Molecular Structure Description. The Electrotopological State. By Lemont B. Kier and Lowell H. Hall. Forward by Gerald M. Maggiora. Academic Press, San Diego, CA. 1999. xx + 245 + 41 pp. 16 x 35 cm. ISBN 0-12-406555-4. $99.95.

This work by the authors, Kier and Hall, is an extension of their approach to molecular description using topological parameters. The book contains a forward by Gerald Maggiora, a preface, 10 chapters, and a copy of the E-Calc software on CD used for generation of the descriptors whose origins are described in the book. In addition a brief user's guide to the software is provided as a separate 41-page section. Terms and definitions are also included in the additional section.

The forward by Gerald Maggiora provides a needed introduction to the book as it tries to tie together the prior connectivity work of Kier and Hall with the work discussed here. The preface then makes a case for the use of the electrotopological state descriptors in combinatorial chemistry.

Chapter 1 serves as an introduction with a brief and rather superficial discussion of molecular structure. It is implied, without proof, that 3-dimensional structure is embedded in topological and graph-based representations.

In Chapter 2 the electrotopological state is developed and compared with other commonly used structure−property related descriptors. Partial charges, Taft constants, hydrophobic fragment constants, and some quantum mechanically based descriptors are included, but the examples cited are simple hydrocarbons, for the most part. Chapter 3 contains a discussion of the extension of the indices to more complex molecules.

Chapter 5 focuses on strategies for the use of electrotopological state descriptors in conjunction with some commonly used data analytic methods. The remainder of the book is a compilation of applications, the majority of which are simple regression based structure−activity studies of homologous series or mono- and/or disubstituted aromatic compounds.

The CD included was installed on a PC with somewhat more than the stated minimum hardware requirements. The program, E-Calc, installed easily and, via the instructions included in the text, was somewhat user friendly. It contains a structure-drawing menu which worked well with simple molecules, but more complex molecules, such as a morphinan, were difficult to draw and, once drawn, were not accurately displayed. The descriptors were easily calculated, however. The help menu was quite limited and should be extended if it is to be generally useful.

The jury is still out on the use of electrotopological state descriptors. They have a number of short comings, and these were alluded to by the authors in the preface. Perhaps they may be useful as purely empirical indices which can be computed and assigned to members of complex libraries. Should the vector that results be unique, and this is not discussed in the book, it would be a method for filtering libraries prior to more quantitative studies of their structure−activity. In summary, topological descriptors have found limited use in structure−activity work, and for those who use them or wish to become more familiar with their use, this book should be a helpful text.

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