Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2012**, *28* (12): 2783-2789
doi: 10.3866/PKU.WHXB201210122

基于 1*H*-苯并咪唑-2-羧酸的三个镧系超分子化合物的结构、热分解动力学和荧光性质

段林强[1] 乔成芳[1,2] 魏青[1,*] 夏正强[1] 陈三平[1,*]
张国春[2] 周春生[2] 高胜利[1,2]

([1]西北大学化学与材料科学学院, 合成与天然功能分子化学教育部重点实验室, 西安 710069;
[2]商洛学院化学与化学工程系, 陕西省尾矿资源综合利用重点实验室, 陕西 商洛 726000)

Structures, Thermodecomposition Kinetics and Luminescence Properties of Three Lanthanide-Based Supramolecular Compounds with 1*H*-Benzimidazole-2-carboxylic Acid

DUAN Lin-Qiang[1] QIAO Cheng-Fang[1,2] WEI Qing[1,*] XIA Zheng-Qiang[1]
CHEN San-Ping[1,*] ZHANG Guo-Chun[2] ZHOU Chun-Sheng[2] GAO Sheng-Li[1,2]

([1]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an 710069, P. R. China*; [2]*Department of Chemistry and Chemical Engineering, Shaanxi Key Laboratory of Comprehensive Utilization of Tailing Resources, Shangluo University, Shangluo 726000, Shaanxi Province, P. R. China*)

*Corresponding authors. WEI Qing, Email: weiqq@126.com. CHEN San-Ping, Email: sanpingchen@126.com; Tel: +86-29-88302604.

Powder X-ray patterns simulated for compound **2**(a) and measured for compound **3**(b). Selected bond lengths (nm), bond angles (°) and hydrogen-bonding interactions for **1** and **2** are in the supporting information. CCDC 874298 and 874297 contain the crystallographic data for the compounds **1** and **2**, respectively. These data can be obtained free of charge *via* the Internet at http://www.ccdc.cam.ac.uk/data_request/cif or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: ＋(44) 1223-336-033, E-mail: deposit@ccdc.cam.ac.uk).

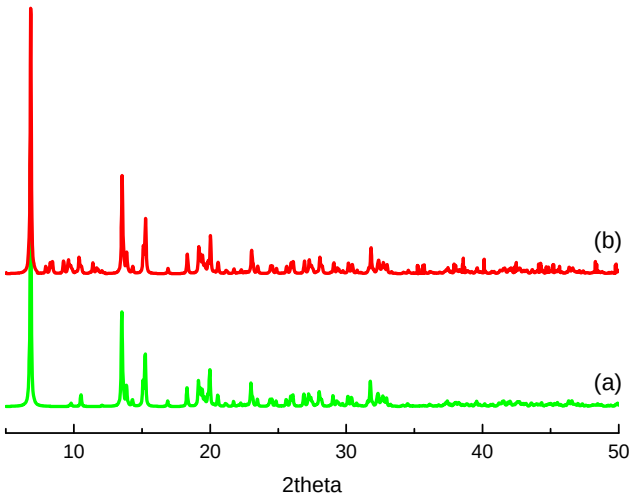

Fig.S1　Powder X-ray patterns simulated for compound 2(a) and measured for compound 3(b)

