



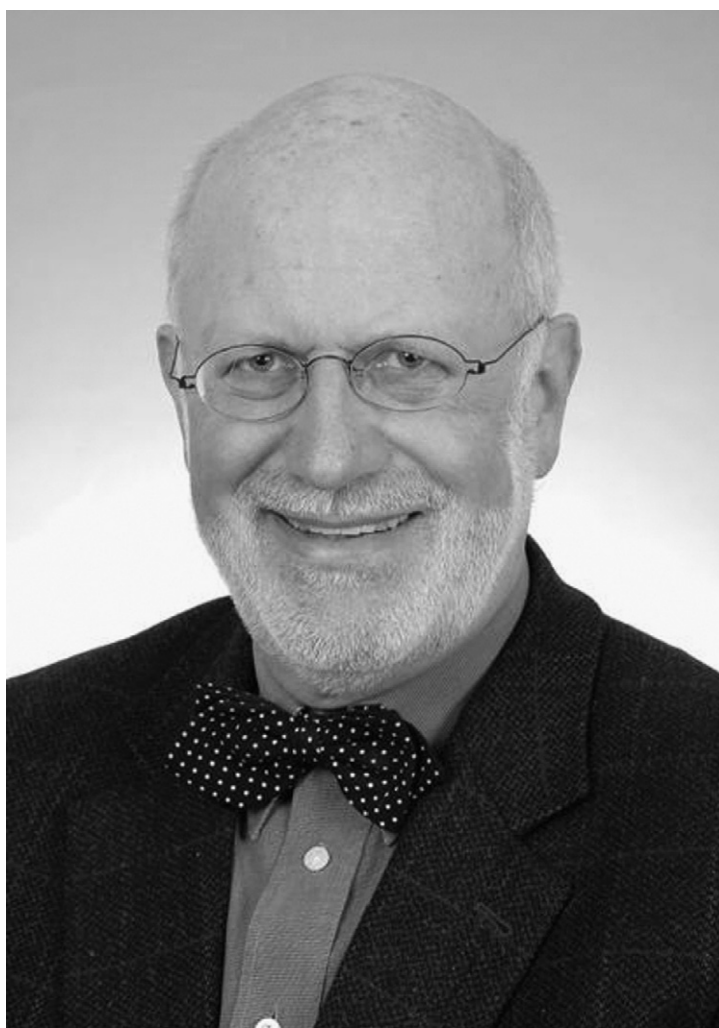
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Preface



In memory of Dr. Karlheinz Schmidt
(1945 - 2008)

In 2001 the German scientific community felt that research in the field of molecular magnetism was not as firmly established in Germany as in other nations and that a concerted effort was necessary to strengthen research in this area. Therefore, a proposal was submitted to the *Deutsche Forschungsgemeinschaft* (DFG, German Research Council) for installation of a “Schwerpunktprogramm” (priority programme) with the title “Molecular Magnetism”, which would focus on the study of the magnetic properties of discrete molecules and coordination polymers. The main research objectives of this priority programme were the preparation of new, magnetically interesting materials, the investigation of the magnetic properties of these materials by physical methods, and the description and explanation of magnetic properties on the basis of theoretical models. In order to achieve these objectives, the priority programme was particularly planned to include research groups from chemistry and physics.

The programme was limited to the study of discrete and supramolecular molecules which contain at least two spin carriers, and to the investigation of molecules which are capable of undergoing temperature-, light- or pressure-induced spin crossover or valence tautomerism. While coordination polymers deriving from molecular precursors were included as objects of study in this programme, the investigation of typical solid state materials (e.g. metal oxides) and metallic phases was explicitly excluded. In addition to determining the magnetic exchange coupling between spin carriers, the study of spin dynamics by physical methods was one major effort in this research programme. Some goals included in the programme were the synthesis and the characterization of new single molecule magnets (SMM), the study of substances, which change their spin state in response to variation of temperature or pressure or to irradiation by light, and the search for an adequate description of the underlying theoretical basis of magnetic properties.

In addition to furthering research in the field of molecular magnetism, the initiators of this priority programme wanted to achieve some broader goals. They wanted to enhance communications between the research groups originating from different scientific communities by providing annual meetings for the participating groups. These meetings served as platforms for the sharing of resources and expertise among the research groups from inorganic and organic chemistry and those from experimental and theoretical physics. Thereby new interdisciplinary collaborations could be established and new scientific partnerships could be promoted. Further goals were to provide training for young co-workers by organizing workshops and to support especially young independent researchers in their work in order that research in molecular magnetism would continue to thrive even after the priority programme has ended. By this means this research programme would have a long-lasting impact on the scientific communities in Germany. A third objective of this research programme consisted in the increase of national and international visibility of German research in the field of molecular magnetism, thereby attracting new research groups to enter this fascinating research area.

The proposal to establish the priority programme “Molecular Magnetism” for the duration of three funding periods, each lasting 2 years, was granted by the DFG in June 2001. The first funding period started in 2002 with 31 participating groups, 29 from Germany and one each from France and Italy. The priority programme ended with a final meeting in February 2009.

This special volume of CCR includes the final reports of most of the participating research groups in this priority programme. Overall it comprises seventeen reviews. Some of these were written by researchers from different groups, demonstrating the strong ties of cooperation established over the years among the participating members of the priority programme. If one cares to classify the contributions, three major areas of interest can be identified. The majority of the contributions is primarily concerned with

synthetic strategies to control magnetic interactions between spin centers by changing the nuclearity of the complexes, the topology of spin centers and the type of bridging ligands. Some of the more prominent goals of the research described in these contributions include deriving magnetostructural relationships on the basis of these new complexes and increasing the total spin and/or the magnetic anisotropy in order to achieve new single molecule magnets with higher blocking temperatures. The second group of contributions concentrates more on experimental methods used to characterize and interpret the properties of magnetic materials. Since the physical characterization of complexes is also included in those contributions of the first section, the association of some of the individual reports to the first group rather than to the second may appear to be arbitrary. I hope I did not offend any of the involved authors by doing so. The last group of contributions is comprised of reports dealing with various aspects of spin crossover properties.

