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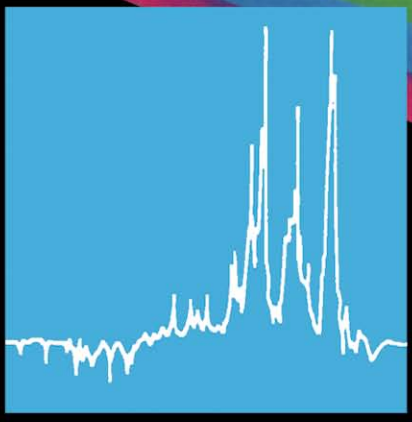

NMR for Liquid Fossil Fuels

Leonidas Petrakis
David Allen

Elsevier

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NMR for Liquid Fossil Fuels

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Volume 1 **NMR for Liquid Fossil Fuels**
by L. Petrakis and D. Allen

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NMR for Liquid Fossil Fuels

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PREFACE

High resolution nuclear magnetic resonance (NMR) of liquid fuels has provided valuable information on the molecular structures present in these fuels. The chemical insight gained through NMR studies has the potential to significantly enhance the development of processes for the utilization of fossil energy. For this potential to be fully realized, the users of NMR information must be able to effectively communicate with NMR experts. Conversely, the NMR experts must understand the type of information that users will attempt to derive from their spectra. The goal of this book is to strengthen the lines of communication between NMR experts and users in the area of NMR of liquid fuels.

The book is divided into two parts. The first part presents elements of relevant NMR phenomenology, including a definition of the most important NMR parameters, an introduction to Fourier transform NMR and a discussion of newer pulse techniques. This discussion of NMR phenomenology is not exhaustive, and it is not aimed at NMR experts. Rather, it attempts to introduce sufficient background material for the non-expert user so that NMR experts and users can work together more efficiently. This first part concludes with many examples from the authors' own work as well as from the literature. The review is not intended as a complete and critical review of the voluminous literature on the subject. Rather, it is intended to illustrate both the techniques presented in the book and also the range of applications and the great potential of the techniques.

The second part of the book addresses the interpretation of NMR spectra and is based to a very large extent on the work of the authors, who have used NMR in a variety of applications to fossil fuels. First, an overview of data interpretation methods is presented. Then, detailed presentations are made on the three most common methods of interpreting NMR spectra: calculation of average molecular parameters, average molecule construction and functional group analysis. Another section is devoted to the use of the NMR characterizations in engineering calculations. Throughout Part Two, examples are drawn from heavy petroleum crudes, shale oils, coal liquids and synthetic mixtures. Comparisons and contrasts among these various fuels are made, and the potential of the NMR techniques is discussed vis-a-vis their ability to produce data relevant to kinetics and processes for conversion and upgrading of fuels. A section is also included on the nature of asphaltenes and contributions made by NMR for their characterization.

We hope that the book will appeal to a wide range of professionals. Those who use NMR to characterize liquid fossil fuels or those who provide NMR

assistance to fossil fuel scientists and technologists should find it of primary interest. In addition, people interested in getting into the field, graduate students and those who manage and fund research in the utilization of liquid fossil fuels should find it of interest. One of us (LP) used some of this material in a pilot graduate course at the University of Wyoming, while the other of the authors (DA) uses the book as one of the texts for a course at UCLA on Molecular Spectroscopy of Complex Systems.

We acknowledge the cooperation and considerable help of the people who made this book possible. First, we thank Phyllis Gilbert for her great skill and patience in laying out and typing the manuscript. We also thank Carol Hicks for her preparation of the figures; Dimitris Liguras for help in assembling the final copy; Don Young for obtaining the spectra of octylbenzene; J. Kiebert and J. Friederich for their encouragement and editing of the manuscript; and Lina Petrakis for her encouragement and understanding.

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Hiller Highlands, Oakland, CA — Leonidas Petrakis
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PART ONE:

ELEMENTS OF RELEVANT NMR PHENOMENOLOGY