Mössbauer Spectroscopy and Transition Metal Chemistry

In modern coordination chemistry, the development of new compounds with well-defined properties, functions, and reactivities depends on the knowledge of the interplay between molecular structure and electronic structure. For determining the electronic structure of transition metal complexes, a repertoire of mostly complementary methods is available. These include magnetic properties, EPR, NMR, MCD, vibrational, and photoelectron spectroscopies, and absorption spectroscopy methods using different wavelengths, from the UV/Vis/NIR region for the excitation of valence electrons to X-rays for the excitation of core electrons. Mössbauer spectroscopy provides additional deep insights into the electronic structure of transition metal ions with special nuclear properties. Based on the special properties of the ^{57}Fe nucleus, ^{57}Fe Mössbauer spectroscopy has been applied in the last two decades for the elucidation of the electronic structures in molecular materials and in bio-inorganic chemistry, starting from model compounds and extending to the study of biomolecules. These developments have inspired Philipp Gütlich and Alfred X. Trautwein, now together with Eckhard Bill, to write a revised version of their classic work *Mössbauer Spectroscopy and Transition Metal Chemistry*, which was published in 1978. This is not simply a reprint of the old book, but a completely revised and extended version, as is evident not only in the doubling of the number of pages, but also in the inclusion of developments during the last two decades, especially the wide variety of applications of Mössbauer spectroscopy.

After an introduction to the basic principles of recoil-less nuclear resonance absorption of gamma radiation (Mössbauer spectroscopy), the book presents a more comprehensive overview of the experimental details, which is of particular value for users of the technique. As well as describing the basic arrangement of a Mössbauer spectrometer with standard components, the authors discuss new developments (e.g., in the area of detectors), which are partly based on experience gained from the construction of a Mössbauer spectrometer (MIMOS II) that was specially developed for landings on Mars.

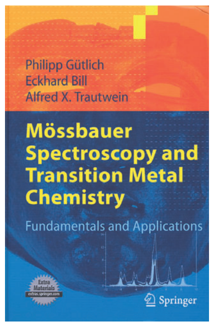
The next chapter describes the three main hyperfine interactions, which yield the classical observables in Mössbauer spectroscopy: isomer shift, quadrupole splitting, and magnetic splitting. Following this description and interpretation based on classical models, Frank Neese and Taras Petrenko provide a chapter on the methodology and the success of quantum-chemical calculations of Mössbauer parameters. In this chapter, the authors have succeeded in providing, besides the theoretical foundations, a deeper understanding for the interpretation of isomer shifts and quadrupole splittings as experimental parameters for the description of metal-ligand bonding in the framework of MO theory.

In another new chapter, Steen Mørup describes magnetic relaxation phenomena in Mössbauer spectra. As well as discussing the relaxation mechanisms and their effects on Mössbauer spectra, he describes an application to superparamagnetic samples. If the chapter had covered not only magnetic nanoparticles but also their molecular analogs, namely single-molecule magnets, it would have been of particular benefit for transition metal chemists.

Besides ^{57}Fe, nuclei of some other transition metals are also suitable for Mössbauer spectroscopy. Chapter 7 provides an overview of the basics, the problems, and the applications of using different transition metals for Mössbauer spectroscopy. This summary leads to the conclusion that ^{57}Fe is the nucleus that is best suited for routine measurements because of its outstanding properties, which is evidenced by the fact that ^{57}Fe Mössbauer spectroscopy is by far the most widely used version of the technique.

Although the chapter "Some special applications" already existed in the first edition of this book, the content in this new edition has completely changed. Whereas applications in solid-state chemistry were the focus in the first edition, in this new one three main fields of application are presented, which correspond to the research interests of the authors during the last 20 years. The first two sections are on spin-crossover and on compounds with unusual spin states and formal oxidation states. The third section deals with the application of the Mössbauer spectrometer MIMOS II, which has been especially developed with backscattering measurement geometry for missions on Mars. Besides the details of these Mars expeditions, some results of the measurements are presented. In particular, it has been possible to identify some iron-containing minerals on Mars that could only have been formed with an abundance of water.

The last chapter gives an overview of Mössbauer spectroscopy using synchrotron radiation, which is a rapidly developing area. The method of nuclear resonance forward scattering yields Mössbauer spectra in the time domain, whereas nuclear inelastic scattering is based on the simultaneous excitation of Mössbauer absorptions and vibrations, which allows one to determine element-



Mössbauer Spectroscopy and Transition Metal Chemistry
Fundamentals and Applications. Edited by Philipp Gütlich, Eckhard Bill and Alfred X. Trautwein.
Springer, Berlin 2011. 620 S., hardcover, € 203.25.—ISBN 978-3540884279

specific vibrational modes involving the Mössbauer nuclei. It would have been useful to coordinate this chapter with the part on nuclear inelastic scattering by Frank Neese and Taras Petrenko.

In summary, the book by Gütlich, Bill, and Trautwein is an excellent combination of basics, methodologies, and applications of Mössbauer spectroscopy in transition metal chemistry. This book is not only strongly recommended for everyone who uses Mössbauer spectroscopy, but will also be of great benefit for coordination chemists, as it deals with the electronic structure of transition metal complexes. As a special bonus, the book is accompanied by a CD-ROM with a selection of examples of applications of Mössbauer spectroscopy by several work groups, and some compilations on theoretical methods. A special highlight is a Powerpoint presentation (286 transparencies) of a lecture series on Mössbauer spectroscopy by Philipp Gütlich, which is especially well-suited for teaching purposes.

Thorsten Glaser
Lehrstuhl für Anorganische Chemie I
Universität Bielefeld (Germany)

DOI: 10.1002/anie.201104962