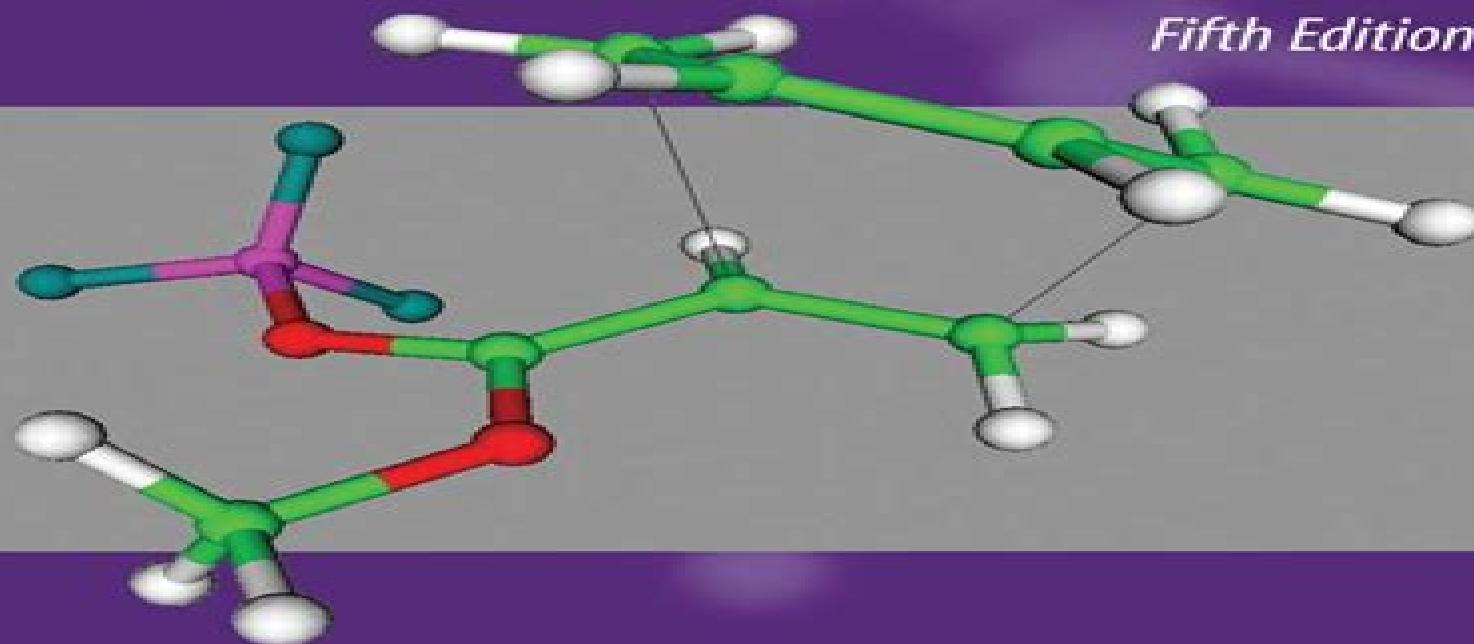


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Fifth Edition



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Errol G. Lewars,2024-06-04 This is the fourth edition of the successful textbook on computational chemistry which continues to provide a comprehensive introduction to the theory and practice of computational chemistry Notable updates include a review of references up to mid 2023 encompassing recent developments in scientific journals books and software The evolving prominence of density functional theory DFT is emphasized and attention is given to the increasing application of artificial intelligence in computational chemistry The book maintains key features from the previous edition delving into the mathematical intricacies of ab initio and density functional methods at an introductory level Clear explanations of matrix methods are provided offering a direct approach to obtaining energy levels and molecular orbitals Additionally each chapter includes sets of Easier and Harder drill questions with suggested answers at the end of the book enhancing the learning experience The book is intended for upper year undergraduate and graduate students studying computational and theoretical chemistry and for self study by researchers in universities and industry to whom

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