

1. Record Nr.	UNINA9910790974603321
Autore	Datta Sambhu N
Titolo	Theoretical and computational aspects of magnetic organic molecules / / Sambhu N. Datta, Indian Institute of Technology, Bombay, India, Carl O. Trindle, University of Virginia, USA, Francesc Illas, Universitat de Barcelona, Spain
Pubbl/distr/stampa	London : , : Imperial College Press, , [2014] 2014
ISBN	1-908977-22-1
Descrizione fisica	1 online resource (x, 335 pages) : illustrations (some color)
Collana	Gale eBooks
Disciplina	541/.378
Soggetti	Magnetochemistry Molecular orbitals Molecules - Magnetic properties
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Introduction to magnetism -- Organic molecules, radicals, and spin states -- Theoretical methodologies -- Molecular orbital description of magnetic organic systems -- Qualitative methods for predicting molecular spin states -- Quantum chemical calculations: structural trends -- Strongly coupled magnetic molecules -- Photomagnetic effects -- Transition metal complexes -- Computational studies of inorganic clusters and solid -- Systems -- A look ahead.
Sommario/riassunto	Organic materials with extraordinary magnetic properties promise a wide range of light, flexible, and inexpensive alternatives to familiar metal-based magnets. Individual organic molecules with high magnetic moments will be the foundation for design and fabrication of these materials. This book provides a systematic understanding of the structure and properties of organic magnetic molecules. After a summary of the phenomenon of magnetism at the molecular level, it presents a survey of the challenges to theoretical description and evaluation of the magnetic character of open-shell molecules, an