Molecular Cluster Magnets

In April 2012, Jeffrey Mervis wrote in *Science* that about 1.2 zettabytes (1.2×10^{21} bytes) of electronic data are generated every year by humans.[1] The world is going to face critical problems to store this enormous amount of data that increases inexorably. This is why nowadays a considerable amount of international research activity is orientated towards the synthesis of nanometer-scale magnetic systems, with the long-term goal to reduce the size of the magnetic units that code information in storage devices. Different approaches have been used to obtain single-domain magnetic particles, but the beginning of the 1990s marked the discovery of single-molecule magnets (SMMs), which raised the hope that information might be stored in a single molecule. In the 20 years since then, numerous SMMs and related molecule-based magnets have been discovered, and a broad research community is currently working on new systems with improved magnetic characteristics. In 2006, Dante Gatteschi, Roberta Sessoli, and Jacques Villain published *Molecular Nanomagnets* (Oxford University Press), the first book describing the chemistry as well as the physics of these nanomagnets.

The book *Molecular Cluster Magnets* is not intended to be a new comprehensive text on the subject—instead the editor, Richard Winpenny, has assembled recent contributions and reviews from leading experts, to supplement and update the contents of the reference book by Dante Gatteschi and co-authors. The book is divided into six independent chapters covering new aspects of the chemistry (first two chapters) and physics of molecular magnets.

The first chapter, by Laurence K. Thompson and co-authors, is devoted to "Supramolecular 2D [$n \times n$] Transition-metal Grids". All the aspects of the synthetic strategy to design molecular grids are discussed, from the convergent self-assembly of the metal ions and engineered ligands to the thermodynamic parameters that must be considered in such rationalized chemistry. The authors review in great detail magnetic complexes of this type, ranging from simple [2×2] grids up to an amazing [5×5] example that can be observed even on a surface, as shown by the astonishing Figure 32. The authors finish their chapter with an interesting discussion about the possible use of such molecular grids in future nanoscale devices for quantum computing.

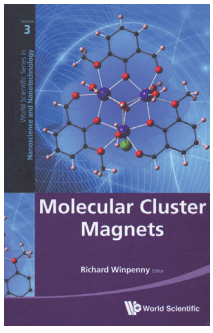
The second chapter, by Guillem Aromi, Eric McInnes, and Richard Winpenny, reviews "Recent Synthetic Results Involving Single-Molecule Magnets" from 2005 to 2008, and follows an earlier review by Guillem Aromi and Euan Brechin,[2] which summarized progress before 2005. The enormous amount of literature on SMMs is summarized in a very elegant way, briefly introducing important theoretical aspects and then describing successively new Mn-, Fe-, Ni-, and Co-based SMMs and related systems. A large part of this chapter is also devoted to the very active area of molecular magnets involving 4f elements, including heterometallic 3d–4f systems.

The second part of the book is orientated towards the physics, theory, and important techniques in the field of molecular magnets. Boris Tsukerblat and Alex Tarantul review in 70 pages the wonderful world of the V_{15} complex. Everything you have always wanted to know about this unique complex is "summarized" in this chapter: molecular structure, spin and interaction topology, and the questions of magnetic frustration, anisotropy, antisymmetric exchange, etc. Experimental results obtained by EPR, NMR, INS magnetization measurements, muon scattering experiments, and Rabi oscillation are also described, always in combination with deep theoretical discussion.

In Chapter 4, Tatiana Guidi explains in a very didactic and pedagogic way how neutron spectroscopy can be used to study the physical characteristics of molecular magnetic systems. Starting from basic theoretical and technical information, the author illustrates with well-chosen examples the advantages of neutron spectroscopy for investigating exchange interactions, energy spectra, magnetic anisotropy, spin dynamics, and quantum coherence in molecular nanomagnets.

Chapter 5, by Eric J. L. McInnes, deals with "Recent Developments in EPR Spectroscopy of Molecular Nanomagnets", including a nice overview of the modeling of EPR (electron paramagnetic resonance) beyond the macro-spin approximation, experimental studies of pairs of molecular complexes, and how pulsed EPR can be used to study spin dynamics and coherence. This review is well provided with literature references, and the many relevant papers and reviews cited in the introduction will be especially useful for newcomers to the field.

The last chapter is devoted to "Simulating Computationally Complex Magnetic Molecules". Starting from the Heisenberg model, Larry Engelhardt and Christian Schröder describe the "arsenal" of theory that is available to simulate the properties of magnetic complexes. Quantum Monte-Carlo and classical spin dynamics methods are explained, together with their limitations and advantages compared with the matrix diagonalization technique. Selected magnetic complexes and their experimental properties are used to illustrate the appropriate ways of applying each approach.



