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A Nanosized Heteronuclear {Fe18Tb6} Coordination Wheel Based on Pivalate and Triethanolamine Ligands

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Abstract

Ring-like systems assembled from metal ions and organic ligands attract attention due to variety of their useful properties and aesthetic beauty of their structure. A new nanosized heteronuclear [Fe18Tb6(piv)12 (tea)6(Htea)18(N3)6]·n(solvent) (1) (where Hpiv = pivalic acid) wheel-shaped cluster was synthesized by reacting of oxo-linked trinuclear Fe(III) pivalate precursors and terbium(III) nitrate with triethanolamine (H3tea) and sodium azide in the mixture of ethanol and acetonitrile under ultrasonic irradiation. Cluster 1 was characterized by elemental analysis and IR-spectroscopy. Single-crystal X-ray diffraction analysis shows that 18 iron(III) and 6 terbium(III) ions in 1 define a ring and are linked by 6 bridging pivalate and 24 triethanolamine ligands. Additionally, six pivalates and six azides completed the coordination sphere of the metal atoms in 1. In the resulting wheel core, three iron(III) and one terbium(III) ions generate six repeated {Fe3Tb} sequential fragments along the ring. The outer diameter of the {Fe18Tb6} wheel is ca. 3.5 nm, the inner diameter is ca. 1.0 nm, and the thickness of this molecular wheel is ca. 1.3 nm. In the crystal structure, the packing of bulky wheel-shaped clusters results in the formation of infinite channels fulfil with solvent molecules. Upon removal of solvent molecules this structure reveals a huge total potential solvent accessible volume of ca. 26% per unit cell volume.

Keywords: iron, lanthanides, coordination clusters, X-ray structure

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