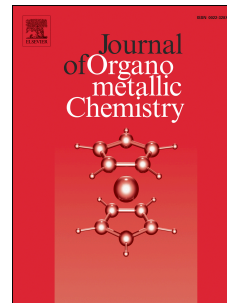


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# Slow Magnetic Relaxation in a Neodymium Metallocene Tetraphenylborate Complex

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## Abstract

Lanthanide-based single-molecule magnet research has historically focused on molecules of the highly anisotropic Dy<sup>3+</sup> and Tb<sup>3+</sup> ions, while studies on the lighter, more abundant lanthanides are still relatively scarce. Recent advances with Dy<sup>3+</sup> metallocene complexes in particular have led to some truly exceptional systems and the highest relaxation barrier to date, in excess of 1200 cm<sup>-1</sup>. Even still, the design and understanding of systems incorporating the earlier lanthanides is arguably of great importance if the field is to shift in the direction of identifying systems for practical application. Herein, we present magnetic characterization of the mononuclear metallocene complex Cp\*<sub>2</sub>Nd(BPh<sub>4</sub>) (Cp\* = pentamethylcyclopentadienyl anion), which exhibits slow magnetic relaxation with a relaxation barrier of  $U_{\text{eff}} = 29(1) \text{ cm}^{-1}$  in the presence of a small dc magnetic field, illustrating that the metallocene ligand framework can also be utilized in the design of single-molecule magnets of the earlier lanthanides. We also discuss dynamic magnetic susceptibility data for the Cp\*<sub>2</sub>Ho(BPh<sub>4</sub>) and Cp\*<sub>2</sub>Er(BPh<sub>4</sub>) congeners, which reveal that this particular ligand field is best suited to lanthanides ions exhibiting an oblate 4f electron density.

## 1. Introduction

The discovery of slow magnetic relaxation in the mononuclear lanthanide complexes [LnPc<sub>2</sub>]<sup>-</sup> (Ln = Tb<sup>3+</sup>, Dy<sup>3+</sup>; Pc<sup>2-</sup> = phthalocyanine dianion) signified a turning point in the field of molecular magnetism [1]. Indeed, prior to the discovery of the dynamic magnetic properties of these complexes, spin-coupled transition metal cluster compounds represented the primary focus of molecular magnetism research, following the initial discovery of slow magnetic relaxation for Mn<sub>12</sub>O<sub>12</sub>(O<sub>2</sub>CMe)<sub>16</sub>(H<sub>2</sub>O)<sub>4</sub> [2, 3]. Although the lanthanides were certainly recognized at this time for their large moments arising from the degeneracy of the 4f orbitals, their potential for building high spin clusters via superexchange is generally limited because of this characteristic. The research landscape became rich for new investigations when Ishikawa and coworkers made the seminal observation that the splitting of the Tb<sup>3+</sup> and Dy<sup>3+</sup> spin-orbit coupled  $J$  ground states in the bis(phthalocyanine) dianion ligand field could generate large  $M_J$  level separations on the order of several hundred wavenumbers, similar to or greater than the splitting of the  $M_S$  manifold

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