Molecular Cluster Magnets
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The late F. A. Cotton would certainly not have appreciated the title of this book, and in particular the use of the word "cluster" to describe simple coordination complexes without metal–metal bonds. This is probably the only criticism that could be made about this book: Richard Winpenny could have found a better title! However, if one does not like the title of the book, that is certainly not a reason to dislike its contents. This new book succeeds in its aim to be a complementary volume to the *Molecular Nanomagnets* textbook by Dante Gatteschi, Roberta Sessoli, and Jacques Villain. Master and PhD students, as well as researchers in the field of molecule-based magnetism, will be delighted to read this book and to use it as a reference source in their research work and future papers.

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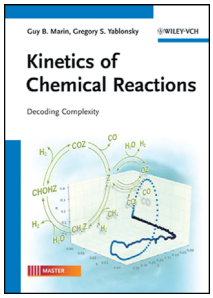
[1] J. Mervis, *Science* **2012**, *336*, 22.
[2] G. Aromi, E. K. Brechin, *Structure and Bonding* **2006**, *122*, 1–67.



Kinetics of Chemical Reactions
Decoding Complexity. By Guy Marin and Gregory S. Yablonsky. Wiley-VCH, Weinheim, 2011. 428 pp., hardcover, € 79.00.—ISBN 978-3527317639

Kinetics of Chemical Reactions

This book was written by two authors from different schools: Prof. Marin was educated in the tradition of the thermodynamics and kinetics school of the Low Countries as well as that of the American school (Prof. Boudart). On the other hand, Gregory Yablonsky had his training in the Soviet-Russian catalysis school (Profs. Mikhail Slin'ko and Georgij Boreskov). He was also a prominent member of the Russian chemico-mathematical team that included Alexander Gorban, Valerij Bykov, Vladimir Elokhin, and Mark Lazman. The different backgrounds of the authors are reflected in the book. Another welcome aspect is that the book also includes many results from Soviet science, which are not widely known.

The book is divided into 12 chapters. The first chapter describes the approach adopted. Three types of chemical kinetics are covered: applied kinetics, detailed kinetics, and mathematical kinetics. The goal of applied kinetics is to obtain kinetic relationships for the design of efficient catalytic processes and reactors. The study of detailed kinetics is aimed at reconstructing the detailed mechanism of a reaction, based on kinetic and non-kinetic (adsorption, desorption, spectrometric) data. Quantum-chemical methods are not taken into account. Mathematical kinetics deals with the analysis of various mathematical, mostly deterministic, models that are used in chemical kinetics. The book focuses on the correspondence between observed kinetic behavior and "hidden" detailed mechanisms, and presents it as the main problem of chemical kinetics. The chapter ends with a short review of the history of kinetics.

The second chapter introduces fundamental definitions of concepts such as elementary reactions and homogeneous expressions, and explains the difference between the reaction rate and the net rate of formation of a product. A reference to the *IUPAC Gold Book* is given.

The third chapter presents material and heat balances for the standard types of chemical reactors, followed by an analysis of some important types of reaction schemes taking place in those reactors. In particular, the ability to distinguish between parallel and consecutive reactions based on kinetic fingerprints is discussed. A subsection is devoted to the question of whether it is possible to extract the values of the rate of chemical transformation without any assumptions about the kinetic model. The chapter ends with complex diagnostics of kinetic experiments in heterogeneous catalysis.

Linear algebraic methods in chemical kinetics are discussed in the fourth chapter, which presents three main matrices for describing complex chemical transformations: the molecular and stoichiometric ones, and a matrix of Horiuti numbers. Some mathematical methods of linear algebra, for example the solution of systems of linear equations, are discussed. The approaches are then used for finding key components and key reactions, and other techniques of stoichiometry such as the use of Horiuti numbers are described.

Graph theory as a tool for easily solving mathematical theoretical problems of chemical kinetics are introduced in Chapter 5. Complex reaction networks can be represented by a method that is an advanced modification of already known graphical methods (King–Altman, Volkenshtein–Gol'dshtein, and Horiuti–Temkin), with a focus on "kinetics–mechanism" relationships. Some very useful examples showing how to find the reaction rate for a complex mechanism are presented. The famous Horiuti–Boreskov problem of how to find the rate equation for the reverse reaction, when one knows the expression for the forward reaction and the equilibrium coefficient of the overall reaction, is explained and solved in the general case for linear mechanisms.

The so-called "gray-box" approach for revealing complex reaction mechanisms is introduced in

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