Annual reports on NMR Spectroscopy

Volume 64

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NMR SPECTROSCOPY

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Edited by

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PREFACE

It is my great pleasure to introduce Volume 64 of Annual Reports on NMR. As is usual with this series of cutting edge reports the great importance of NMR in many areas of scientific research is highlighted.

The volume commences with a chapter on Theoretical and Experimental Studies on ^{19}F NMR Shieldings in Mineral Glasses, Zeolites and Related Silsequioxanes by J.A. Tossell. Chapter 2 is on NOE Studies of Solvent–Solute Interactions by G.T. Gerig. Chapter 3 is a state-of-the-art account of DFT Computations of Transition Metal Chemical Shifts by M. Bühl; this is followed by a contribution from D. Huster on Solid-State NMR Studies of Collagen Structure and Dynamics in Isolated Fibrils and in Biological Tissues; J. Kidrič reports on NMR Studies of Beverages; the Contribution of NMR Spectroscopy to Flavour Release and Perception is covered by L. Tavel, E. Guichard and C. Moreau; the final contribution by J.L. White is on Polymer Blend Miscibility.

My gratitude for their very interesting reports is due to all of these contributors. My thanks also go to the production staff at Elsevier for their help in the timely appearance of volumes of Annual Reports on NMR Spectroscopy.

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CHAPTER 1

Theoretical and Experimental Studies on ^{19}F NMR Shieldings in Mineral Glasses, Zeolites and Related Silsesquioxanes

J.A. Tossell

Contents

Abstract

While much attention has been devoted to the measurement and calculation of O NMR shieldings in solid oxides and silicates, F has been seriously neglected. This is because, except for the metal fluorides, F enters most solids as a low-concentration impurity or defect. Yet, the presence of only small amounts of F can exercise enormous influence upon physical properties, such as phase relations and viscosity, and upon chemical reactivity and mechanism of formation. Since the 1990s a number of studies have shown that F NMR shieldings in solids can be calculated quite accurately using quantum methods, which use large flexible basis sets and partially incorporate electron correlation, so long as the cluster model for the solid is adequate. Studies directed toward the assignment of particular unexpected peaks in specific glasses or disordered solids, as well as more general studies of trends in F NMR shifts have both been performed. We now have a good general understanding of the effect of local and mid-range structure about F on its NMR shift. However, for any given site trends often

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