Supporting Information for:

# Sm and Eu(III) Lanthanide Triple Helicate Cages Based on N,N'-Methylene-Bis(Pyridin-4-One)

Yu-Bo Shu, Xiao-Liang Tang and Wei-Sheng Liu\*

Key Laboratory of Nonferrous Metals Chemistry and Resources Utilization of Gansu Province and State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, 730000, China. E-mail: liuws@lzu.edu.cn

## **Table of Contents**

#### **Experimental details**

Fig. S1 IR data of 1

Fig. S2 IR data of 2

Fig. S3 Powder X-ray diffraction pattern of 1

Fig. S4 Powder X-ray diffraction pattern of 2

Fig. S5 Excitation spectra of 1 and 2

Fig. S6 Six sets of  $\pi$ - $\pi$  stacking interactions between one cage and neighboring six units in **1**.

Fig. S7 The interactions of nitrate-nitrate electrostatic repellence in 1.

### **Experimental details**

All reagents were purchased commercially and used without further purification. The ligand N,N'-methylene-bis(4,4'-dihydroxy-bispyridinium)bromide was synthesized according to the literature<sup>S1</sup>. The infrared spectrum was recorded on a Nicolet FT-170SX instrument using KBr discs in the 400–4000 cm<sup>-1</sup> region. Powder X-Ray diffraction (PXRD) patterns were collected with a PANalytical X'Pert Pro Diffractometer operated at 40 kV and 40 mA with Cu *Ka* radiation (step size: 0.0167113°, step time: 10.16 s). Elemental analyses were performed using a Elementar Analysenesysteme GmbH varioEL cube instrument. CD spectra were measured on JASCO J-810, by grinding the crystalline sample with KCl into a pellet (1:200). Fluorescence measurements were made on FLS920 of Edinburgh Instrument and was corrected for instrumental response. Luminescence lifetimes were determined on FLS920 of Edinburgh Instrument, results obtained by fitting with F900 software. Quantum yields were determined by an absolute method using an integrating sphere on FLS920 of Edinburgh Instrument.



Figure S1 IR data of 1.



Figure S2 IR data of 2.



Figure S3 Powder X-ray diffraction pattern of 1.



Figure S4 Powder X-ray diffraction pattern of 2.



Figure S5 Excitation spectra of (a) 1 and (b) 2.



**Figure S6** Six sets of  $\pi$ - $\pi$  stacking interaction between one cage and neighboring six units in **1**.



Figure S7 The interactions of nitrate-nitrate electrostatic repellence in 1.

#### REFERENCES

S1 S. Munavalli, E. J. Poziomek, W. G. Landis, HETEROCYCLES., 1986, 24, 1883.