

## Electronic Supplementary Information

# Fluorescence of a Triple-Stranded Helicate Iron(III) Complex from a Novel Bis- $\beta$ -diketone Ligand: Synthesis, Structure and Spectroscopic Studies

Fang Zou,<sup>a</sup> Xiao Tang,<sup>a</sup> Yuhong Huang,<sup>a</sup> Shigang Wan,<sup>a</sup> Fa Lu,<sup>a</sup> Zhe-Ning Chen,<sup>\*b</sup> Anan Wu<sup>\*a</sup> and Hui Zhang<sup>a</sup>

<sup>a</sup> Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China. E-mail: ananwu@xmu.edu.cn

<sup>b</sup> Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, China. E-mail: zheningchen@gmail.com

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**Table S1.** Selected bond length and angles of complex Fe<sub>2</sub>(BOBA)<sub>3</sub>

Selected bond length(Å)			
Fe(1)-O(1)	Fe(1)-O(2)	Fe(1)-O(3)	Fe(1)-O(4)
2.009(6)	1.996(5)	1.986(6)	1.983(6)
Fe(1)-O(5)	Fe(1)-O(6)	Fe(2)-O(7)	Fe(2)-O(8)
2.005(6)	2.007(5)	1.990(6)	1.988(7)
Fe(2)-O(9)	Fe(2)-O(10)	Fe(2)-O(11)	Fe(2)-O(12)
2.003(5)	2.008(6)	1.965(6)	1.999(6)

Selected Angles (deg)			
O(4)-Fe(1)-O(3)	86.4(2)	O(4)-Fe(1)-O(2)	87.3(2)
O(3)-Fe(1)-O(2)	103.2(2)	O(4)-Fe(1)-O(5)	99.5(3)
O(3)-Fe(1)-O(5)	86.4(3)	O(2)-Fe(1)-O(5)	168.6(3)
O(4)-Fe(1)-O(6)	86.9(3)	O(3)-Fe(1)-O(6)	168.6(2)
O(2)-Fe(1)-O(6)	85.7(2)	O(5)-Fe(1)-O(6)	85.6(2)
O(4)-Fe(1)-O(1)	171.6(2)	O(3)-Fe(1)-O(1)	90.2(2)
O(2)-Fe(1)-O(1)	86.1(2)	O(5)-Fe(1)-O(1)	87.9(2)
O(6)-Fe(1)-O(1)	97.7(3)	O(11)-Fe(2)-O(7)	86.8(2)
O(11)-Fe(2)-O(12)	86.0(2)	O(7)-Fe(2)-O(12)	98.5(2)
O(11)-Fe(2)-O(9)	87.4(2)	O(7)-Fe(2)-O(9)	85.0(2)
O(12)-Fe(2)-O(9)	172.4(3)	O(11)-Fe(2)-O(8)	170.8(3)
O(7)-Fe(2)-O(8)	86.9(3)	O(12)-Fe(2)-O(8)	88.3(3)
O(9)-Fe(2)-O(8)	98.7(3)	O(11)-Fe(2)-O(10)	99.8(3)
O(7)-Fe(2)-O(10)	168.7(3)	O(12)-Fe(2)-O(10)	91.2(2)
O(9)-Fe(2)-O(10)	86.2(2)	O(8)-Fe(2)-O(10)	87.4(3)

**Table S2.** Selected bond length and angles of complex Cd(BOBA)<sub>2</sub>(py)<sub>3</sub>

Selected bond length(Å)			
Cd(1)-O(2)	Cd(1)-N(1)	Cd(1)-O(4)	Cd(1)-N(3)
2.312(5)	2.342(6)	2.346(5)	2.351(6)
Cd(1)-N(2)	Cd(1)-O(3)	Cd(1)-O(1)	
2.382(6)	2.498(5)	2.596(6)	

