Synthesis, XRD, EMR, magnetic, and optical studies of trigonal and triclinic dinuclear MNM-analogous Gd^{3+} complexes

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Rok wydania

2025

Czasopismo

Journal of Magnetism and Magnetic Materials

Numer woluminu

628

Strony

173184/1-173184/10

DOI

10.1016/j.jmmm.2025.173184

Kolekcja

Naukowa

Streszczenie

Two structurally similar dinuclear Gd^{3+} complexes are newly synthesized as potential molecular nanomagnets (MNMs): $[Gd_2(\mathbf{L^1})_3](NO_3)_3$ (**1** symmetric) and $[Gd_2(\mathbf{L^2})_3(NO_3)_3]$ (**2** dissymmetric). Characterization by variety of experimental techniques: XRD, EMR, magnetic measurements, and optical spectroscopy was carried out. The EMR and magnetic measurements reveal that the two Gd^{3+} complexes show very weak exchange interactions. Hence these complexes can be classified as the MNM-analogous complexes. The zero-field splitting (ZFS) parameters bkq were fitted from EMR spectra using the forms of the zero-field splitting Hamiltonian (H_{ZFS}) suitable for Gd^{3+} ions at various symmetry sites. This enabled exposing the role of site symmetry for proper interpretation of spectroscopic and magnetic properties of these Gd^{3+} complexes. Several fitting schemes were employed to investigate the relative importance of each *k*-rank bkq′s for Gd^{3+} ions. The distinction between *actual* (low/high) site symmetry and *apparent* (lower/higher) site symmetry was introduced. Since for triclinic site symmetry (complex **2**), infinite number of physically equivalent ZFSP sets exist, to assess equivalence of independently obtained sets, we utilize the invariant quantities and standardization. Our findings clearly demonstrate the importance of the low and high symmetry aspects in EMR studies. This paper prepares grounds for an in-depth study of the symmetry aspects inherent in the modelled ZFSP sets for the two complexes. These aspects are not well recognized as yet and thus are frequently overlooked in literature. Their elucidation is crucial since improper treatment of the low and high symmetry aspects may potentially lead to erroneous interpretations of compounds' properties.

Język

Angielski

Typ publikacji

Artykuł

Słowa kluczowe

EMR/EPR, XRD, Magnetic measurements, Zero-field splitting, Dinuclear Gd3+ complexes, Molecular nanomagnets, Symmetry aspects

Adres publiczny

http://dx.doi.org/10.1016/j.jmmm.2025.173184

Strona internetowa wydawcy

http://www.elsevier.com