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this graduate level text explains the modern in depth approaches to the calculation of electronic structure and the properties of molecules largely self contained it features more than 150 exercises 1989 edition

this important book collects together state of the art reviews of diverse topics covering almost all the major areas of modern quantum chemistry the current focus in the discipline of chemistry synthesis structure reactivity and dynamics is mainly on control a variety of essential computational tools at the disposal of chemists have emerged from recent studies in quantum chemistry the acceptance and application of these tools in the interfacial disciplines of the life and physical sciences continue to grow the new era of modern quantum chemistry throws up promising potentialities for further research reviews of modern quantum chemistry is a joint endeavor in which renowned scientists from leading universities and research laboratories spanning 22 countries present 59 in depth reviews along with a personal introduction written by professor walter kohn nobel laureate chemistry 1998 the articles celebrate the scientific contributions of professor robert g parr on the occasion of his 80th birthday list of contributors w kohn m levy r pariser b r judd e lo b n plakhutin a savin p politzer p lane j s murray a j thakkar s r gadre r f nalewajski k jug m randic g del re u kaldor e eliav a landau m ehara m ishida k toyota h nakatsuji g maroulis a m mebel s mahapatra r carbó dorca nagy i a howard n h march s b liu r g pearson n watanabe s ten no s iwata y udagawa e valderrama x fradera i silanes j m ugalde r j boyd e v lude a v v karasiev l massa t tsuneda k hirao j m tao j p perdew o v gritsenko m gr ning e j baerends f aparicio j garza a cedillo m galván n r vargas e engel a h ck r n schmid r m dreizler j poater m sol m duran j robles x fradera p k chattaraj a

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some knowledge of the principles of quantum mechanics and how they are applied to theoretical chemistry it is generally agreed should be part of the education of all chemists this instruction in quantum chemistry is either added to the more traditional topics of physical chemistry or given separately at syracuse university it forms the third semester of the physical chemistry sequence while a wide variety of textbooks and monographs on the subject of quantum chemistry exists the author of the present text found that none of them was satisfactory for his purposes i e none fit his ideas of what subjects should be discussed and in what way this book is presented with the hope that others with similar experiences will agree with him and endorse his conclusions the undergraduate student to whom our attentions are directed is a chemistry major but probably will not go on to graduate school in physical chemistry he may take several more chemistry courses as an undergraduate and then seek a position in industry or perhaps he will do graduate work in organic or inorganic chemistry of course one never stops hoping that as a result of this first course he will decide to learn more quantum chem istry

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