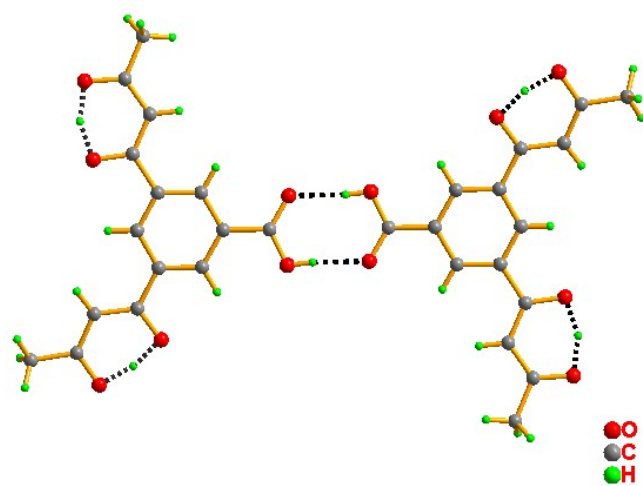
Selected Angles (deg)			
O(2)-Cd(1)-N(1)	134.5(2)	O(2)-Cd(1)-O(4)	88.2(2)
N(1)-Cd(1)-O(4)	136.9(2)	O(2)-Cd(1)-N(3)	91.2(2)
N(1)-Cd(1)-N(3)	89.2(2)	O(4)-Cd(1)-N(3)	96.5(2)
O(2)-Cd(1)-N(2)	89.9(2)	N(1)-Cd(1)-N(2)	85.7(2)
O(4)-Cd(1)-N(2)	89.6(2)	N(3)-Cd(1)-N(2)	173.8(2)
O(2)-Cd(1)-O(3)	141.5(2)	N(1)-Cd(1)-O(3)	83.9(2)
O(4)-Cd(1)-O(3)	53.30(19)	N(3)-Cd(1)-O(3)	93.0(2)
N(2)-Cd(1)-O(3)	89.9(2)	O(2)-Cd(1)-O(1)	52.52(19)
N(1)-Cd(1)-O(1)	82.3(2)	O(4)-Cd(1)-O(1)	140.68(19)
N(3)-Cd(1)-O(1)	84.1(2)	N(2)-Cd(1)-O(1)	91.79(19)
O(3)-Cd(1)-O(1)	165.9(2)		

**Table S3.** Selected bond length and angles of ligand BOBA

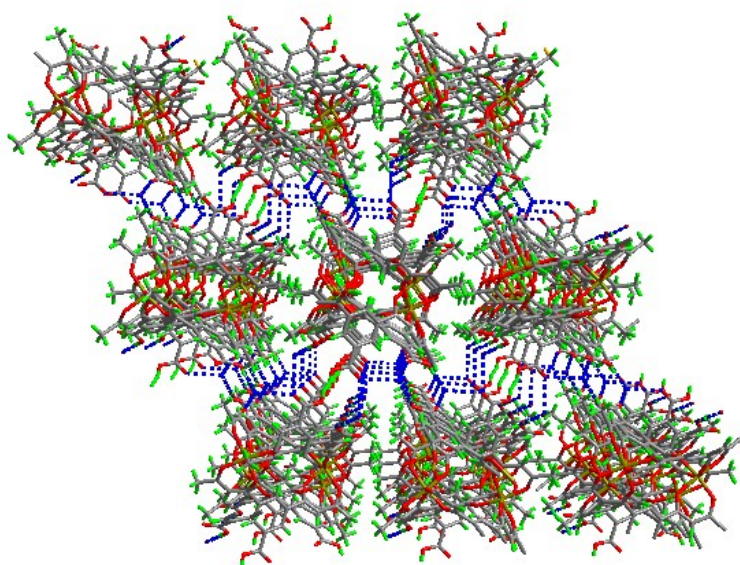
Selected bond length(Å)			
O(2)-C(11)	O(4)-C(9)	C(3)-C(4)	C(3)-C(2)
1.278(4)	1.288(4)	1.381(5)	1.387(5)
C(3)-C(11)	O(6)-C(15)	O(1)-C(13)	O(3)-C(7)
1.480(5)	1.236(4)	1.277(4)	1.279(4)
O(5)-C(15)	C(12)-C(13)	C(12)-C(11)	C(1)-C(2)
1.272(4)	1.384(5)	1.393(5)	1.379(5)
C(1)-C(6)	C(1)-C(15)	C(4)-C(5)	C(6)-C(5)
1.381(5)	1.485(5)	1.388(5)	1.389(5)
C(9)-C(8)	C(9)-C(10)	C(5)-C(7)	C(8)-C(7)
1.382(5)	1.486(5)	1.480(5)	1.388(5)
C(13)-C(14)			
1.487(5)			

