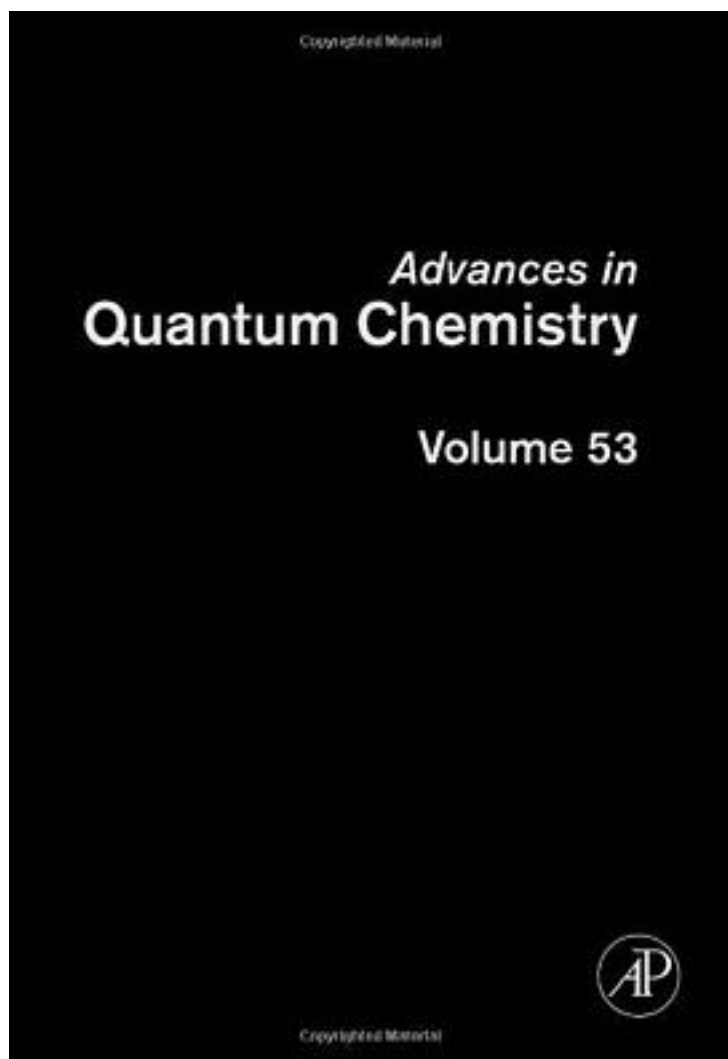


Advances in Quantum Chemistry



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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. "Advances in Quantum Chemistry, Volume 51" deals with various aspects of mathematical versus chemical applications. Some parts belong to established scientific domains, where technical progress has been crucial for the development of modern quantum chemistry as well as the quantification problem in spectral resonance analysis. The first chapter in the volume, concerns the calculation of molecular electronic structure to high accuracy, using a variety of one and two-body schemes in the coupled cluster family of methods. Chapter 2 is devoted to Angular Momentum Diagrams. In chapters 3 and 4, the authors portray Chemical Graph Theory (CGT). Advances quantum mechanical signal processing through the fast Pade transform (FPT) are covered in Chapter 5. The concluding chapter gives a mathematical view of molecular equilibria using a Density-Functional Theory (DFT) description. Features include: published articles, invited reviews and proceedings of major international conferences and workshops; compiled by the leading international researchers in quantum and theoretical chemistry; and, highlights the important, interdisciplinary developments.

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