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	ISBN	3-319-90781-6
	Edizione	[1st ed. 2018.]
	Descrizione fisica	1 online resource (405 pages)
	Disciplina	543.0877
	Soggetti	Spectrum analysis
		Microscopy
		Physics
		Solid state physics
		Statistical physics
		Spectroscopy and Microscopy
		Numerical and Computational Physics, Simulation
		Spectroscopy/Spectrometry
		Solid State Physics
		Statistical Physics and Dynamical Systems
	Lingua di pubblicazione	Inglese
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	Nota di contenuto	1 Introduction -- 2 Principles of NMR spectroscopy -- 3 NMR Spectroscopy and Molecular Dynamics - an Outlook -- 4 Nuclear spin relaxation effects in NMR spectra -- 5 Discrete Molecular Dynamics and NMR Line Shape Effects. Intramolecular Exchange -- 6 Discrete Molecular Dynamics and NMR Line Shape Effects. General Exchange -- 7 Rotational tunneling in stick NMR spectra of solids -- 8 Quantum molecular dymanics in liquid-phase NMR spectra -- 9 Quantum mechanical rate processes in NMR spectra -- A Selected properties of matrices -- B Derivation of a general DNMR lineshape equation -- C Nuclear permutation symmetry in NMR spectra.
	Sommario/riassunto	The book provides a detailed account of how condensed-phase molecular dynamics are reflected in the line shapes of NMR spectra. The theories establishing connections between random, time-

dependent molecular processes and lineshape effects are exposed in depth. Special emphasis is placed on the theoretical aspects, involving in particular intermolecular processes in solution, and molecular symmetry issues. The Liouville super-operator formalism is briefly introduced and used wherever it is beneficial for the transparency of presentation. The proposed formal descriptions of the discussed problems are sufficiently detailed to be implemented on a computer. Practical applications of the theory in solid- and liquid-phase studies are illustrated with appropriate experimental examples, exposing the potential of the lineshape method in elucidating molecular dynamics NMR-observable molecular phenomena where quantization of the spatial nuclear degrees of freedom is crucial are addressed in the last part of the book. As an introduction to this exciting research field, selected aspects of the quantum mechanics of isolated systems undergoing rotational tunnelling are reviewed, together with some basic information about quantum systems interacting with their condensed environment. The quantum theory of rate processes evidenced in the NMR lineshapes of molecular rotors is presented, and illustrated with appropriate experimental examples from both solid- and liquid-phase spectra. In this context, the everlasting problem of the quantum-to-classical transition is discussed at a quantitative level. The book will be suitable for graduate students and new and practising researchers using NMR techniques.