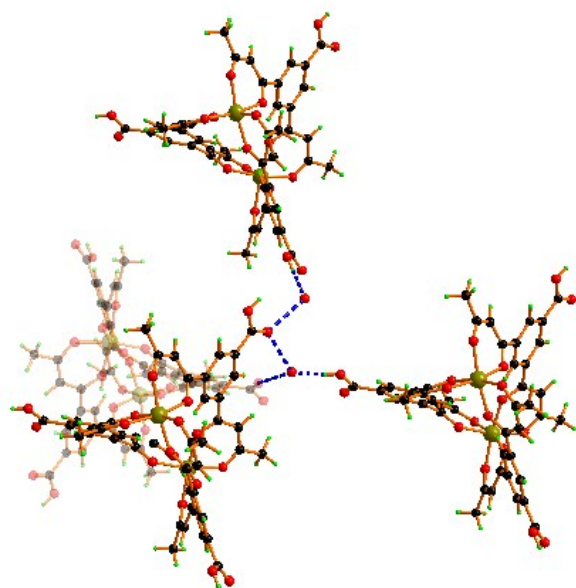
Selected Angles (deg)			
C(4)-C(3)-C(2)	118.6(3)	C(4)-C(3)-C(11)	122.7(3)
C(2)-C(3)-C(11)	118.7(3)	C(13)-C(12)-C(11)	120.1(3)
C(2)-C(1)-C(6)	120.5(3)	C(2)-C(1)-C(15)	119.9(3)
C(6)-C(1)-C(15)	119.6(3)	C(3)-C(4)-C(5)	121.6(3)
C(1)-C(6)-C(5)	119.8(3)	C(1)-C(2)-C(3)	120.5(3)
O(4)-C(9)-C(8)	122.3(3)	O(4)-C(9)-C(10)	116.0(3)
C(8)-C(9)-C(10)	121.7(3)	C(4)-C(5)-C(6)	119.0(3)
C(4)-C(5)-C(7)	118.7(3)	C(6)-C(5)-C(7)	122.3(3)
C(9)-C(8)-C(7)	121.2(3)	O(3)-C(7)-C(8)	121.2(3)
O(3)-C(7)-C(5)	115.2(3)	C(8)-C(7)-C(5)	123.6(3)
O(2)-C(11)-C(12)	120.1(3)	O(2)-C(11)-C(3)	116.1(3)
C(12)-C(11)-C(3)	123.8(3)	O(6)-C(15)-O(5)	123.9(3)
O(6)-C(15)-C(1)	120.3(3)	O(5)-C(15)-C(1)	115.8(3)
O(1)-C(13)-C(12)	121.9(3)	O(1)-C(13)-C(14)	115.7(3)
C(12)-C(13)-C(14)	122.4(3)		



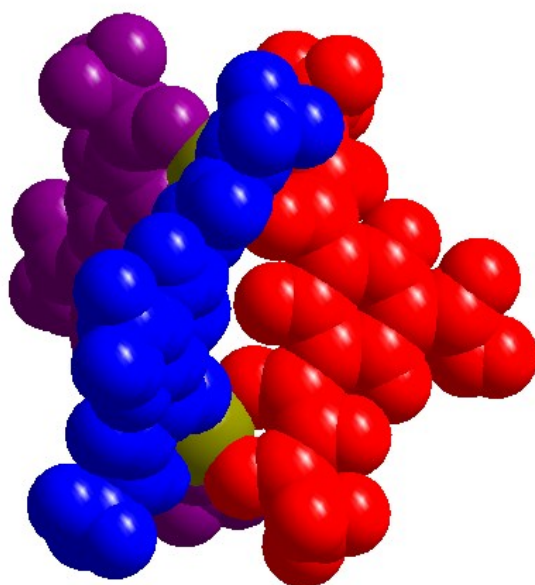
**Fig. S1** Dimer structure of ligand BOBA molecular showing intermolecular hydrogen bonds



