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Effects; 5.5 Non-Relativistic Theory of EPR and NMR Parameters; 5.6 Relativistic Theory of Magnetic Properties; 5.7 The Leading Relativistic Corrections; 5.8 Concluding Remarks; Part B NMR Parameters, Methodological Aspects; 6 Chemical Shifts with Hartree-Fock and Density Functional Methods; 6.1 Introduction; 6.2 Linear Response and the Gauge Origin Problem
6.3 Determination of the First-Order Orbitals
6.4 Distributed Gauge Origins, IGLO and GIAO Approaches; 6.5 Distributed Gauge Origins in Real Space, a "Continuous Set of Gauge Transformations"; 6.6 Beyond Pure Density Functional Theory; 6.7 Conclusions; 7 Spin-Spin Coupling Constants with HF and DFT Methods; 7.1 Introduction; 7.2 The Calculation of Indirect Nuclear Spin-Spin Coupling Constants; 7.3 Examples of Applications; 7.4 Conclusions; 8 Electron-Correlated Methods for the Calculation of NMR Chemical Shifts; 8.1 Introduction; 8.2 Theoretical Background
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8.4 Special developments; 8.5 Numerical Results; 8.6 Summary and Outlook; 9 Semiempirical Methods for the Calculation of NMR Chemical Shifts; 9.1 Introduction; 9.2 Methods; 9.3 Representative Applications; 9.4 Concluding Remarks: Limitations of Semiempirical Methods for the Calculation of NMR Parameters; 10 Ro-Vibrational Corrections to NMR Parameters; 10.1 Introduction; 10.2 Perturbation Theory; 10.3 Other Approaches for Calculating Vibrationally Averaged NMR Properties; 10.4 Examples of Vibrational Contributions to NMR Properties
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13.2 Nuclear Shielding and Spin-Spin Coupling

Sommario/riassunto

This is the first book to present the necessary quantum chemical methods for both resonance types in one handy volume, emphasizing the crucial interrelation between NMR and EPR parameters from a computational and theoretical point of view. Here, readers are given a broad overview of all the pertinent topics, such as basic theory, methodic considerations, benchmark results and applications for both spectroscopy methods in such fields as biochemistry, bioinorganic chemistry as well as with different substance classes, including fullerenes, zeolites and transition metal compounds. The chapters
