

which is now widely used by the non-specialist. His assessment of the reliability of the various methods in predicting the correct inversion barriers for hydrides also applies to their reliability in other conformational problems. He points out that, with too small a basis set, even *ab initio* calculations can lead to incorrect results.

In the second chapter, entitled "Organic molecules. Studies by semi-empirical methods," J. K. Fernandez Alonso describes the semiempirical techniques more thoroughly. His examples of the smaller molecules overlap Veillard's somewhat, but most of the examples are of the larger molecules.

The third chapter, entitled "Molecules of pharmacological interest," by R. E. Christoffersen, has a somewhat different format. It deals with calculations on the pharmacological molecules themselves. The separation of molecules by their pharmacological effects is especially valuable in view of the dismal state of indexing of quantum-chemical calculations that have been performed on pharmacological molecules. There is at present no way to search for such calculations without knowing the precise molecule or general family of molecules on which the calculations were performed. The literature is covered in this chapter only through 1974. One hopes that every two or three years a chapter updating this one will appear as part of the series.

In the last chapter, entitled "Proteins, nucleic acids and their constituents," B. Pullman cogently describes the fundamentals of the PCILO (perturbative configuration interaction based on localized orbitals) method derived by his group as well as the more empirical, potential-function methods used by other investigators. The large majority of examples in this chapter have been calculated by Pullman using the PCILO method, and the comparisons of the computed conformational energy maps with the known experimental results are truly impressive.

All four of the authors have searched the literature thoroughly and have presented their subjects coherently. In several chapters, the introductory sections, which summarize theoretical and computational methods and give extensive references to the original articles, will be especially useful to the nonspecialist. One looks forward to the subsequent volumes in the series.

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
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