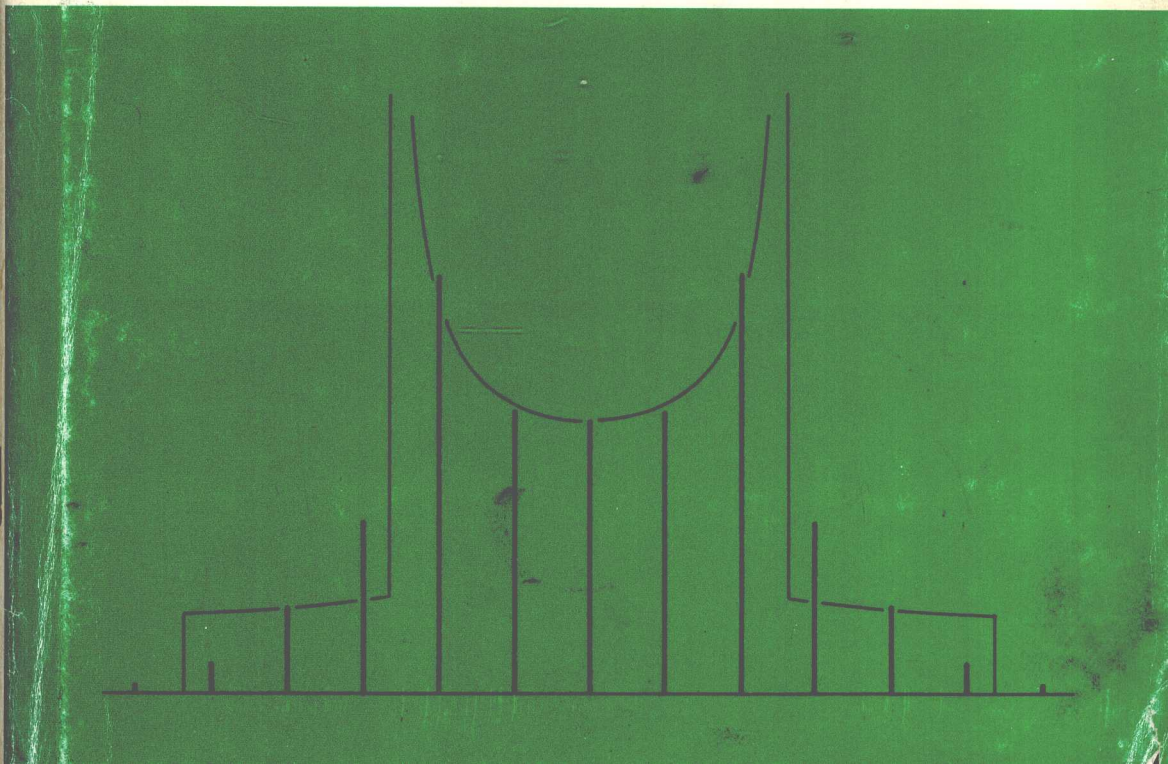
New Directions in Chemical Analysis

Proceedings of the Third Symposium
of the
Industry-University Cooperative Chemistry Program
of the
Department of Chemistry, Texas A&M University
March 31–April 3, 1985

Editor

Bernard L. Shapiro



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College Station, Texas 77843
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Volume 1 (1983) Organometallic Compounds

Volume 2 (1984) Heterogeneous Catalysis

Foreword

Chemistry has been referred to as the "central science," interfacing with most aspects of the physical sciences, engineering, and medicine. The multiple facets of chemistry have in turn a central, common need for qualitative and quantitative identification of chemical species.

The present volume illustrates the cardinal role of analytical chemistry, with contributions ranging from the characterization of surfaces to separations, and from strategies for data measurement and interpretation to methodologies for elucidating the chemistry of the life process. It is unusual to have a broad range of advanced contributions in a compact book format. We are indebted to the fifteen distinguished authors for participating in this venture designed to foster the awareness and exchange of information among subdisciplines of analytical chemistry.

This volume represents the proceedings of a three-day symposium organized by a Steering Committee with the following

membership: D. L. Cocke (TAMU), J. F. Haw (TAMU), T. B. Malloy, Jr. (Shell), C. R. Martin (TAMU), R. A. Nadkarni (Exxon), M. W. Rowe (TAMU), D. H. Russell (TAMU), R. W. Sims (Monsanto), L. O. Wheeler (Celanese), R. L. Windham (Texaco), and L. Wolfram (SOHIO). It is a distinct pleasure and privilege to thank my colleagues for their help in selecting the scientific program.

On behalf of the Steering Committee, I am pleased to acknowledge the financial support the Industry-University Cooperative Chemistry Program provided for holding the symposium and for publishing these Proceedings. Last but not least, kudos go to Dr. Abraham Clearfield and Ms. Elizabeth Porter for organizing the meeting, and to Dr. Bernard L. Shapiro for the meticulous editing of this volume.

