Proceedings of the XIIIth International Symposium on NQR Spectroscopy

Providence Rhode Island, USA, July 23-28, 1995. Z. Naturforsch. **51 a**, 315-804 (1996)



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This volume contains the Proceedings of the XIII International Symposium on Nuclear Quadrupole Interactions (NQI), held in Providence, Rhode Island, from July 23rd to 28th, 1995; it is dedicated to the memory of Professor Alarich Weiss, a former chairman of the International Committee and one of the founders of this series of Symposia, who died on October 10th, 1995, after a long illness. During the Providence Symposium, he became the first recipient of the NQI Award, presented for his outstanding contributions to nuclear quadrupole resonance research and for the work he did in developing and strengthening the NQI community. This was but the last of a series of honours and awards which he received during his lifetime for contributions to physical chemistry which included not only the study of nuclear quadrupole and nuclear magnetic resonance in solids, but other fields as diverse X-ray and neutron crystallography, preparative inorganic chemistry, the transport properties of liquids, compleximetric titrations, intermetallic systems, and hydrogen absorption in alloys.

Alarich Weiss was born on February 2nd, 1925 in Bavaria. He studied physics at Erlangen, Mainz and Darmstadt. While studying for his Ph.D. degree under Professor Helmut Witte on the electron density distribution in calcium fluoride, he also worked with his brother Armin Weiss in the field of preparative inorganic chemistry and X-ray crystal structure analysis, with some emphasis on compounds of silicon and mercury. This collaboration was so productive that seventeen papers were published before his first work on calcium fluoride appeared in 1957.

In the period 1956 to 1957, he spent one year with Professor Walter J. Moore in Bloomington, Indiana and a further year at the Carnegie Institute of Technology in Pittsburgh. In 1958 he returned to the Institute of Physical Chemistry at the Technische Hochschule of Darmstadt to begin his first research work on quadrupole interactions in the solid state. His first paper in this field, published in this journal in 1960, was on ²³Na quadrupole interactions in a single crystal of sodium nitrite, an experimental technique which was to interest him for the rest of his life, and to which he made many important contributions. In 1962, he finished his post-graduate degree (Habilitation) in physical chemistry and became a professor in 1965, by which time he had already published six papers on nuclear quadrupole interactions, whilst continuing the collaboration with Armin Weiss. In 1967 he accepted an invitation to occupy a full professorial position at the University of Münster, but returned to Darmstadt in 1972 to a chair in chemical spectroscopy in the Institute of Physical Chemistry at the Technische Hochschule, where he stayed for the rest of his working career, except during guest professorships at the Universities of Madras, Geneva and Nagoya.

His earlier studies on 23 Na quadrupole interactions in single crystals of NaNO₂, Na₂S₂O₆ · 2H₂O, and Na₂SO₄ were followed by an extensive series of investigations of NQR in polycrystalline samples by means of a very diverse range of nuclei including 35 Cl, 79,81 Br, 27 Al and 127 I. At the same time he developed methods of studying Knight shifts in the NMR spectra of intermetallic compounds of nuclei such as 113 Cd and 205 Tl. An important instrumental contribution during these years was the development of a 4π goniometer for the study of quadrupole interactions in single crystals from their Zeeman splitting patterns, which several years later was modified and became a microcomputer controlled device for the accurate determination of the full quadrupole tensor, even when the asymmetry parameter was close to zero. The techniques of NMR and NQR were skilfully used to investigate a wide range of problems in solid state chemistry, such as the study of the electron density distribution in ionic crystals, covalency in organic compounds, crystal field effects and their temperature dependence, phase transitions in a variety of organic and inorganic crystals, and spin lattice relaxation and its relation to molecular motion in many different compounds. Dipole-dipole inter-

actions in ¹H NMR were used to determine the positions of protons, and ²H NMR in crystal hydrates to investigate hydrogen bonding and the dependence of the ²H quadrupole coupling parameters on the crystal environment.

