

Low symmetry aspects in electron magnetic resonance (EMR) and optical spectroscopy of coordination compounds of transition ions: Crucial notions and issues, literature survey and database

Autorzy

Czesław Rudowicz

Muhammed Açıkgöz

Mirosław Karbowiak

Rok wydania

2024

Czasopismo

Coordination Chemistry
Reviews

Numer woluminu

512

Strony

215865/1-215865/43

DOI

10.1016/j.ccr.2024.215865

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

EMR and optical spectroscopy are important techniques enabling characterization of transition 3d/4f ions in coordination compounds, which often exhibit low symmetry sites. Low symmetry aspects are largely unexplored as yet due to lack of consistent methodology and guidelines, which has often led to their neglect or employing orthorhombic or higher symmetry approximations. To alleviate these problems, we provide comprehensive elucidation of low symmetry aspects in EMR, which are also relevant, to a great extent, for optical spectroscopy. Based on extensive survey of EMR-related monographs, reviews, selected papers and computer programs, definitions of the crucial notions underlying EMR studies of 3d/4f ions at low symmetry sites are systematized and their interrelationships clarified. Peculiar issues at the interface between theory, computations, and experiment, which affect proper interpretation of EMR data for low site symmetry systems, are discussed. Outline of the shortcomings, which may lead to employing deficient procedures in analysis of EMR data, is provided to help avoiding such deficiencies. To ensure comprehensive and up-to-date coverage, the survey of reviews and selected papers is supplemented by database of EMR studies of low site symmetry systems listing source references provided in Supplementary Materials. This review provides grounds for specialized reviews of low symmetry aspects occurring in: (i) studies of molecular nanomagnets containing transition ions, and (ii) density functional theory/ab initio modeling of zero-field splitting and crystal-field parameters.

Słowa kluczowe

Electron magnetic resonance (EMR), spectroscopy, Optical spectroscopy, Low symmetry aspects, Zero-field splitting parameters, Crystal field parameters, Transition ions

Adres publiczny

<http://dx.doi.org/10.1016/j.ccr.2024.215865>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-10-07 07:24:11

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/qqZdniE>.