Preface

MULTINUCLEAR NMR spectroscopy is certainly one the most powerful experimental techniques for the characterization of the local structures in solution and in the solid state. The versatility of the technique has drawn the involvement of many scientific groups, leading to an extremely dynamic field of research. Focusing on solid state NMR, Spanish scientific community is small and scattered throughout the national geography, nonetheless contributing very actively to different fields of Science and Technology. In this context, we initiated the organization of a course on solid state NMR with a dual purpose: to strengthen the communication and collaboration among the Spanish scientific community working in the field, and to disseminate the technique and its applications in the solid state among researchers and students. The first Solid-State NMR Training Course was imparted on 2014, at the Instituto de Cerámica y Vidrio, Consejo Superior de Investigaciones Científicas (ICV-CSIC). The success of this initiative prompted us to organize a second edition the following year. This year will be presented the fourth edition of this training course.

After the second edition, we considered the publication of a book focused on the applications of NMR in the solid state gathering all topics covered through the above mentioned teaching experience. The illustration of the state of the art of the applications of NMR may assist in exploring the possibilities that this spectroscopy can offer in the analysis of solid materials emphasizing its strength when compared to other experimental techniques. This book could be useful as a starting material for future courses.

The title *Applications of NMR spectroscopy in the solid state* refers to the fact that this book gives an overview on the contribution of the technique in various research areas, differing from other approaches available in the literature, some of them more focused in theory and methods. We have attempted to explore the application of the technique in the characterization of structural and behavioral aspects of both natural and synthetic materials, although the contents of each chapter have been adapted to the particular experience of the authors. The book is separated into four parts, with a total of fourteen independent chapters.

The first part covers basic theoretical background and is composed of two chapters addressed to a wide audience, useful as a first approach for non-specialist in NMR. Chapter 1 defines basic concepts, including relevant NMR interactions and its possible cancelation by means of high-resolution techniques. Chapter 2 describes the modern methods of spectral simulation and theoretical calculations of NMR parameters by *ab initio* procedures.

The second part contains five chapters describing the use of NMR to explore the local structure of a wide variety of natural and synthetic materials, including crystalline and non-crystalline solids and glasses. For example, chapter 3 is devoted to the application of NMR for the elucidation of crystal structures of minerals (i.e., natural crystals) as a particular exploration of the increasingly popular field of the NMR crystallography. Chapter 4 focuses on ceramic materials, in terms of raw materials for traditional and advanced technological applications of ceramics, and chapter 5 addresses the particular application of certain ceramics to the immobilization of radionuclides. Cementitious materials are explored in detail in chapter 6, particularly from the point of view of ^{27}Al and ^{29}Si nuclei. Finally, glasses and glass-ceramic materials are developed in chapter 7, from silicate and borosilicate systems to phosphates and the study of the structural role of certain anions in glasses.

The third part of the book is dedicated to materials and compounds of interest in energy production, transformation and storage, and related applications. It is comprised of four chapters, including the contribution in relevant structural aspects of zeolites in chapter 8, and *in-situ* heterogeneous catalyst in chapter 9; chapter 10 refers to the study of structural factors that affect cation mobility in solid electrolytes, paying particular attention to lithium phases; and chapter 11 describes paramagnetic interactions and mobility of cations in solid electrodes.

The fourth part in the book describes organic compounds, including active pharmaceutical ingredients (APIS), with special consideration to polymorphism and co-crystals in chapter 12. In chapter 13, polymers are discussed, with special emphasis on the relationship between the macroscopic properties and the physicochemical structure, molecular mobility and processing conditions. Finally, chapter 14 refers to solid proteins, where solid state NMR spectroscopy is emerging as an essential method for the determination of three-dimensional structures of insoluble peptides and proteins and for the characterization of their dynamics.

We know that the field of solid-state NMR is much broader than exposed in this work, but we have concentrated on the expertise of the authors, in charge of the scientific contents. We would like to thank numerous editorials for their permission to reproduce previously published figures and tables in our book, as well as the reviewers for their disinterested reading and constructive criticisms.

THE EDITORS