In eight contributions the synthesis and coordination chemistry of new complexes with varying nuclearity and the characterization of their magnetic properties are reviewed. The rich coordination chemistry of dinuclear first-row transition metal complexes with macrocyclic hexamine-dithiophenolate ligands, and the experimental and theoretical results of the magnetic study of these complexes are described by Kersting, Kortus et al. The utilization of various dinuclear metal complexes as building blocks for the controlled synthesis of tetranuclear complexes and the study of these complexes by high-field EPR and pulsed-field magnetization is the focus of the review by Chaudhuri, Büchner, Klaus, Kersting and Meyer. Plass gives an account of the coordinative properties of aminoglucose and tritopic triaminoguanidine ligands used in preparing oligo- and polynuclear complexes with specific magnetostructural properties in a controlled way. The possible coordination modes of bridging 2,6-bis(hydroxymethyl)phenol ligands leading to polynuclear complexes, which in the case of a nonadecanuclear mixed-valence manganese cluster can even result in the highest spin ground state ever recorded for a discrete complex, are highlighted in the contribution of Glaser, Powell et al. Atanasov, Comba et al. present their results on cyanometalate-bridged magnetic clusters, which allows them to study the magnetic anisotropy by experimental and theoretical means. The synthesis, as well as the structural and magnetic characterization of gigantic polyoxo-tungstate and -molybdate complexes which contain additionally paramagnetic d- or f-block metal ions, are reviewed by Kortz, A. Müller, van Slageren, Schnack, Dalai and Dressel in their contribution. In their review, Sessoli and Powell outline their synthetic efforts to obtain new single molecule magnets based on complexes containing lanthanide ions alone or in combination with first-row transition metal ions. In the last review of this section, Train, Baumgarten et al. examine closely the prospects that pure organic radicals as well as coordination complexes of these organic radicals might render in building molecule-based magnetic materials.

The second group of reviews focuses primarily on the application of specific physical methods in studying magnetic molecules. In two reviews, the combination of temperature-dependent magnetic susceptibility, magnetic field-dependent magnetization and MCD spectroscopic measurements is portrayed as being a powerful tool in extracting important electronic parameters, such as the zero-field splitting or the exchange coupling constants. While Neese, Bill, Chaudhuri et al. illustrate in their report the applicability of these methods on weakly exchange-coupled dinuclear metal complexes, Haase et al. summarize their results of an investigation on several high-spin cobalt(II) complexes. Kaupp and Köhler demonstrate in their review the advantages that the combination of NMR spectroscopic and theoretical methods can offer in the analysis of spin density distributions within magnetic molecules. P. Müller et al.

present their results of STM spectroscopic investigations of various magnetic molecules, which allow them to map isolated single magnetic molecules as well as functional units within a supramolecular entity.

Five reviews present new results in the research field of spin crossover complexes. Thus, in two contributions (Gütlich et al. and Kurth, Pietsch, Haase et al.) the synergetic effects between spin crossover and the phase transition of liquid crystals are illustrated. Trautwein, Schünemann et al. give an overview on new developments in studying the spin crossover phenomenon by experimental and theoretical methods. In the report by Weber, crystal-engineering-type strategies are presented showing how cooperativity can be increased between spin crossover units in the solid state in a planned way by utilizing appropriate mononuclear building blocks as starting material. Krüger provides an overview on spin crossover complexes with various octahedral metal ions containing tetraazamacrocyclic ligands.

The priority programme “Molecular Magnetism” was entrusted to the care of Dr. Karlheinz Schmidt, the representative of the *Deutsche Forschungsgemeinschaft* who was responsible for overseeing this priority programme as well as for consulting and advising me and other members in all kinds of administrative or organisational problems and questions. Unfortunately and regrettably Dr. Schmidt died of cancer on March 4, 2008.

Dr. Schmidt (born in 1945 in Witten) studied chemistry in Göttingen, receiving his doctorate there in 1973 with a dissertation in inorganic chemistry under the supervision of Prof. Dr. Achim Müller. After joining the Head Office of the *Deutsche Forschungsgemeinschaft* in Bonn in 1976, he served in several positions within the DFG; he was in charge of overseeing the research funding and research programs in the fields of inorganic, analytical, applied and macromolecular chemistry for many years. Then, in 2001 he became the Head of the Chemistry and Process Engineering Divi-

sion. In this position he was engaged in initiating a pan-European research funding network in chemistry. In 2004 he also took over responsibility for coordination of the European ERA Chemistry Network. His outstanding achievements in promoting European cooperation in research were acknowledged in 2005 when he was awarded the Carl-Duisberg-Medal of the German Chemical Society.

Many German researchers, not only in the field of chemistry, grieve for Dr. Schmidt. Many of us are indebted to him for his invaluable advice in obtaining research funding from the DFG and, thereby, for his help in establishing our own careers. We have lost more than an officer of the DFG, we have lost a valued mentor in science and a dear friend. The members of this research priority programme would like to thank him for all the help and support that he gave us over the years and have therefore decided to dedicate this final report to his memory.

Finally, in the name of all members of the priority programme, I would like to thank the *Deutsche Forschungsgemeinschaft* for its financial support; and I wish you, dear reader, a pleasant time reading this special issue of CCR.

Coordinator of the priority programme

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