The theoretical aspects of the subject were not neglected; detailed studies were performed on electrical interactions in solids, the calculation of Sternheimer anti-shielding factors, electron polarizabilities, and methods of deriving lattice sums in ionic crystals. There were a number of papers on NMR in intermetallic and metal-hydrogen systems, the dielectric properties of solids, pyro-electricity and superconductivity, subjects denoting the wide range of Alarich Weiss's interests in physical chemistry. In these fields, he published a total of over 350 scientific papers. He also wrote with Wolfgang Pies volume 7 of the New Series of Landolt-Börnstein numerical data. This volume on "The Crystal Structure of Inorganic Compounds" is itself subdivided into 15 large subvolumes.

This work brought him world-wide recognition and many scientific honours, of which the award from the Japan Society for the Promotion of Science is worthy of mention. His research group in Darmstadt became renowned internationally as a centre of excellence in nuclear quadrupole resonance spectroscopy, and many scholars were trained there or came to visit his Institute from abroad. Alarich Weiss's international reputation and high standing in science led to many invitations to serve on scientific organisations. He was president of the Bunsen-Gesellschaft for Physical Chemistry and for many years a member of the executive committee of the German Chemical Society. He was strongly committed to the work of the Alexander von Humboldt Foundation, where he held the office of Vice-President of the central selection committee of the Foundation. He and his wife Elisabeth personally advised and helped the Humboldt fellows who came to Darmstadt.

His contribution to his chosen fields of research was immense and will continue to influence all who work with nuclear quadrupole interactions. It is appropriate that this volume should be dedicated to his memory, as it contains some of his last papers in a long and distinguished series, many of which were published in this journal.

P. C. Schmidt and J. A. S. Smith

Preface

These Proceedings contain papers based on a selection of talks presented at the XIIIth International Symposium on Nuclear Quadrupole Interactions, which was held at Brown University in Providence, Rhode Island, USA, during the period 23–28 July 1995. This was the first Symposium to carry the expanded title Nuclear Quadrupole Interactions in place of the Nuclear Quadrupole Resonance Spectroscopy employed for the twelve prior meetings. The breadth of topics and experimental techniques evident in the papers of these Proceedings reflect that broadening of the scope of the symposia to embrace all experimental and theoretical work on nuclear quadrupole interactions. This change was adopted by the International Committee on NQR Spectroscopy at the XIIth International Symposium in Zurich, Switzerland in July 1993. In a corresponding action, the name of the Committee was changed to the International Committee on NQI. Some 170 papers were presented at the XIIIth Symposium which involved more than 120 participants and their guests from 28 countries, including 15 scientists from Russia, the Ukraine, and Armenia. The papers in the Proceedings are organized in the following sections:

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The International Committee on Nuclear Quadrupole Interactions, and the Organizing Committee for the XIIIth International Symposium, gratefully acknowledge support and sponsorship by the following agencies, companies, individuals and institutions:

Dr. Vartan Gregorian, President, Brown University
Dr. Frank Rothman, Provost, Brown University
Brown University
U.S. Department of Energy/Lawrence Berkeley Laboratory
U.S. National Science Foundation
Tecmag, Inc.
RITEC, Inc.

It is a pleasure to acknowledge the advice and assistance of Dr. J. A. S. Smith of Kings College, London and Dr. Detlev Brinkmann of the University of Zurich who hosted the XIth and XIIth Symposia in London (1991) and Zurich (1993), respectively. The extensive imaginative work of the Organizing Committee, and the contributions of the participants and their guests, brought about a Symposium that was highly productive scientifically and most pleasant an occasion socially. The members of the Organizing Committee were:

Professor Philip J. Bray (Chairman)	Brown University
Professor Tara P. Das	State University of New York at Albany
Professor Robert A. Marino	Hunter College
Dr. Gary L. Petersen	RITEC, Inc. and Brown University
Professor Alexander Pines	University of California at Berkeley
Professor P. Craig Taylor	University of Utah
Professor Gary P. Wulfsberg	Middle Tennessee State University

We are grateful to the Editor of the Zeitschrift für Naturforschung, Prof. A. Klemm, for his excellent cooperation and to the Managing Editor, Mrs. T. Littmann, for her efficient and swift handling of the papers and for her patience. The editing of the Proceedings was done by Gary Wulfsberg and Robert Marino.