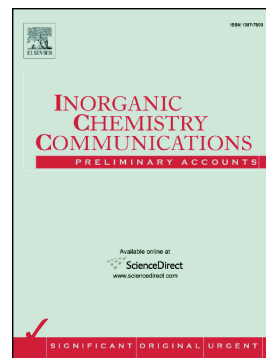


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Fine-tuning of the molecular structures and magnetic anisotropy analysis of two mononuclear dysprosium–sulfur complexes

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ABSTRACT: Two mononuclear sulfur-based dysprosium complexes [(dte)₃Dy(bipy)] (**1Dy**, dte⁻ = diethyldithiocarbamate anion, bipy = 2,2'-bipyridine) and [(dte)₃Dy(dmbipy)]·0.68CH₃CN (**2Dy**, dmbipy = 4,4'-dimethyl-2,2'-bipyridine) were successfully synthesized and structurally characterized by X-ray diffraction. The Dy^{III} centers of **1Dy** and **2Dy** are eight-coordinated by six S atoms from three dte⁻ ligands and two N atoms from bipy (**1Dy**) or dmbipy (**2Dy**). Magnetic measurements reveal that the magnetic properties of **2Dy** are obviously better than those of **1Dy**. Theoretical calculations based on the molecular crystal structures are performed to analyze the difference of the magnetic behavior in two complexes.

Keywords: dysprosium-sulfur complexes; magnetic properties; magnetic anisotropy; ligand modifications

Lanthanide-based single-ion magnets (Ln-SIMs) have been a hot research topic in the field of molecular magnetism.[1] Ln-SIM is the type of the molecule which contains only one paramagnetic lanthanide ion and can produce the magnetic memory effect below certain temperature. Dysprosium-based SIMs with ligated atoms such as C[2, 3], N[4, 5], O[6, 7], S[8, 9] and halogen[10, 11] dominate in the reported Ln-SIMs owing to the anisotropic characteristic of the Kramers ion Dy^{III}[12-15]. Higher blocking temperature and energy barrier are pursued under the theoretical guidance that a strong crystal field in one direction and/or high molecular symmetry is favorable for Dy^{III} ion. [12-15] In our previous work, we have successfully synthesized a S-ligated Dy-SIM [(dbm)₂Dy(dte)(phen)] (dbm⁻ = dibenzoylmethanoate anion, phen = phenanthroline) by replacing two dte⁻ ligands with two dbm⁻ ligands to gain a strong axial ligand field based on a S-ligated field-induced Dy-SIM [(dte)₃Dy(phen)].[9] We also noticed that the crystal field constructed by dte⁻ ligands is weak in [(dte)₃Dy(phen)] and the bond length of Dy-S is longer than that of Dy-N[9], which inspires us to investigate the effect of ancillary ligands on the magnetic properties in the [(dte)₃Dy(L)] type molecules. Therefore, we chose 2,2'-bipyridine (bipy) and bipy with two electron-donating methyl groups 4,4'-dimethyl-2,2'-bipyridyl (dmbipy) as the ancillary ligands and successfully synthesized two complexes [(dte)₃Dy(bipy)] (**1Dy**) and [(dte)₃Dy(dmbipy)]·0.68CH₃CN (**2Dy**). Magnetic measurements and theoretical calculations were performed to study their magnetic properties and magnetic anisotropy.

All reactions were carried out under atmospheric conditions. Detailed syntheses procedures are described in the supporting information. **1Dy** and **2Dy** crystallize in monoclinic $P2_1/c$ space group and orthorhombic $Pbca$ space group respectively. As shown in Fig. 1, **1Dy** consists of one central ion - Dy^{III}, three dte⁻ ligands each of which is bonded to Dy^{III} via two sulfur atoms, and one bipy ligand bonded to Dy^{III} via two nitrogen atoms. The structure of **2Dy** is similar with **1Dy** except that the bipy ligand is replaced by a dmbipy ligand. SHAPE software[16] was applied in the analyses of the local geometry of two complexes with the values being 1.873 (triangular dodecahedron D_{2d} , **1Dy**) and 3.564 (biaugmented trigonal prism C_{2v} , **2Dy**). The shortest distance between adjacent Dy^{III} ions of **1Dy** and **2Dy** are 9.5253(2) Å, 9.080 Å respectively. Detailed data are shown in Table S1 and S2. The elemental analysis and PXRD data (Fig. S1) were examined to check the purity of the sample.

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