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Autor: Robin K. Harris

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The term "NMR Crystallography" has only recently come into common usage, and even now causes raised eyebrows within some parts of the diffraction community. The power of solid-state NMR to give crystallographic information has considerably increased since the CPMAS suite of techniques was introduced in 1976. In the first years of the 21st century, the ability of NMR to provide information to support and facilitate the analysis of single-crystal and powder diffraction patterns has become widely accepted. Indeed, NMR can now be used to refine diffraction results and, in favorable cases, to solve crystal structures with minimal (or even no) diffraction data. The increasing ability to relate chemical shifts (including the tensor components) to the crystallographic location of relevant atoms in the unit cell via computational methods has added significantly to the practice of NMR crystallography. Diffraction experts will increasingly welcome NMR as an allied technique in their structural analyses. Indeed, it may be that in the future crystal structures will be determined by simultaneously fitting diffraction patterns and NMR spectra.

This Handbook is organised into six sections. The first contains an overview and some articles on fundamental NMR topics, followed by a section concentrating on chemical shifts, and one on coupling interactions. The fourth section contains articles describing how NMR results relate to fundamental crystallography concepts and to diffraction methods. The fifth section concerns specific aspects of structure, such as hydrogen bonding. Finally, four articles in the sixth section give applications of NMR crystallography to structural biology, organic & pharmaceutical