

Control of magnetic anisotropy by macrocyclic ligand distortion in a family of Dy-III and Er-III single molecule magnets

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Abstract

A family of hexaazamacrocyclic lanthanide complexes, $[\text{Ln}(\text{L}-n)(\text{NCS})(3)]$ ($\text{Ln}(\text{III}) = \text{Dy}, \text{Er}; n = 1-3$) has been synthesized and characterized by single-crystal X-ray diffraction, magnetic measurements and ab initio calculations. Macrocyclic ligands (L-n) differ in the lateral spacers, which are aliphatic chains with two and three carbons (for L-n, $n = 1$ and 2 , respectively), and an aromatic ring for $L-n = 3$. Modification of the macrocycle spacer tunes planarity and rigidity of the equatorial coordination for both oblate (Dy) and prolate (Er) lanthanide ions. Ac-susceptibility studies showed that four of the six complexes are field induced single molecule magnets (SMMs). Trends in magnetic relaxation properties are rationalized with the aid of ab initio multireference calculations, highlighting the combined influence of macrocycle planarity, lanthanide electronic density distribution and intermolecular interactions for the achievement of slow demagnetization.

Keywords

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