Book Review

Ab Initio Molecular Orbital Theory, by W. J. Hehre, L. Radom, P. v. R. Schleyer and J. A. Pople, John Wiley & Sons, 1986, 548 pp., £81.80p.

This book concerns the basic topics of quantum chemistry necessary in order to perform *'ab initio'* molecular orbital calculations. Moreover it gives a relatively complete and analytical picture of the results which have been obtained or, potentially, can be obtained using such a calculation technique.

After a brief but interesting prologue, we have chapters 1 and 2 which give a synthetic but sufficiently complete review of the theoretical background.

Chapter 3 is concerned with several subjects more strictly connected to undertaking the calculations. More specifically, methods for evaluation of molecular integrals, solution of self-consistent equations, use of molecular symmetry, evaluation of energy gradient, etc.

The most interesting part of the book is contained within chapters 4, 6 and 7. In fact chapter 4 deals with the choices to be made when performing a calculation, particularly the atomic basis set of Gaussian functions, the method for evaluating the electron correlation, the molecular geometry to be considered, etc. The set of choices forms a 'model'. In chapter 6 the authors give an extended and analytical review of the performance of the models, especially with regard to some observables like equilibrium geometries, vibrational frequencies and related thermodynamic properties, molecular conformations and barriers to rotation, thermodynamic stabilities, molecular charge distributions, electric dipole moments, etc. Finally the last chapter, the 7th, concerns the applications of the theory. Amongst various subjects particular attention is paid to intramolecular interactions, reactive intermediates and reaction potential surfaces.

Overall the book is very interesting because it fills a gap within the literature on quantum chemistry which is lacking in such works. In fact the performance of a model as a function of the molecular system and the selection of the most suitable model are very important points to enable correct use of the quantum mechanical calculation as a means of answering chemical problems.

Unfortunately in the book only the ground state is studied and no calculation technique for electronic excited states is considered. However, I think that the book is very useful and that it is especially recommendable to those who carry out quantum mechanical calculations using some of the programs available today (e.g. the GAUSSIAN series) without having a critical knowledge of the performance of the calculation model which is in fact fundamental in order to produce meaningful answers from a chemical point of view.

Luigi Oleari