Book Review

Understanding Molecular Properties (edited by J. Avery, J.P. Dahl and A.E. Hansen), D. Reidel Publishing Company, Dordrecht, Boston, Lancaster, Tokyo, 1987, x + 598 pages, DFl 225, $98, £78.75. ISBN 90-277-2419-9.

This volume presents the proceedings of a symposium in honour of Professor Carl Johan Ballhausen, which was held at the Royal Danish Academy of Sciences and Letters, between April 4th and 5th 1986, as part of the celebrations associated with Professor Ballhausen's sixtieth birthday. To have such a volume and symposium dedicated to you is a true tribute, and the list of contributors reads like a "Who's Who" of coordination chemistry and chemical physics. The volume opens with an (undated) quote from Ballhausen, "Today we realize that the whole of chemistry is one huge manifestation of quantum phenomena", and the thirty-seven contributions to this volume admirably illustrate this point.

If one were forced to pick a single area in which Professor Ballhausen has made his most important contribution, it would have to be the experimental and theoretical study of transition metal complexes, with particular emphasis being placed on the the application of ligand field theory. This subject, of absolutely prime importance to all coordination chemists, forms the basis of the first third of this volume. The articles in this section discuss the electronic spectroscopy of metal-metal σ-symmetry interactions (V.M. Miskowski and H.B. Gray), metal-metal bonds in edge-sharing bioctahedra (F.A. Cotton), recent developments in inorganic spectroscopy (E.I. Solomon, A.A. Gewirth and S.L. Cohen), exchange effects in polynuclear chromium(III) complexes (H.U. Güdel), Jahn-Teller distortion of the $^4T_1(G)$ state of $[MnCl_4]^{2-}$ in Cs_3MnCl_5 (P. Day, A.C.W.P. James and J.R.G. Thorne), *ab initio* calculation of electronic transitions in transition metal complexes (H. Johansen), the cellular ligand-field model (M. Gerloch), the orthonormal operator formulation of symmetry-based ligand fields, with rhombohedral hierarchies as a general example (C. Schäffer), high- and low-spin interconversion in a series of tris(pyridylmethylamine)iron(II) complexes (L. Christiansen and H. Toftlund), tetracyanobiimidazole, a polyploid of distinction (P.G. Rasmussen), and the intensities of vibronic origins in transition metal complex ions (C.D. Flint and R. Acevedo).

Part II of this volume contains papers dealing with the theoretical treatment of reaction rates, and include accounts of photon echoes on multilevel systems (D.J. Tannor and S.A. Rice), solvent dynamical and

symmetrized potential aspects of electron transfer rates (R.A. Marcus), a theoretical approach to chemical reactions at solid surfaces (G.D. Billing), and the use of electron beams in surface analysis (P.J. Møller and F. Grønlund). The third section deals with various aspects of spectroscopy, and includes insights into hæmoglobin dynamics from resonance Raman spectroscopy (T.G. Spiro), spin uncoupling in the 6s Rydberg states of iodomethane (J.A. Dagata and coworkers), spectroscopy as a probe of intermolecular interactions (A.J. McCaffery), solvent, temperature and band asymmetry features of optical charge-transfer transitions in solute molecules in liquids and glasses (A.M. Kjær and J. Ulstrup), a theory of vibrational optical activity (P.J. Stephens), understanding molecular optical activity (A.E. Hansen and T.J. Bouman), optical activity (CD and CPL) as a probe of ion pairing and solution structure of macrocycle complexes (R.A. Palmer and coworkers), optical properties of large molecules in the Frenkel exciton approximation (J. Avery and S. Hvidt) and two-photon spectroscopy of lanthanide(III) complexes (W. Strek and J. Sztucki). Part IV describes 'floppy' molecules and the liquid state, and includes articles discussing the problems of rigid/floppy or solid/liquid molecules (R.S. Berry), understanding floppy molecules (B.T. Sutcliffe and J. Tennyson), stability and conformation of silicon–carbon compounds, especially [SiC_2], [Si_2C] and [Si_3] (J. Oddershede, J.R. Sabin and G.H.F. Diercksen), water and aqueous solutions (A. Hvidt), and the effect of structure and solvation on the thermodynamic parameters for the formation of singly and doubly charged ions of organic compounds in solution (O. Hammerich and V.D. Parker). The final section is concerned entirely with computational quantum chemistry, and contains accounts of the energies of three-electron atomic systems calculated by Hylleraas type wave functions (K. Hijikata, I. Matsubara and M. Maruyama), Hartree-Fock pathology and large molecules (J.-L. Calais and J. Delhalle), the relation between relativity and periodic trends within a triad of transition metals (T. Ziegler), a symmetric group approach to the calculation of electronic correlation effects in molecules (S. Rettrup and coworkers), the transverse susceptibility of spin-S Ising chains (I. Chatterjee), and chemical bond and electronic states of transition metal containing diatomic molecules (I. Shim).

The above detailed contents list has been included in order to illustrate the broad range of absolutely fascinating chemistry covered in this volume, the wide field of chemistry and physics which Professor Ballhausen's own work has influenced, and its particular relevance to coordination chemistry. My only adverse criticisms of this book would be the rather diverse mixture of camera-ready copy styles, ranging from the immaculate (*e.g.* E.I. Solomon *et al.* and R.A. Marcus) to the rather tatty (*e.g.* M. Gerloch),

and the patchy nature of the index. However, these are minor complaints about a volume which is a real tribute to Professor Ballhausen and his work. It is also, however, a reflection of modern Danish chemistry, the high quality of which is reflected in so many of the articles in this splendid book. This book should be in every chemistry library and, at its reasonable price, on many personal bookshelves.

Although published by Reidel, this book is sold and distributed by Kluwer Academic Publishers.

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