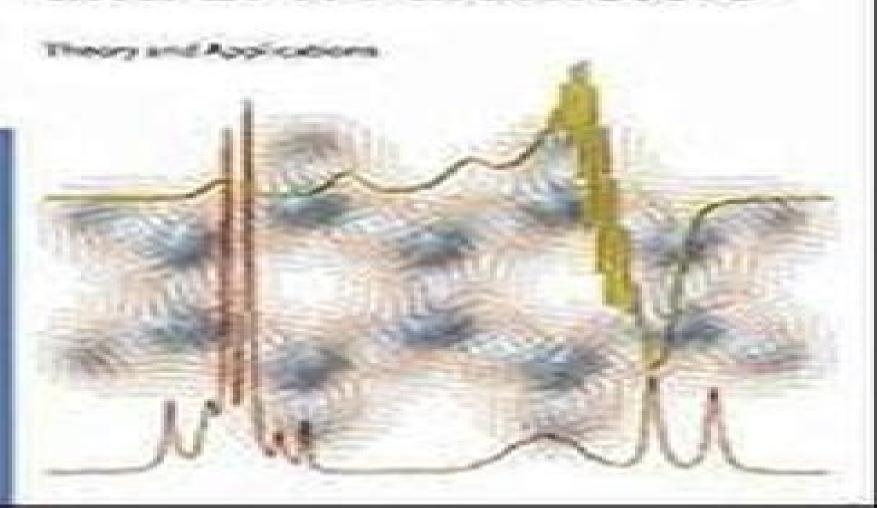
Calculation of NMR and EPR Parameters



Calculation Of Nmr And Epr Parameters Theory And Applications

D. M. P. Mingos, Robert Crabtree

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and in which the nature of interactions and reactions in solution is being studied Annual Reports on NMR Spectroscopy has established itself as a premier means for the specialist and non specialist alike to become familiar with new techniques and applications of NMR spectroscopy Provides updates on the latest developments in NMR spectroscopy Includes comprehensive review articles Highlights the increasing importance of NMR spectroscopy as a technique for structural **High Resolution NMR Spectroscopy** Juha Vaara, 2013-06-08 The theory and quantum chemical determination calculations of the spectral parameters of nuclear magnetic resonance NMR are well established in the case of diamagnetic closed shell molecules In contrast NMR calculations of paramagnetic open shell molecules pNMR are scarce limited by both assumptions within the underlying theoretical background as well as the availability of computational implementations We discuss the systematic development of pNMR theory that recently culminated in a novel general and systematic electronic structure approach for the shielding tensor and the associated chemical shift for paramagnetic open shell atoms molecules and nonmetallic solids The approach has now been extended for the first time to a higher than doublet spin state as well as arbitrary spatial symmetry. The approach is formulated without reference to spin susceptibility in contrast to the contemporary experimental procedure and approximate quantum chemical treatment of axial zero field splitting As a result of the systematic procedure all the temperature dependent hyperfine shielding terms are generalized and for example the leading order nonrelativistic dipolar term now provides an isotropic chemical shift contribution for species with triplet and higher spin multiplicity Recent first principles quantum chemical calculations of pNMR chemical shifts are reviewed both using the novel theory as well as earlier approaches **Advances in Physical Organic Chemistry** John P. Richard, 2007-12-08 Advances in Physical Organic Chemistry provides the chemical community with authoritative and critical assessments of the many aspects of physical organic chemistry. The field is a rapidly developing one with results and methodologies finding application from biology to solid state physics Reviews the application of quantitative and mathematical methods towards understanding chemical problems Multidisciplinary volumes cover organic organometallic bioorganic enzymes and materials topics Comprehensive Organometallic Chemistry III D. M. P. Mingos, Robert Crabtree, 2006-12-26 Comprehensive Organometallic Chemistry COMC III Third Edition 13 Volume Set is aimed at the specialist and non specialist alike It covers the major developments in the field in a carefully presented way with extensive cross references COMC III provides a clear and comprehensive overview of developments since 1993 and attempts to predict trends in the field over the next ten years Applications of organometallic chemistry continue to expand and this has been reflected by the significant increase in the number of volumes devoted to applications in COMC III Organic chemists have edited the volumes on organometallic chemistry towards organic synthesis this is now organized by reaction type so as to be readily accessible to the organic community Like its predecessors COMC 1982 and COMC II 1995 this new work is the essential reference text for any chemist or technologist who needs to use or apply organometallic compounds Also available

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