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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