



Nuclear Magnetic Shieldings and Molecular Structure (Paperback)

By -

Springer, Netherlands, 2012. Paperback. Condition: New. Language: English . Brand New Book ***** Print on Demand *****.Modern approaches to the theoretical computation and experimental determination of NMR shielding tensors are described in twenty-nine papers based on lectures presented at the NATO ARW. All of the most popular computational methods are reviewed and recent progress is described in their application to chemical, biochemical, geochemical and materials science problems. Experimental studies on NMR shieldings in gases, liquids and solids are also included, with special emphasis placed upon the relationship between NMR shielding and geometric structure and upon tests of the accuracy of the various computational methods. Qualitative MO schemes and semiempirical approaches are also considered in light of the computational results. This is a valuable book for anyone interested in how the NMR shielding tensor can be used to determine the geometric and electronic structures of molecules and solids. (abstract) Modern methods for computing and measuring nuclear magnetic resonance shielding tensors are described in papers by a great number of leaders in the field. The most popular methods for quantum mechanically calculating NMR shielding tensors are reviewed and many applications of these methods are described to problems in chemistry, biochemistry, geochemistry and...



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