Structural Systematic Design of Organic Templated Samarium Sulfates and Their Luminescence Property

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Table S1 Selected bond lengths (Å) and angles (°) for **1-4**.

		1			
Sm(1)-O(18)	2.511(4)	O(21)-Sm(2)-O(5)	81.17(13)	O(21)-Sm(2)-O(7)	101.32(13)
Sm(1)-O(8)	2.519(3)	O(14)-Sm(2)-O(5)	55.87(11)	O(14)-Sm(2)-O(7)	73.15(12)
Sm(2)-O(21)	2.315(4)	O(7)-Sm(2)-O(5)	72.77(11)	O(13)-Sm(3)-O(11)	89.93(12)
Sm(2)-O(14)	2.491(3)	O(21)-Sm(2)-O(10)	76.93(12)	O(16)-Sm(3)-O(2)	69.92(11)
Sm(2)-O(7)	2.516(4)	O(14)-Sm(2)-O(10)	125.06(11)	O(4)-Sm(3)-O(2)	55.12(10)
Sm(2)-O(5)	2.533(3)	O(7)-Sm(2)-O(10)	55.69(11)	O(17)-Sm(3)-O(2)	118.34(11)
Sm(2)-O(10)	2.533(3)	O(5)-Sm(2)-O(10)	117.25(11)	O(13)-Sm(3)-O(2)	145.82(11)
Sm(3)-O(16)	2.396(3)	O(16)-Sm(3)-O(4)	88.77(12)	O(11)-Sm(3)-O(2)	124.22(11)
Sm(3)-O(4)	2.437(3)	O(16)-Sm(3)-O(17)	76.92(11)	O(16)-Sm(3)-O(8)	135.62(11)
Sm(3)-O(17)	2.464(3)	O(4)-Sm(3)-O(17)	74.23(11)	O(4)-Sm(3)-O(8)	135.61(11)
Sm(3)-O(13)	2.493(3)	O(16)-Sm(3)-O(13)	86.48(12)	O(17)-Sm(3)-O(8)	110.28(11)
Sm(3)-O(11)	2.525(3)	O(4)-Sm(3)-O(13)	151.74(11)	O(13)-Sm(3)-O(8)	54.95(11)
Sm(3)-O(2)	2.631(3)	O(17)-Sm(3)-O(13)	77.56(12)	O(11)-Sm(3)-O(8)	74.35(11)
Sm(3)-O(8)	2.642(3)	O(16)-Sm(3)-O(11)	132.48(11)	O(2)-Sm(3)-O(8)	129.93(10)
O(18)-Sm(1)-O(8)	55.78(11)	O(4)-Sm(3)-O(11)	73.03(11)	O(17)-Sm(3)-O(11)	56.12(11)
		2			
Sm(1)-O(23)	2.328(5)	O(13)-Sm(1)-O(22)	84.41(16)	O(10)-Sm(1)-O(8)	66.49(14)
Sm(1)-O(13)	2.376(5)	O(6)-Sm(1)-O(22)	153.30(18)	O(15)-Sm(2)-O(21)	77.99(18)
Sm(1)-O(6)	2.457(5)	O(23)-Sm(1)-O(26)	76.24(17)	O(15)-Sm(2)-O(4)	152.28(18)
Sm(1)-O(22)	2.471(4)	O(13)-Sm(1)-O(26)	154.41(16)	O(21)-Sm(2)-O(4)	87.4(2)
Sm(1)-O(26)	2.472(5)	O(6)-Sm(1)-O(26)	117.37(17)	O(15)-Sm(2)-O(20)	83.16(18)
Sm(1)-O(10)	2.627(5)	O(22)-Sm(1)-O(26)	75.95(17)	O(21)-Sm(2)-O(20)	95.5(2)
Sm(1)-O(8)	2.699(5)	O(23)-Sm(1)-O(10)	77.96(16)	O(4)-Sm(2)-O(20)	74.85(18)
Sm(2)-O(15)	2.313(5)	O(13)-Sm(1)-O(10)	68.87(15)	O(15)-Sm(2)-O(3)	126.72(17)
Sm(2)-O(21)	2.337(5)	O(6)-Sm(1)-O(10)	55.30(15)	O(21)-Sm(2)-O(3)	154.89(17)
Sm(2)-O(4)	2.357(5)	O(22)-Sm(1)-O(10)	141.55(15)	O(4)-Sm(2)-O(3)	71.71(17)

