# *Additions and Corrections*

**Synthesis of [70]Azafulleroids: Investigations of Azide Addition to $C_{70}$** [*J. Am. Chem. Soc.* **1997**, *119*, 943−946]. CHERYL BELLAVIA-LUND AND FRED WUDL*

Page 944, Scheme 1: Structures $C_1$(d,c) and $C_1$(c,d) should read $C_1$(e,d) and $C_1$(d,e), respectively. Consequently, the same change should be made in the first paragraph of the Conclusion section.

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**Energy Transfer in Rigidly-Linked Heterodinuclear Ru(II)/Fe(II) Polypyridyl Complexes: Distance and Linkage Dependence** [*J. Am. Chem. Soc.* **1995**, *117*, 5881−5882]. S. L. LARSON, S. M. HENDRICKSON, S. FERRERE, D. L. DERR, AND C. MICHAEL ELLIOTT*

Page 5882, Table 1, Figure 2, and Text: The slope of the linear least-squares fit to the data listed in Table 1 and presented in Figure 2 was incorrectly reported in Figure 2 and the text as "$\beta$". On the basis of the customary definition of $\beta$, the value reported, 0.87 Å$^{-1}$, is actually $\beta$/2.303. Thus, the correct value for $\beta$ is 2.00 Å$^{-1}$. As a consequence, the arguments presented at the end of the next to the last paragraph before the Acknowledgement concerning the detailed nature of the donor/acceptor coupling are weakened.

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# *Book Reviews*

**NMR as a Structural Tool for Macromolecules: Current Status and Future Directions**. Edited by B. D. Nageswara Rao and Marvin D. Kemple (Indiana University−Purdue University at Indianapolis). Plenum: New York, 1996. ix + 382 pp. $120.00. ISBN 0-306-45313-4.

From the elegantly phrased introduction to the research articles and the interesting panel discussions, this volume represents a useful summary of the field of high-resolution NMR of macromolecules as of late 1994−1995. The book is a compendium of the lectures and discussions which constitute the proceedings of a symposium at Indiana University−Purdue University at Indianapolis organized by Drs. B. D. Nageswara Rao and Marvin D. Kemple. Its objectives are to present a description of the current status and future directions of NMR spectroscopy as a structural method for the investigation of biomolecular structure and dynamics.

The widespread applicability and importance of modern NMR methodologies to the chemical and biochemical communities is well-known. In this regard the book represents a useful avenue to this vast literature. The strength of this particular collection of articles is that the principles and scope of current research involving high-resolution NMR methods are presented and illustrated within the framework of various applications as described by leading practitioners of the art. In large part, this is due to the good judgment of the organizers of the conference in the selection of topics and the quality of the participants and discussants. The unifying motifs which make NMR spectroscopy such an attractive and exciting field of endeavor are well brought out by these various applications. The book accurately captures the spirit and flavor of the symposium, in that after each paper the recorded discussion is included, which lends a perspective not found otherwise. Another aspect is that there are three complete recorded panel discussions dealing with contemporary issues in high-resolution NMR spectroscopy, which are lead by distinguished contributors to the field and involve expert discussants.

In the choice of applications, the natural role of NMR spectroscopy as a cohesive feature that lends a degree of unity to the various disciplines is illustrated. This is, of course, a part of the culture of NMR spectroscopy. Although this reviewer tends to be somewhat biased against compendia of manuscripts which are often superseded or published elsewhere, or soon become out of date, the volume appears to be useful. What holds this particular collection together is the distinguished authors and interesting subject material described in the detailed and specialized research articles. In addition, one is drawn to the interesting panel discussions which are logically and clearly organized, with distinguished moderators and discussants. These offer a current and unedited perspective on the status of the field which is not typically found in books or articles. In this manner the theme of the book is accurately captured in a format which integrates the various NMR principles illustrated by the various contributions. It is this facet that is perhaps valuable for the beginning NMR enthusiast and graduate student entering the field. Unfortunately too little of the volume is devoted to this aspect; this reviewer would have preferred at least twice the amount of material, but alas the conference is over.