**Fig. S2** Perspective views of hydrogen bond network and  $\pi$ - $\pi$  stacking interactions in BOBA.



**Fig. S3** Perspective views of hydrogen bonds interactions in complex Fe<sub>2</sub>(BOBA)<sub>3</sub>.



**Fig. S4** Space fill representation of complex  $\text{Fe}_2(\text{BOBA})_3$ , the nonmetal atoms of three strands and iron atoms are differently colored for clarity



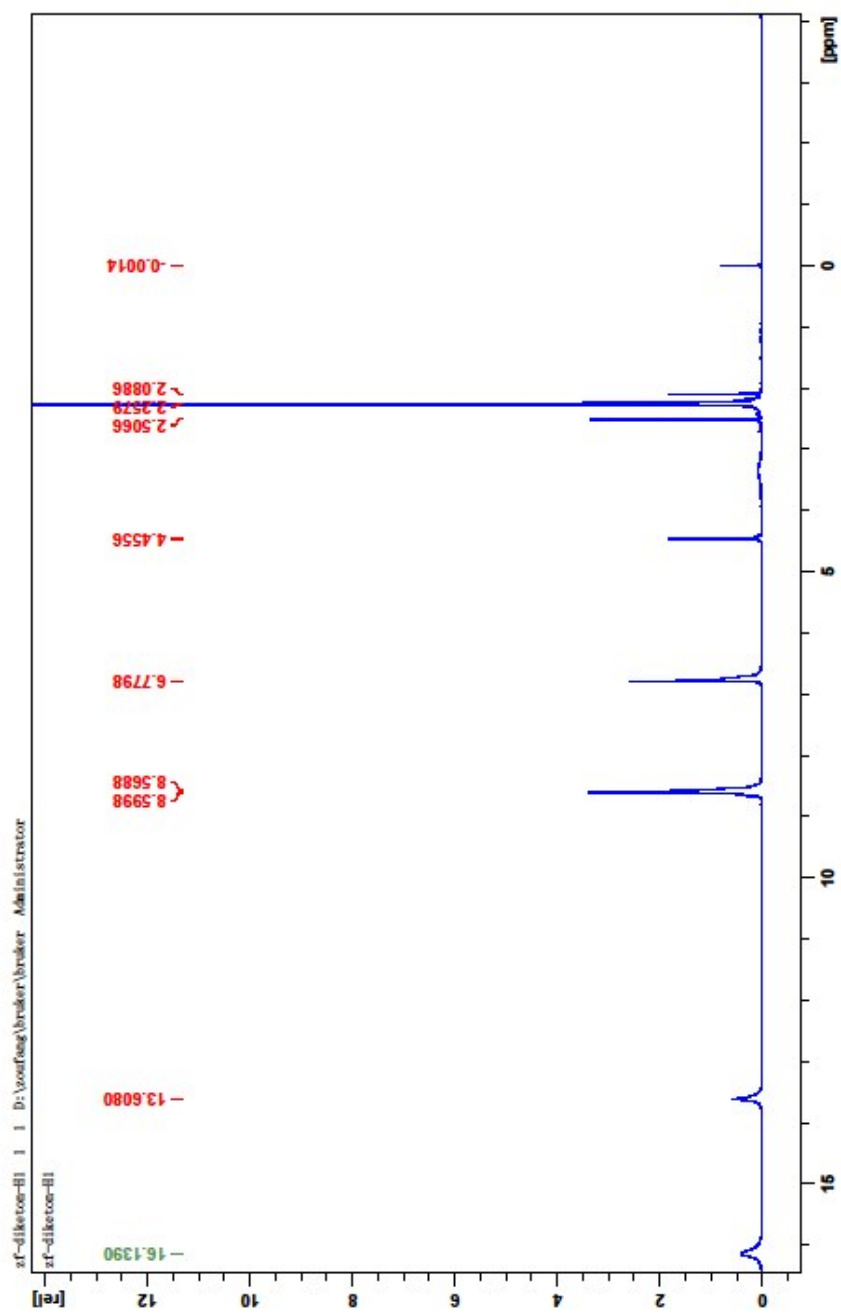
