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Determination And Interpretation Of Molecular Wave Functions

Joseph M. Harrer, James G. Beckerley



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The Determination and Interpretation of Molecular Wave Functions Erich Steiner, 2009-03-19 First published in 1976 this monograph presents an exposition of some of the more important theoretical and computational techniques that have been developed for the determination and interpretation of molecular wave functions Although a comprehensive theory of the electronic structure and bonding in molecules had been developed by 1960 only with the advent of the electronic computer in the late 1950s did it become possible to perform accurate non empirical calculations for molecules of chemical interest indeed much of the subsequent evolution of the theory has occurred in parallel with the development of computing machines and techniques

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