Table S1 Selected bond lengths (nm) and bond angles (°) for 1 and 2

Compound **1**			
Sm(1)-O(4)#1	0.2351(4)	Sm(1)-N(4)	0.2535(5)
Sm(1)-O(2)#2	0.2402(4)	Sm(1)-N(1)	0.2576(5)
Sm(1)-O(5)	0.2408(4)	Sm(1)-N(5)	0.2577(5)
Sm(1)-O(3)	0.2457(4)	O(2)-Sm(1)#3	0.2402(4)
Sm(1)-O(1)	0.2497(4)	O(4)-Sm(1)#4	0.2351(4)
O(4)#1-Sm(1)-O(2)#2	81.65(14)	O(5)-Sm(1)-N(4)	137.24(14)
O(4)#1-Sm(1)-O(5)	79.33(14)	O(3)-Sm(1)-N(4)	65.63(15)
O(2)#2-Sm(1)-O(5)	119.17(14)	O(1)-Sm(1)-N(4)	70.03(15)
O(4)#1-Sm(1)-O(3)	81.52(15)	O(4)#1-Sm(1)-N(1)	152.18(15)
O(2)#2-Sm(1)-O(3)	156.96(15)	O(2)#2-Sm(1)-N(1)	126.02(15)
O(5)-Sm(1)-O(3)	72.70(13)	O(5)-Sm(1)-N(1)	83.41(15)
O(4)#1-Sm(1)-O(1)	139.58(14)	O(3)-Sm(1)-N(1)	72.55(16)
O(2)#2-Sm(1)-O(1)	70.79(14)	O(1)-Sm(1)-N(1)	63.52(14)
O(5)-Sm(1)-O(1)	139.97(14)	N(4)-Sm(1)-N(1)	92.82(17)
O(3)-Sm(1)-O(1)	114.07(15)	O(4)#1-Sm(1)-N(5)	120.01(16)
O(5)-Sm(1)-N(5)	65.07(14)	O(2)#2-Sm(1)-N(4)	97.39(15)
O(4)#1-Sm(1)-N(4)	85.38(16)	O(2)#2-Sm(1)-N(5)	76.52(15)
O(3)-Sm(1)-N(5)	125.85(15)	N(4)-Sm(1)-N(5)	151.91(17)
O(1)-Sm(1)-N(5)	82.19(15)	N(1)-Sm(1)-N(5)	70.44(17)
Symmetry transformations used to generate equivalent atoms:			
#1 -x+1/2, y-1/2, -z+1/2;		#2 -x+3/2, y-1/2, -z+1/2;	
#3 -x+3/2, y+1/2, -z+1/2;		#4 -x+1/2, y+1/2, -z+1/2.	
Compound **2**			
Ho(1)-O(2)#1	0.2302(3)	Ho(1)-O(5)	0.2461(3)
Ho(1)-O(4)	0.2363(3)	Ho(1)-N(3)	0.2496(4)
Ho(1)-O(6)#2	0.2373(3)	Ho(1)-N(5)	0.2526(4)
Ho(1)-O(1)	0.2413(3)	O(2)-Ho(1)#3	0.2302(3)
Ho(1)-N(1)	0.2461(4)	O(6)-Ho(1)#4	0.2373(3)
O(2)#1-Ho(1)-O(4)	78.91(12)	N(1)-Ho(1)-O(5)	70.59(12)
O(2)#1-Ho(1)-O(6)#2	80.88(11)	O(2)#1-Ho(1)-N(3)	152.21(12)
O(4)-Ho(1)-O(6)#2	118.98(12)	O(4)-Ho(1)-N(3)	84.17(12)
O(2)#1-Ho(1)-O(1)	81.78(12)	O(6)#2-Ho(1)-N(3)	126.81(12)
O(4)-Ho(1)-O(1)	71.72(11)	O(1)-Ho(1)-N(3)	72.00(12)
O(6)#2-Ho(1)-O(1)	157.13(12)	N(1)-Ho(1)-N(3)	93.74(14)
O(2)#1-Ho(1)-O(5)	138.29(11)	O(5)-Ho(1)-N(3)	64.61(11)
O(4)-Ho(1)-O(5)	141.50(11)	O(2)#1-Ho(1)-N(5)	120.00(13)
O(6)#2-Ho(1)-O(5)	70.26(11)	O(4)-Ho(1)-N(5)	65.93(12)
O(1)-Ho(1)-O(5)	115.21(11)	O(6)#2-Ho(1)-N(5)	76.44(13)
O(2)#1-Ho(1)-N(1)	84.00(13)	O(1)-Ho(1)-N(5)	125.54(12)
O(4)-Ho(1)-N(1)	136.85(12)	N(1)-Ho(1)-N(5)	152.70(13)
O(6)#2-Ho(1)-N(1)	96.61(13)	O(5)-Ho(1)-N(5)	82.29(12)
O(1)-Ho(1)-N(1)	66.77(12)	N(3)-Ho(1)-N(5)	71.16(13)
Symmetry transformations used to generate equivalent atoms:			
#1 -x+1/2, y+1/2, -z+1/2;		#2 -x+3/2, y+1/2, -z+1/2;	
#3 -x+1/2, y-1/2, -z+1/2;		#4 -x+3/2, y-1/2, -z+1/2.	

Table S2 Hydrogen-bonding interactions in 1 and 2

Compound **1**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6N)...O(6)#1	0.86	1.99	0.2818(7)	159.9
N(3)-H(3)...O(5)#2	0.86	1.94	0.2788(7)	166.4
N(2)-H(2)...O(1)#3	0.86	1.92	0.2723(6)	155.7
Symmetry transformations used to generate equivalent atoms:				
#1 -x+1, -y+1, -z; #2 -x+1/2, y+1/2, -z+1/2; #3 -x+3/2, y+1/2, -z+1/2.				
Compound **2**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(4)#1	0.86	1.91	0.2753(5)	165.5
N(4)-H(4A)...O(5)#2	0.86	1.89	0.2679(5)	152.3
N(6)-H(6A)...O(3)#3	0.86	2.04	0.2857(6)	159.5
Symmetry transformations used to generate equivalent atoms:				
#1 -x+1/2, y-1/2, -z+1/2; #2 -x+3/2, y-1/2, -z+1/2; #3 -x+1, -y+1, -z.				