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Recensio

P. O. Löwdin: Advances in Quantum Chemistry 7. p. XVI + 457, New York–London: Academic Press 1973, DM 90,—.

The editor's goal is to emphasize the links of quantum chemistry to the traditional fields of mathematics, physics, chemistry and biology. In this sense, this volume is well balanced. The twelve articles cover a range from molecular integrals to DNA.

The first two articles by E. O. Steinborn and K. Ruedenberg convince us that the management of computational aspects like the speed of integral evaluation is still unfortunately an important ingredient of quantum chemical calculations. The advantage of certain atomic coordinate systems and their transformation to molecular coordinates is the subject of the first article. It focusses on rotations and translations of spherical harmonics and reviews the standard literature on the subject. The other paper deals with transformations from real to complex atomic and molecular orbitals and their relative advantages. How to relate the theory of the symmetric group to applications in numerical computations is a question asked by G. A. Gallup in an article on spin-free Hamiltonians. There is a long history involved from Yamanouchi, Kotani, Löwdin, Matsen to Goddard.

In a remarkably clear presentation, K. Johnson explains his Xa Scattered-Wave Method and its present applications. With the examples of MnO_4^- and SF_6 he demonstrates its advantage over present LCAO calculations in terms of computer time and "accuracy" of orbital energies. He hopes that this method will enable us to investigate metal bonding in enzymes and proteins in the near future. New methods in Hartree-Fock-theory is also the topic of a paper by S. Huzinaga, D. McWilliams and A. A. Cantu. Projection operator techniques are reviewed in the light of possible application for virtual orbitals and separability of many-electron-systems. In a series of three articles A. E. S. Green developes under collaboration with J. N. Bass, J. H. Wood and R. A. Berg an analytic independent particle approach for atoms. The two parameters of his statistical model are adjusted to fit the atomic Hartree-Fock energies computed by Mann for atoms up to $Z = 103$. The use in electron-atom scattering is outlined. The other two articles deal with modifications for the parameter adjustment and applications to ionization of rare gas atoms.

A. T. Amos and B. L. Burrows are concerned with solvent-shift effects on electronic spectra and exited state dipole moments and polarizabilities. Electrostatic type interactions and dispersion correction and their relation to experimental data are discussed. A. C. Hurley adopts the facy title of thermochemistry in the Hartree-Fock Approximation for an article dealing with high-accuracy (1 kcal/mole) energy calculations of small molecules. He tries to extrapolate from Hartree-Fock limits and pair correlation energies to heats of formation for larger systems.

The last two chapters are dedicated to large molecular systems of biological interest. R. Rein gives an analysis in terms of charge distributions and multipole moments, diamagnetic susceptibilities and ESCA shifts. Calculations reported are based on various semiempirical MO methods. A particular system, namely DNA, is the exclusive topic for J. J. Ladik. Spectrum and charge transport appear as of specific interest.

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