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# *Book Reviews*

**Peter Politzer, Donald G. Truhlar: Chemical Applications of Atomic and Molecular Electrostatic Potentials,** Plenum Press: New York–London 1981

This books contains the papers of an ACS symposium on the role of the electrostatic potential in chemistry held in 1980 in Houston and organized by Peter Politzer. The editors have broadened the scope and included also several specially invited contributions. The eighteen articles are in the three categories: i) Atoms, molecules and complexes in gas phase, ii) biomolecules, iii) crystal phase preceded by an introduction. The editors point out that relations exist between the energy of a system and its electrostatic potential, in particular at the nuclei of the systems. One way to establish such a relation is via the electronic density. It is hoped that this would allow a better prediction of total energies than many of the present *ab initio* or semiempirical procedures. Two articles deal with this subject. Although it is tempting to try to derive total energies from experimental measurements of e.g. X-ray diffraction via density functional theory without referring to wavefunctions, the present state of the art presented in these articles seems far removed from this goal. The elegant formulas derived between energy and potential can be successfully applied if a rigorous formula between potential and charge is known. Even in atoms, approximations have to be introduced which distinguish between a core and a valence region and parameterize the remaining degrees of freedom.

In the first category, we find articles concerning fundamental aspects on correlation energy from atomic Hartree–Fock electrostatic potentials at nuclei, the base-nuclear potential compared to electron density contours, atomic multipole expansions of molecular charge densities and different uses of the electrostatic potential. The emphasis by the various contributors is more on qualitative than on quantitative use. Articles on electron scattering follow concerning electrostatic potentials of free molecules derived from electron diffraction results, effective potentials for intermediate-energy electron scattering and adiabatic polarization potentials for the water and nitrogen molecules. Attempts are made here to compare calculated and experimental cross sections. The final section in this chapter is on molecular structure and interactions which are analyzed with respect to the electrostatic potential. The chapter on biomolecules uses the electrostatic potential as a measure of reactivity. The last chapter on crystals treats X-ray diffraction and transition metal ions. The articles are referred to more than forty authors, among them many prominent, which we cannot name all in detail.

Altogether, this is a very stimulating book. It suggests an alternative approach to structure and bonding, daring to oppose the main stream. We should certainly be glad to learn more about the structural dependence between energy and electrostatic potential as another way of understanding quantum chemistry, not replacing but complementing the wave function method. In this sense, this book will be a useful addition to the existing literature in quantum chemistry.

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