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Book review

I. G. Csizmadia (ed.): Progress in theoretical organic chemistry. III. Molecular structure and conformation. Amsterdam: Elsevier 1982, 344 pp

Some 20 years ago one could hardly have anticipated that many of the real problems of organic chemistry would one day be solved by *ab initio* computations. Nowadays, computational organic chemistry is a well-established branch of science. The third volume of the series *Progress in theoretical organic chemistry* consists of six review papers. Four of these deal with topics covered by the subtitle "Molecular structure and conformation", namely "Structural consequences of hyperconjugation" (L. Radom), "Quantitative orbital analysis of the conformational preference in methyl derivatives" (F. Bernardi and A. Bottoni)," The nonclassical polyhedral organic molecules and ions" (V. I. Minkin and R. M. Minyaev), and "Analytic equations for conformational energy surfaces" (M. R. Peterson and I. G. Csizmadia). The article by M. A. Robb, "Correlation energy as a stabilizing factor in molecular structure", is more concerned with small molecules such as F_2, HF, O_3, and C_2H_2. The paper by G. Naray-Szabó and T. Bleha, "Quantum chemical studies of the mechanism of enzyme action", deals with quantum biochemistry. The computations reviewed in this book are mainly *ab initio* on the SCF/STO-3G level, for the larger molecules also of the semi-empirical type, or by means of empirical atom-pair potentials. Qualitative MO-pictures are still widely used. The book contains enough material to be of interest to any computational chemist.

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