College Station, Texas
May 1985

Emile A. Schweikert

Professor of Chemistry

Director, Center for
Trace Characterization

Chairman, 1985 IUCCP
Research Symposium

Preface

It is hard for me to comprehend the phenomenal growth which has characterized Texas A&M University since I joined the faculty in 1976. Similarly, the parallel growth in the Bryan-College Station area has been nothing short of astounding. No doubt these two phenomena are related, but the factors which made this growth possible - the enlargement of the student body and the greater emphasis on graduate study and research - have begun to plateau.

In a similar vein, the heyday of intense oil exploration and production also has slowed and Texas is looking for greater diversification to provide continued and long-term economic health. In this connection her universities will play a leading role and cooperative efforts which involve major industrial concerns become ever more important.

The Industry-University Cooperative Chemistry Program (IUCCP) was founded in 1982 to promote dialogue and an interchange of ideas between these two strongly interdependent

types of organizations. Our annual IUCCP symposium is predicated on fostering such a dialogue and brings together industrial, university, and other scientists in a relatively informal and relaxed setting. An international flavor has been fostered by the inclusion of foreign scientists in the programs.

This year's program, "New Directions in Chemical Analysis," featured invited lectures by an outstanding array of scientists who are on the cutting edge of their respective specialties. This volume and the earlier two, Organometallic Compounds: Synthesis, Structure, and Theory and Heterogeneous Catalysis, testify to the high quality of the presentations. But equally important are the informal discussions which ensued at the mixer, poster session, wine and cheese party, and final banquet.

In planning and executing such a conference, a great deal of work is required by many people. Thanks are due Professor Emile Schweikert, our Program Chairman, and the Analytical Chemistry faculty at Texas A&M, as well as to the industrial members of the organizing committee - Dr. T. B. Malloy, Jr. (Shell); Dr. R. A. Nadkarni (Exxon); Dr. R. W. Sims (Monsanto); Dr. L. O. Wheeler (Celanese); Dr. R. L. Windham (Texaco); and Dr. L. Wolfram (SOHIO) - for arranging the scientific program.

Thanks also are due Elizabeth Porter and her staff for all the social arrangements and myriad other functions required to ensure that the conference events proceeded smoothly and to make our conferees feel welcome and comfortable. Special thanks are due our editor, Dr. B. L. Shapiro, and the Texas A&M University Press, whose labors resulted in the visible evidence before you.

Finally, we are indebted to our industrial sponsors, without whose generous support none of this would be possible.

College Station, Texas
May 1985

Abraham Clearfield

Professor of Chemistry

Director, Industry-University
Cooperative Chemistry Program

This volume is the third in the annual series of Proceedings of the Research Symposia sponsored by the Industry-University Cooperative Chemistry Program of the Department of Chemistry at Texas A&M University. As with the previous volumes, rapidity of publication has been a principal concern. To facilitate this goal, the approach has been to have the articles prepared by the authors in camera-ready format.

With the ubiquity of the word processor and computer, some variety of type fonts has resulted, but the goal of timely

publication has been aided. To maximize readability and the similarity of visual impact, the double-spaced style of the previous Proceedings volumes has been maintained. It was felt that the extra readability for scientific notation, etc., was more important than the relatively small savings in space which could have resulted from single-spaced presentation.

The articles in this volume appear, for the most part, in the order in which the corresponding lectures were presented at the Symposium, whose organization is thus mirrored.

It is a pleasure to acknowledge the extent and excellence of the work done by Russel R. Kirk, Elizabeth Porter, and Letetia L. Beggs. Their important contributions, involving formatting some of the chapters, preparing the front and back matter, creating the author index, etc., were dispatched in a diligent and highly professional manner and enabled the many chapters to be integrated into a consistent whole.

College Station, Texas
May 1985

Bernard L. Shapiro

Professor of Chemistry
Editor, IUCCP Proceedings Volumes

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New Directions in Solid State Mass Spectrometry: The Role of the Matrix in the Formation of Gas Phase Molecular Ions

Ronald D. Macfarlane

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Abstract

Mass spectrometry is one of the important methods for chemical analysis. The applicability of mass spectrometry to a particular problem depends on the ability to form gas phase molecular ions of the molecules of interest. Methods have been developed in recent years to solve the problem of involatility for molecules that have strong intermolecular binding and have been referred to as particle-induced desorption methods. The desorption process can be stimulated by the surface excitation of a condensed matrix using energetic particles. The 252-Cf-plasma desorption technique is one of these methods. The details of this method are briefly described along with some results that reflect the ability to desorb molecular ions of large biomolecules and the role of the matrix in the ionization-desorption process.