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Authored by Paul Hewitt, the pioneer of the enormously successful "concepts before

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This is the third edition of the successful text-reference book that covers computational chemistry. It features changes to the presentation of key concepts and includes revised and new material with several expanded exercises at various levels such as 'harder questions' for those ready to be tested in greater depth - this aspect is absent from other textbooks in the field. Although introductory and assuming no prior knowledge of computational chemistry, it covers the essential aspects of the subject. There are several introductory textbooks on computational chemistry; this one is (as in its previous editions) a unique textbook in the field with copious exercises (and questions) and solutions with discussions. Noteworthy is the fact that it is the only book at the introductory level that shows in detail yet clearly how matrices are used in one important aspect of computational chemistry. It also serves as an essential guide for researchers, and as a reference book.

The rivers run into the sea, yet the sea is not full Ecclesiastes What is quantum chemistry? The straightforward answer is that it is what quan tum chemists do. But it must be admitted,

that in contrast to physicists and chemists, "quantum chemists" seem to be a rather ill-defined category of scientists. Quantum chemists are more or less physicists (basically theoreticians), more or less chemists, and by and large, computationists. But first and foremost, we, quantum chemists, are conscious beings. We may safely guess that quantum chemistry was one of the first areas in the natural sciences to lie on the boundaries of many disciplines. We may certainly claim that quantum chemists were the first to use computers for really large scale calculations. The scope of the problems which quantum chemistry wishes to answer and which, by its unique nature, only quantum chemistry can answer is growing daily. Retrospectively we may guess that many of those problems meet a daily need, or are say, technical in some sense. The rest are fundamental or conceptual. The daily life of most quantum chemists is usually filled with grasping the more or less technical problems. But it is at least as important to devote some time to the other kind of problems whose solution will open up new perspectives for both quantum chemistry itself and for the natural sciences in general.

Almost all branches of chemistry and material science now interface with organometallic chemistry - the study of compounds containing carbon-metal bonds. The widely acclaimed serial Advances in Organometallic Chemistry contains authoritative reviews that address all aspects of organometallic chemistry, a field which has expanded enormously since the publication of Volume 1 in 1964. Provides an authoritative, definitive review addressing all aspects of organometallic chemistry Useful to researchers within this active field and is a must for every modern library of chemistry High quality research book within this rapidly

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This work was begun quite some time ago at the University of Oxford during the tenure of an Overseas Scholarship of the Royal Commission for the Exhibition of 1851 and was completed at Banga lore when the author was being supported by a maintenance allowance from the CSIR Pool for unemployed scientists. It is hoped that significant developments taking place as late as the beginning of 1965 have been incorporated. The initial impetus and inspiration for the work came from Dr. K. Mendelssohn. To him and to Drs. R. W. Hill and N. E. Phillips, who went through the whole of the text, the author is obliged in more ways than one. For permission to use figures and other materials, grateful thanks are tendered to the concerned workers and institutions. The author is not so sanguine as to imagine that all technical and literary flaws have been weeded out. If others come across them, they may be charitably

brought to the author's notice as proof that physics has become too vast to be comprehended by a single onlooker. E. S. RAJA GoPAL Department of Physics Indian Institute of Science Bangalore 12, India November 1965 v Contents Introduction ..... .