Essential Practical NMR for Organic Chemistry

Essential Practical NMR for Organic Chemistry S. A. Richards and J. C. Hollerton
 ISBN: 978-0-470-71092-0

Essential Practical NMR for Organic Chemistry

S. A. RICHARDS
AND
J. C. HOLLERTON

WILEY
A John Wiley and Sons, Ltd., Publication

This edition first published 2011

Registered office
John Wiley & Sons, Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, United Kingdom

Library of Congress Cataloguing-in-Publication Data

Richards, S. A.
Essential practical NMR for organic chemistry / S.A. Richards, J.C. Hollerton.
p. cm.
Includes bibliographical references and index.
ISBN 978-0-470-71092-0 (cloth)
1. Proton magnetic resonance spectroscopy. 2. Nuclear magnetic resonance spectroscopy. I. Hollerton, J. C. (John C.), 1959- II. Title.
QD96.P7R529 2011
543′.66–dc22

2010033319

A catalogue record for this book is available from the British Library.

Print ISBN: 9780470710920
ePDF ISBN: 9780470976395
oBook ISBN: 9780470976401
ePub ISBN: 9780470977224

Set in 10.5/12.5pt Times by Aptara Inc., New Delhi, India.
Printed in Singapore by Fabulous Printers Pte Ltd.

We would like to dedicate this book to our families and our NMR colleagues past and present.

Contents

Introduction

This book is an up-to-date follow-up to the original "Laboratory Guide to Proton NMR Spectroscopy" (Blackwell Scientific Publications, 1988). It follows the same informal approach and is hopefully fun to read as well as a useful guide. Whilst still concentrating on proton NMR, it includes 2-D approaches and some heteronuclear examples (specifically ^{13}C and ^{19}F plus a little ^{15}N). The greater coverage is devoted to the techniques that you will be likely to make most use of.

The book is here to help you select the right experiment to solve your problem and to then interpret the results correctly. NMR is a funny beast – it throws up surprises no matter how long you have been doing it (at this point, it should be noted that the authors have about 60 years of NMR experience between them and we still get surprises regularly!).

The strength of NMR, particularly in the small organic molecule area, is that it is very information rich but ironically, this very high density of information can itself create problems for the less experienced practitioner. Information overload can be a problem and we hope to redress this by advocating an ordered approach to handling NMR data. There are huge subtleties in looking at this data; chemical shifts, splitting patterns, integrals, linewidths all have an existence due to physical molecular processes and they each tell a storey about the atoms in the molecule. There is a *reason* for *everything* that you observe in a spectrum and the better your understanding of spectroscopic principles, the greater can be your confidence in your interpretation of the data in front of you.

So, who is this book aimed at? Well, it contains useful information for anyone involved in using NMR as a tool for solving structural problems. It is particularly useful for chemists who have to run and look at their own NMR spectra and also for people who have been working in small molecule NMR for a relatively short time (less than 20 years, say!. . .). It is focused on small organic molecule work (molecular weight less than 1000, commonly about 300). Ultimately, the book is pragmatic – we discuss cost-effective experiments to solve chemical structure problems as quickly as possible. It deals with some of the unglamorous bits, like making up your sample. These are necessary if dull. It also looks at the more challenging aspects of NMR.

Whilst the book touches on some aspects of NMR theory, the main focus of the text is firmly rooted in data acquisition, problem solving strategy and interpretation. If you find yourself wanting to know more about aspects of theory, we suggest the excellent, *High-Resolution NMR Techniques in Organic Chemistry* by Timothy D W Claridge (Elsevier, ISBN-13: 978-0-08-054818-0) as an approachable next step before delving into the even more theoretical works. Another really good source is Joseph P. Hornak's "The Basics of NMR" website (you can find it by putting "hornak nmr" into your favourite search engine). Whilst writing these chapters, we have often fought with the problem of statements that are partially true and debated whether to insert a qualifier. To get across the fundamental ideas we have tried to minimise the disclaimers and qualifiers. This aids clarity, but be aware, almost everything is more complicated than it first appears!

Thirty years in NMR has been fun. The amazing thing is that it is still fun . . . and challenging . . . and stimulating even now!

Please note that all spectra included in this book were acquired at 400 MHz unless otherwise stated.