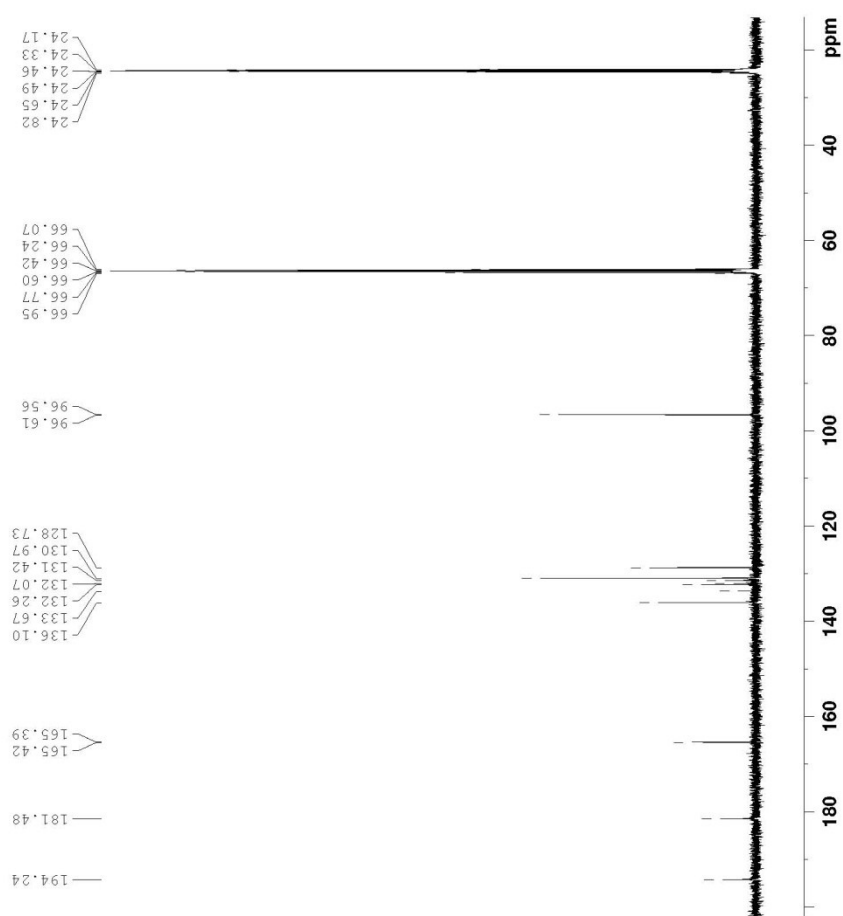
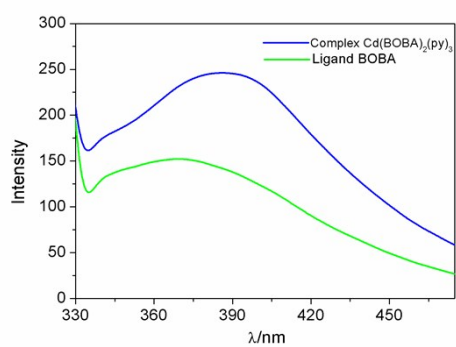


Fig. S5  $^1\text{H}$  NMR (500 MHz) spectra of ligand BOBA in  $(\text{CD}_3)_2\text{CO}$



**Fig. S6**  $^{13}\text{C}$  NMR (500 MHz) spectra of ligand BOBA in THF- $d_8$



**Fig. S7** Emission spectra of ligand BOBA and complex Cd(BOBA)<sub>2</sub>(py)<sub>3</sub> ( $\lambda_{exc} = 289 \text{ nm}$ ,  $5.0 \times 10^{-6} \text{ M}$  in degassed H<sub>2</sub>O).