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Book Reviews

I. G. Csizmadia: Theory and Practice of MO Calculations on Organic Molecules.
Amsterdam and New York: Elsevier Scientific Publishing Company 1976.
x + 378 pp., price: Dfl. 100.00/US-$38.50

It is really astonishing how much material the author has condensed into approximately 370 pages of which the book consists. The presentation, nevertheless, is very clear and by no means too concentrated; it is even suitable for those readers who still know little about SCF calculations.

However, the book is especially intended for the organic chemist, but it may be said that all chemists will profit by reading it as it starts off with an introduction to basic mathematics for molecular orbital calculations (an introduction which will also be sufficient for the German chemist).

Following the introduction, the theory of closed and open electron shells is treated. Concerning this topic, practically everything of basic interest is contained in the book, but sometimes in a very concise form.

Chapter 4, treating the proper selection of basis sets, merits special praise. It deserves particular appreciation as the reader is told, in detail, which programs are offered at present in the QCPE exchange program, details being given as to their proper application in the individual case.

Finally, mathematical derivations of the basic equations are added in an appendix.

Most of the readers will accept the fact that the text is typewritten; however, it would be desirable to have the book translated into German.

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