DESCRIPTION

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.
ABOUT THE AUTHOR

**Martin Kaupp** is Professor at the Institut für Anorganische Chemie at Universität Würzburg. He was born in Stuttgart and studied chemistry in Stuttgart and Cincinnati, before carrying out his PhD thesis in Erlangen. After postdoctoral work at Max-Planck-Institut für Festkörperforschung in Stuttgart and at Université de Montréal, Canada, he completed his habilitation in Theoretical Chemistry in Stuttgart, before moving to Würzburg in November 1999. His wide research interests include development and applications of quantum chemical methods to calculate NMR and EPR parameters, density functional theory, relativistic effects, bioradicals, and various aspects of computational bioinorganic, inorganic, and organometallic chemistry.

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**Vladimir G. Malkin** is a Leading Research Scientist at the Institute of Inorganic Chemistry of the Slovak Academy of Sciences (Bratislava, Slovak Republic). He was born in Russia and carried out his studies of Physics in the Novosibirsk). He was an Alexander von Humboldt fellow at the Ruhr-Universität Bochum, Germany before he was working at the Université de Montréal, Canada. His major interests include development of quantum-chemical methods for non-relativistic and relativistic calculation of NMR and EPR parameters using Density Functional theory as well as new general approaches in quantum chemistry.

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