As a rule the first part of the volume deals with the structure and dynamics of macromolecules, mainly proteins, and includes a number of interesting contributions, starting with the keynote lecture by Nobelist Richard Ernst. The various applications illustrate the possibilities of contemporary NMR methodologies as applied to proteins in solution. The panel discussion led by Wagner addresses the issues of (i) structure generation via nuclear Overhauser enhancements (NOEs) and indirect dipolar couplings ($J$ couplings), (ii) structure refinement and the role of force fields, and (iii) the dynamics of macromolecules. In fact, many of the observations in high-resolution NMR spectroscopy of macromolecules in solution (NOE, $T_{1Z}$, $T_2$, $T_{1\rho}$ etc.) correspond to the spectral densities of motion which manifest both equilibrium and dynamical quantities. It appears that many workers in the field are relatively new to the dynamics literature; a generalized anisotropic diffusion model is adopted which is identical to the formalism widely used in the literature on surfactant micelles and lipid bilayers. The second set of articles also deals with structure and dynamics and includes several articles on nucleic acids and protein−nucleic acid interactions; the topics and quality of the research is fascinating. Next, the panel discussion led by Markley considers the extension of solution NMR techniques to large molecules, meaning proteins. The topics include (i) the role of sample conditions and mutagenesis, (ii) isotopic labeling strategies

and expression systems, (iii) pulse sequence modules for larger proteins, (iv) the use of very high magnetic fields, (v) large sample sizes, and (vi) data acquisition techniques. It may come as no surprise that the major features for success are the NMR friendliness of the protein and the salutary effects of ultra-high and ultra-expensive magnetic field strengths. The third set of articles describes applications of high-resolution NMR spectroscopy to proteins and peptides and includes a description of NMR structural methods with a range of interesting applications. Finally, the panel discussion led by Cohn is enlightening in terms of the goals of the conference involving the current status and future directions of NMR and includes a comparison of (i) X-ray crystallography, (ii) NMR spectroscopy, (iii) fluorescence and other spectroscopic methods, and (iv) finally computational methods and model building. This discussion offers a perspective not often found in the published scientific literature.

There are some caveats in that the book deals for the most part with high-resolution NMR spectroscopy of macromolecules, mainly proteins and nucleic acids in solution. The title is slightly misleading since only biological macromolecules are typically considered; the content is restricted mainly to high-resolution multidimensional NMR methods. There is little explicit mention of solid-state NMR spectroscopy, which has found broad applicability to macromolecules such as DNA and the nucleic acids, fibrous proteins, membrane proteins, and supramolecular assemblies of membrane lipids. The volume is principally a collection of manuscripts which has not benefitted from a strong editorial hand or production team. There is little consistency among the various articles; some, written by distinguished NMR spectroscopists, are cursory and a few pages long, while others are more detailed and original contributions. Also, there are some areas where the production of the volume could have been improved substantially. The book appears to involve a modest effort on the part of the publisher, perhaps that is a harbinger of the future of this particular medium for the dissemination of scientific knowledge.

Does the volume succeed in achieving its goals of capturing the current status and future directions of NMR spectroscopy as a structural tool for the investigation of macromolecules? Although the book is restricted for the most part to solution NMR methods, the answer would appear to be a qualified yes. Recognizing that what we have here are the proceedings of a scientific conference, the volume has its utility. Were it not for the cost, the book could be useful for beginning graduate students who wish to assimilate the flavor and range of topics of an exciting scientific symposium, but who have not yet had the opportunity to attend one. My overall recommendation to the aspiring biomolecular NMR spectroscopist is to start with the basics, that is to say acquire a firm background in physical chemistry and spectroscopic methods as found in the established texts. As a guide to the literature or for a specialized graduate course, this book could be a useful adjunct in that it includes a range of applications of high-resolution NMR spectroscopy to biological macromolecules in solution. This can then provide the basis for further detailed discussion and as a guide to the literature. For a research or industrial laboratory the book probably also has some utility, since it provides a perspective that is lacking in research articles of even review articles, due to the inclusion of the recorded discussions and panel discussions. I would be prepared to recommend adoption of the volume as a guide to the methods, personalities, and literature on high-resolution NMR of biological macromolecules in solution up to 1994 and for a contemporary perspective as articulated by some of the leading investigators in the field.

