Theoret. Chim. Acta (Berl.) 48, 267 (1978)

THEORETICA CHIMICA ACTA

Book Review

Lecture Notes in Chemistry, Niketić, S. R., Rasmussen, K.: The Consistent Force Field: A Documentation. Vol. 3. Berlin–Heidelberg–New York: Springer-Verlag, 1977, 212 pp., price: DM 28,80, (US $ 12.70)

The majority of the readers of this Journal may be unfamiliar with the Consistent Force Field (CFF) so a brief introduction may be useful. The CFF (also known under other names, like Molecular Mechanics) is a method for the determination of transferable potential functions for stable, ground-state molecules, mainly for large organic ones. Terms in the potential function, referring to transferable structural units, have an assumed analytical form with free numerical parameters. The latter are determined to give the best overall agreement with experimental data, mainly equilibrium geometries and ΔH values of conformers, and vibrational data. Many CFFs are possible, depending on the compound class and the form of the potential function used, and considerable physical insight is needed to develop a good CFF. Both the form of the potential function and the number of the free parameters requires judicious choice. Good CFFs are known for hydrocarbons (with the exception of conjugated ones), for amides and several other classes of compounds. However, the CFF concept does not lend itself readily to compounds with delocalized electron structure. A typical and successful use of the CFF concept is the prediction of molecular geometries in strained organic molecules. In general, the prediction of vibrational data is less successful, although the classical work of Schachtschneider and Snyder on the force field of aliphatic hydrocarbons shows that this need not be so.

This book by a Yugoslav and a Danish author is an introduction to a program system, developed at the Technical University of Denmark from the original CFF programs of Lifson. This is a very large program system and the reader may wonder why, as the basic mathematics of the CFF is very simple, consisting mainly of taking the first and second derivatives of elementary functions, and of a least-squares procedure. The answer lies in the complexity of the molecules which requires the automatic set-up of approximate Cartesians from line formulas, options for using preselected potential functions, merging and updating data bases, etc. Nevertheless, I often wondered while reading this book whether all this complexity is really needed.

The style of the book is lively but not at all concise; the same story could be told perhaps in half the space. There is a great deal of general science and programming philosophy in it, and trivial formulas abound. Somebody not acquainted with the CFF will probably find it very difficult to grasp the simple essence behind all the details. Individual sections of the author's program are described, from the choice of the algorithm down to the names of the variables. A few tables with CFF parameters are given but nothing is said about the results, the reliability of the parameter values, the relative merits of different CFFs, etc. The book is obviously intended for those who plan to implement a CFF program system, and within this scope it will be undoubtedly useful.

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Received January 20, 1978