

Supplementary information

Multiple-decked Gd(III) Complexes Induced by Hydrogen Bonds Depending on Anions

Kyoung-Tae Youm,^a Hyun Kyung Woo,^a Jaejung Ko,^{*b} and Moo-Jin Jun ^{*a}

^a Department of Chemistry, Yonsei University, Seoul 120-749, Korea. Fax: +82 2 364 7050; Tel: +82 2 2123 2639; E-mail: mjjun@yonsei.ac.kr

^b Departments of Chemistry, Korea University, Chochiwon, Chugnam 339-700, Korea.

1. General procedures

Thermal gravimetric analysis was recorded on a Shimadzu TGA-50H in nitrogen atmosphere. Temperature ranges from 25 °C to 500 °C and is elevated at 10.0 °C / min. The arrangement used to measure magnetic susceptibility by using a Quantum Design/MPMS SQUID (superconducting quantum interface device). SQUID data were collected 5 k from 300 K at 5000 G.

2. Single crystal X-ray analysis.

2-1. {[Gd(btp)(H₂O)₄(NO₃)₂]·2btp·H₂O·MeOH·NO₃} (1)

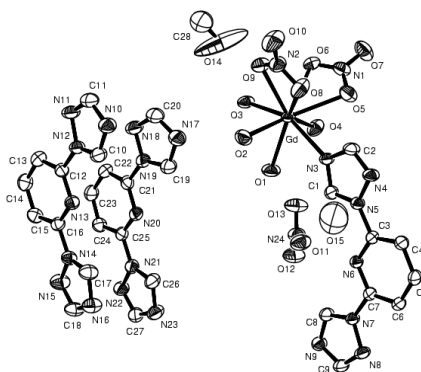


Fig. S1 ORTEP drawing of asymmetric unit of **1**. All the hydrogen atoms are omitted for clarity.

By single X-ray structure analysis represent that the asymmetric unit of complex (**1**) is composed of one Gd ion, five H₂O molecules, one methanol, three nitrate ions and three btp molecules. The coordination number of Gd ion is nine in which two nitrate ions chelate Gd in a η^2 -mode and four H₂O and N atoms from btp bind directly Gd center. The first shell around Gd is arranged in tricapped-trigonal-prismatic architecture.

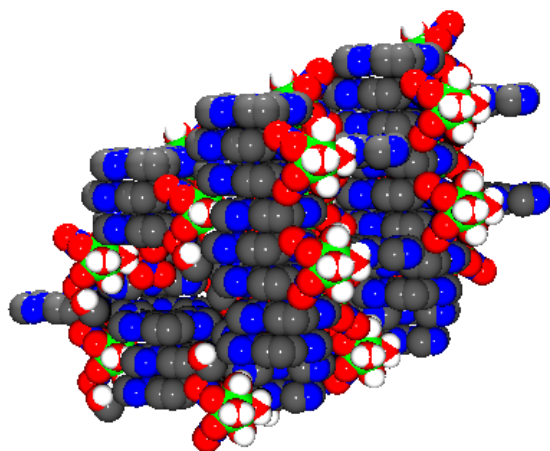


Fig. S2. Space filling diagram presenting π - π stacking pattern of dimeric **1**.

2-2. $\{[\text{Gd}(\text{btp})(\text{H}_2\text{O})_3(\text{MeOH})(\text{NO}_3)_2] \cdot 2\text{btp} \cdot \text{MeOH} \cdot \text{ClO}_4\}$ (**2**)

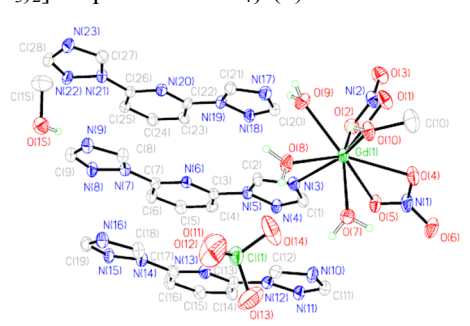


Fig. S3. ORTEP drawing of asymmetric unit of **2**.

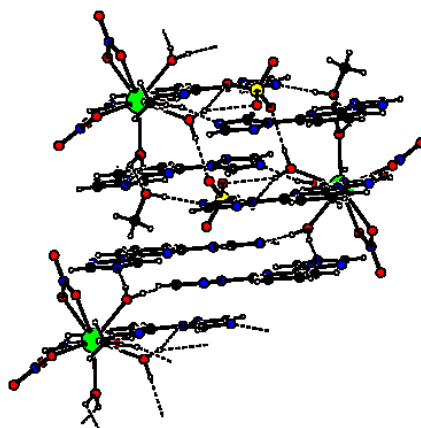


Fig. S4 Hydrogen bond patterns propagating in 1dimensional direction.

3. Magnetic susceptibility study

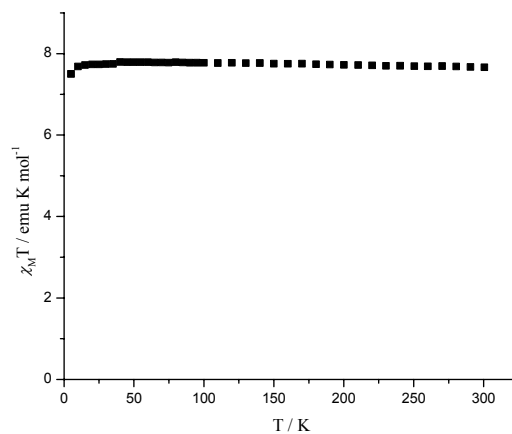


Fig. S5. $X_M T$ vs T curve for **1**

The variable-temperature magnetic susceptibility of **1** in the range 5-300 K reveal that there is no magnetic interaction between Gd(III) centres. The $X_M T$ of 7.83~7.89 emu K mol⁻¹ per Gd(III) of **1** is, within error, identical to the spin-only value of 7.88 emu K mol⁻¹. These data are in agreement with the large separation distances between the neighboring magnetic centres (10.66 Å).