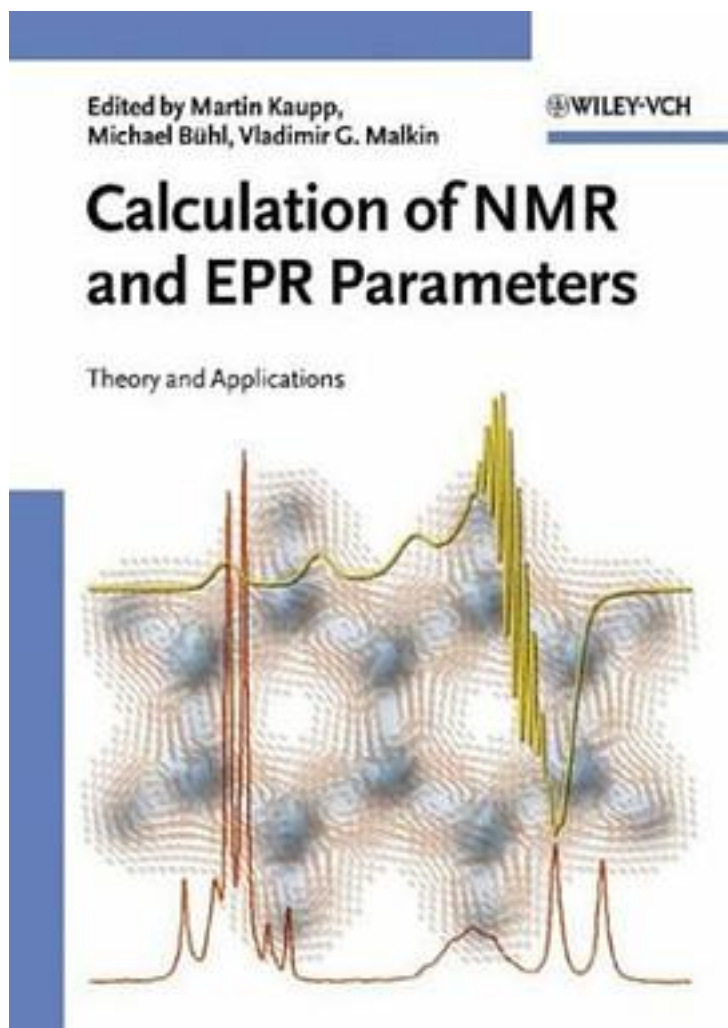


Calculation of NMR and EPR Parameters



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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 have been written by leading experts in a given area, but with a wider audience in mind. The result is the standard reference on the topic, serving as a guide to the best computational methods for any given problem, and is thus an indispensable tool for scientists using quantum chemical calculations of NMR and EPR parameters. A must-have for all chemists, physicists, biologists and materials scientists who wish to augment their research by quantum chemical calculations of magnetic resonance data, but who are not necessarily specialists in these methods or their applications. Furthermore, specialists in one of the subdomains of this wide field will be grateful to find here an overview of what lies beyond their own area of focus.

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