**Michael F. Brown,** *University of Arizona*

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**Monte Carlo and Molecular Dynamics Simulations in Polymer Science**. Edited by Kurt Binder (Johannes-Gutenberg University). Oxford University Press: New York, Oxford, 1995. xiv + 587 pp. $95.00. ISBN 0-19-509438-7.

The introduction of the digital computers into scientific research is fast approaching the half-century mark, and the field of computer simulation applied to molecular systems has developed apace. Computer simulation complements analytical theory and experiment in scientific problem solving and is imbued with some of the characteristics of both: analytical theory frequently involves working out the properties of a model system and comparing calculated results with experiment. However, in complex molecular systems, where the grail is interpretation and prediction of observable phenomena in terms of atomistic interactions and motions, the gap between the model and the desired results is not bridgeable by analytical theory without severe approximations. In a computer simulation, the answers are obtained by running a computer "experiment" on the energy surface or force field representative of a model and calculating observable and other properties of the model system as results. As computer power increases, the behavior of ever more detailed models can be explored for ever more complex systems using simulation.

Computer simulation was introduced into the study of the physics of simple liquids soon after the turn of the century and began to impact molecular science in the 1970's with the appearance of the first serious studies of the structure and dynamics of molecular liquids. A parallel formalism for polymers was soon developed and applied, and by the late 1970's, molecular simulation had been extended to the study of macromolecules. Today we are fortunate enough to have arrived at the point where technology in the form of desktop workstations or parallel supercomputer makes it possible to carry out simulations on in macromolecules on increasingly realistic models of salt solutions and mixed solvents. Computer simulation is thus playing an increasingly important role in fields such as diverse as physical organic chemistry, structural biology and polymer physics, the subject of this volume of technical articles.

*Monte Carlo and Molecular Dynamics Simulations in Polymer Science* is a multiauthored treatise aimed at communicating molecular simulation theory and methodology applicable to the structure, molecular motions, and physical properties of polymers. Professor Kurt Binder of the University of Maine and 12 distinguished colleagues in the field have succeeded in this volume in providing a valuable but very high level technical overview. Molecular simulation capabilities are now readily available to scientists at all levels in the form of "molecular modeling" programs, but the complexity of problems and the wide range of both length scales and time scales on which molecular phenomena occur make naive use of these programs as a "black box" a risky business. The motivation for this volume is that foundational knowledge of what simulation is all about, what methods are applicable to a given problem, and what the strengths and weaknesses various methodological approaches entail are all essential to successful scientific problem-solving, and this attitude clearly prevails in the various articles.

The treatise begins with an introduction and overview by Prof. Binder on general aspects of computer simulation techniques and applications in polymer physics. Nine chapters follow which collectively provide an in-depth treatment of simulation theory and methods applied particularly to amorphous polymers in solution, melts, or solid states covering a spectrum of topics ranging from the primarily theoretical (*Monte Carlo Methods for the Self-Avoiding Walk* by Alan Sokal of NYU) to the applied (*Simulations of Studies of Polymer Melts at Interfaces*). Additional topics covered also include Monte Carlo Methods for the Self-Avoiding Walk, Simulations of Tethered Chains, Long Range Interaction Problems in the Simulation of Charged Polymers, Entanglement Effects in Melts and Networks, Molecular Dynamics of Glassy Polymers, Monte Carlo Simulation of the Glass Transition, Simulational Approaches to Polymer Blends, and Block Copolymers and Polymer Melts. The treatment in each case is definitely at the cutting edge of polymer science, with presentations aimed at advanced research students and experienced practitioners. The volume contains a wealth of methodological detail and leading references to the original literature and is not only a valuable reference for researchers but a possible supplement for graduate courses in polymer physics, engineering, and materials science. Prof. Sokal's article concludes with a thoughtful set of practical recommendations and list of open problems, and the volume would have been even more useful and connected if each of the other article would have provided a similar concluding section.

In summary, this treatise provides a valuable perspective on theory, methodology, and selected applications of computer simulation to polymer physics and contains a unique collection of articles that will be of interest to those exploring the macroscopic behavior of macromolecules with atomistic models. The reader of this book will find it filled to the brim with timely current theory and valuable methodological details, many of interest to those working in the area of biological macromolecules as well as in polymer physics.

**David L. Beveridge,** *Wesleyan University*

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