Spectroscopic and magnetic studies of erbium(III)-TEMPO complex as a potential single-molecule magnet : interplay of the crystal-field and exchange coupling effects.

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2016

Czasopismo

Chemical Physics Letters

Numer woluminu

662

Strony

163-168

DOI

10.1016/j.cplett.2016.09.033

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Crystallographic, spectroscopic, and magnetic studies of three-center systems: lanthanoid-Ln^{3+} ions doubly-coordinated by TEMPO (2,2,6,6-tetramethylpiperidin-1-oxyl) radicals [Ln-$TEMPO_2$] are reported. The temperature dependence of alternating-current magnetic susceptibility indicates the single-molecule-magnet behavior of Er-$TEMPO_2$, exhibiting relatively slow magnetization relaxation. Well-resolved absorption spectra were obtained only for Er-$TEMPO_2$. Other samples yielded spectra not amenable for meaningful interpretation. The crystal-field parameters (CFPs) determined from the measured Er^{3+}-energy levels served as starting CFPs for fitting the direct-current magnetic susceptibility result. Compatibility of the so-determined and fine-tuned CFPs, and interplay between crystal-field-related effects and exchange-coupling effects are considered. Exchange couplings in Ln-$TEMPO_2$ appear antiferromagnetic and unexpectedly large.

Słowa kluczowe

single-molecule magnets, Spectroscopic properties, magnetic susceptibility, absorption spectra, Crystal-field parameters, Exchange coupling constants, Ln-TEMPO complexes

Adres publiczny

http://dx.doi.org/10.1016/j.cplett.2016.09.033

Strona internetowa wydawcy

http://www.elsevier.com