

Advances in Quantum Chemistry, Volume 50: Response Theory and Molecular Properties



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Advances in Quantum Chemistry presents surveys of current developments in this rapidly developing field that falls between the historically established areas of mathematics, physics, chemistry, and biology. With invited reviews written by leading international researchers, each presenting new results, it provides a single vehicle for following progress in this interdisciplinary area. This volume continues the tradition with high quality and thorough reviews of various aspects of quantum chemistry. It contains a variety of topics on the use of quantum mechanical methods to calculate molecular properties including response properties. Linear and non-linear response methods have been developed and implemented for most of the approximate wave functions used in quantum chemistry, giving a range of computational methods of varying cost and accuracy. Thus it is presently possible to calculate for example excitation energies, linear and nonlinear optical properties, one- and multi-photon transition rates, and magnetically induced transition moments for a wide range of molecules and target accuracies. These calculations aid in the interpretation of a wide range of spectroscopy including electron spin resonance, nuclear magnetic resonance and magnetic circular dichroism and general laser spectroscopy.

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