

Additions and Corrections

The Purine-2-amino Group as the Critical Recognition Element for Sequence-Specific Alkylation and Cross-Linking of DNA by Mitomycin C [*J. Am. Chem. Soc.* **1998**, 120, 11581–11593]. MARIA TOMASZ,* ARUNANGSHU DAS, KIT S. TANG, MARJIN G. J. FORD, ANDREW MINNOCK, STEVEN M. MUSSER, AND MICHAEL J. WARING

Page 11589, line 4, line 8: References 15, 16 should be corrected to 35, 36, 38. Reference 38 was not listed in the original version and should be added:

(38) Millard, J. T.; Spencer, R. J.; Hopkins, P. B. *Biochemistry* **1998**, 37, 5211–5219.

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Book Reviews

Conceptual Perspectives in Quantum Chemistry. Edited by J.-L. Calais and E. S. Kryachko. Kluwer Academic Publishers: Dordrecht, Netherlands. 1997. 553 pp. \$395.00. ISBN 0-792-34688-2.

The stated aim in this third volume of a series puts an emphasis on revisiting concepts in theoretical chemistry as opposed to the more obvious quantitative advances. The topics are varied enough that there should be something of interest to all quantum chemists, although varying in quality also. The price restricts it primarily to libraries. Nesbet gives an authoritative review of recent advances in two areas for computations on solids. One is “full potential” multiple scattering theory (MST), correcting the standard MST which used the muffin-tin potential in solids with disappointing results. He gives several means of addressing the difficulties associated with full potential MST, particularly convergence. Nesbet also discusses Green’s function and linearization methods. In DFT, he discusses a theory based on the density of a reference state rather than the exact density. Hall and Rees cover work in progress for localized atomic hybrids, a very familiar concept to freshman students. They present a matrix-based formalism that includes group theory, with several examples. A goal of the method is interpretation of modern calculations (with nonminimal basis sets) using hybrid orbitals. The chapter by Wooley is one of three in the volume dealing with whether the concept of molecular structure is problematic in quantum chemistry. Wooley gives a description of diffraction experiments using scattering theory and Feynmann diagrams as seen in quantum electrodynamics theory (working in the Coulomb gauge), which he calls molecular electrodynamics. The ninth chapter is by a philosopher, Jeffrey L. Ramsey, countering that many of the “problems” with the concept of molecular structure result from “unnecessarily strong versions of realism, reduction, and theoretical explanation” that makes for interesting reading. He is probably right. The final chapter is a description of P. G. Mezey’s concepts of shape in quantum chemistry: a means for describing the shape of a molecule as an algebraic group, and also for potential energy surfaces by describing classes of paths on the hypersurface. This is a rather abstract chapter. J. F. Ogilvie’s qualitative discussion in *The Chemical Bond* 1996 could have been benefited from an introduction that laid out the points to be discussed, since the chapter lacked coherence and the points were unclear. Truax reviews the use of Lie symmetries in quantum mechanics, which in many cases enables separable solutions for time dependent 1-D and 2-D Schrodinger equations for potentials of a certain form. Coherent

states are discussed, and examples are worked for the harmonic and driven oscillators (1- and 2-D cases). Kast, Brickman, and Berry discuss the interplay between quantum chemistry and molecular dynamics simulations. Included is a stochastic approach to constant temperature that avoids constraining the kinetic energy to be fixed and then brief coverage of constant pressure simulations. The quantum chemistry interplay arises from computation of forces used in dynamics; various methods are discussed such as simulated annealing. Rettrup’s short chapter on the permutational group in many electron theory is more pedagogical and historical in nature, not covering recent advances. It is well written, though. It is followed by a review of developments in many body perturbation and coupled cluster theories by Cremer and He. The work is quite impressive, going up to sixth order (MP6). They also analyze coupled cluster methods and quadratic configuration methods in terms of perturbation theory, and show that QCISD and even QCISD(T) method fail for some molecules because they do not treat the effects of triple excitations in a balanced way. They also develop a size-consistent series of QCI methods. Gianturco and Paesani examine the He–CO system as a case study for van der Waals interactions from various density functionals. Quite a few studies of this nature now exist in the literature, with the general conclusion that the hybrid DFT methods are preferred (B3LYP was not covered in this chapter). Simoes and Gavroglu discuss the historical roles of Linus Pauling and Robert Mulliken in chemical bonding. Quack and Suhm review their ambitious program to characterize the H-bond through studies of HF clusters. They discuss different approaches to solving the problems of potential surfaces for many dimensions, relevant issues being global vs local, analytical vs “on-the-fly”, decomposition into two-body, three-body, etc. terms, and reducing dimensionality. The chapter by Ortiz et al. is an exposition of the application of electron propagator (one-electron Green’s function) to compute IPs and EAs. This is done for second order and higher order methods, with an indication of how they are implemented (including pole searching). Examples of photoelectron spectra are presented that demonstrate the method is efficient and very accurate.

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