restrictions. An index would have been useful. On a more personal level, it is regrettable that the IBB paper was not treated fairly, being cited only in the Preface. In the book it is not mentioned that on the first page of the IBB paper, a footnote explicitly states: *We agree with N. Trinajstić's proposal to call RDSUM the "Harary number"*. This IBB paper also contains correlations which are not mentioned in chapter 4. Also, no mention is made of the monograph edited by J. Devillers and A. T. Balaban "*Topological Indices and Related Descriptors in QSAR and QSPR*", Gordon and Breach, The Netherlands, 1999, or of two other papers (M. V. Diudea, O. Minailiuc, A. T. Balaban, Molecular topology. IV. Regressive vertex degrees (new graph invariants) and derived topological indices, *J. Comput. Chem.* **12** (1991) 527–535; A. T. Balaban, M. V. Diudea, Real number vertex invariants: regressive distance sums and related topological indices, *J. Chem. Inf. Comput. Sci.* **33** (1993) 421–428). In these two papers we emphasized the contributions of nearest neighbors, just as we did in the IBB paper, so that the resulting indices are also related to HI.

Professor Nenad Trinajstić, with his Croatian, Chinese, and Korean co-authors has explored and published many new aspects of the Harary index, and the present book is a good starting point for those that are interested to investigate further the rich possibilities offered by the Harary index and its relatives.

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