Sm(2)-O(20)	2.385(5)	O(26)-Sm(1)-O(10)	118.46(15)	O(20)-Sm(2)-O(3)	92.37(17)
Sm(2)-O(3)	2.428(5)	O(23)-Sm(1)-O(8)	77.28(17)	O(15)-Sm(2)-O(22)	75.34(16)
Sm(2)-O(22)	2.769(4)	O(13)-Sm(1)-O(8)	133.66(16)	O(21)-Sm(2)-O(22)	151.92(15)
O(23)-Sm(1)-O(13)	82.03(18)	O(6)-Sm(1)-O(8)	77.50(16)	O(4)-Sm(2)-O(22)	112.88(18)
O(23)-Sm(1)-O(6)	132.65(17)	O(22)-Sm(1)-O(8)	125.53(17)	O(20)-Sm(2)-O(22)	72.87(17)
O(13)-Sm(1)-O(6)	87.35(16)	O(26)-Sm(1)-O(8)	53.77(15)	O(3)-Sm(2)-O(22)	53.02(15)
O(23)-Sm(1)-O(22)	71.15(18)				
			3		
Sm(1)-O(7)	2.368(2)	O(7)-Sm(1)-O(9)	136.06(7)	O(1)-Sm(1)-O(3)	57.47(6)
Sm(1)-O(9)	2.3832(19)	O(7)-Sm(1)-O(1)	85.71(7)	O(7)-Sm(1)-O(10)	78.35(7)
Sm(1)-O(1)	2.4372(19)	O(9)-Sm(1)-O(1)	133.96(6)	O(9)-Sm(1)-O(10)	57.72(6)
Sm(1)-O(3)	2.4657(18)	O(7)-Sm(1)-O(3)	140.73(7)	O(1)-Sm(1)-O(10)	153.41(7)
Sm(1)-O(10)	2.4946(19)	O(9)-Sm(1)-O(3)	76.76(6)	O(3)-Sm(1)-O(10)	128.78(6)
			4		
Sm(1)-O(6)	2.413(5)	O(6)-Sm(1)-O(1)	57.57(16)	O(1)-Sm(1)-O(5)	150.37(17)
Sm(1)-O(2)	2.437(5)	O(2)-Sm(1)-O(1)	130.92(16)	O(4)-Sm(1)-O(5)	94.92(17)
Sm(1)-O(1)	2.457(4)	O(6)-Sm(1)-O(4)	79.37(18)	O(6)-Sm(1)-O(3)	89.05(17)
Sm(1)-O(4)	2.471(5)	O(2)-Sm(1)-O(4)	74.37(16)	O(2)-Sm(1)-O(3)	130.52(16)
Sm(1)-O(5)	2.501(4)	O(1)-Sm(1)-O(4)	114.67(17)	O(1)-Sm(1)-O(3)	74.99(16)
Sm(1)-O(3)	2.536(5)	O(6)-Sm(1)-O(5)	135.00(16)	O(4)-Sm(1)-O(3)	56.20(15)
O(6)-Sm(1)-O(2)	79.24(16)	O(2)-Sm(1)-O(5)	56.55(16)	O(5)-Sm(1)-O(3)	124.69(16)

Table S2 Hydrogen bonds of compound **1.**

D—H•••A	D—H(Å)	H•••A(Å)	D•••A(Å)	D—H•••A(°)
N6A--H6AD…O13	0.9000	2.5200	3.259(14)	140.00
N6A--H6AD…O20	0.9000	2.1800	2.998(14)	151.00
N1--H1E…O12	0.9000	1.9800	2.841(7)	160.00
N6--H6AE…O5	0.9500	2.5300	3.002(17)	111.00
N6--H6AE…O24	0.9500	2.1000	2.796(15)	129.00
N2--H2D…O11	0.9000	2.4800	2.878(8)	107.00
N2--H2D…O20	0.9000	2.1200	2.912(8)	147.00
N2--H2E…O23	0.9000	2.0500	2.866(9)	150.00
N2--H2E…O11	0.9000	2.5200	2.878(8)	104.00
N3--H3E…O10	0.9000	2.3000	2.775(6)	113.00
N3--H3E…O3	0.9000	2.1500	2.939(5)	146.00
N4--H4E…O7	0.9000	2.4000	3.099(9)	134.00
N4--H4E…O14	0.9000	2.5100	3.323(5)	151.00
N5--H5D…O6	0.9000	2.4400	3.201(12)	143.00
N5--H5D…O12	0.9000	2.1600	2.979(13)	151.00
N5--H5E…O9	0.9000	2.4500	3.169(13)	137.00
N5--H5E…O19	0.9000	2.0400	2.867(14)	152.00
N6--H6D…O22	0.9000	2.3200	3.130(16)	149.00
N6--H6D…O21	0.9000	2.4800	3.176(14)	135.00

N6--H6E…O5	0.9000	2.1500	3.002(17)	158.00
C1--H1A…O19	0.9600	2.4700	3.287(8)	143.00
C1--H1C…O13	0.9600	2.5000	3.233(8)	133.00
C3--H3C…O24	0.9600	2.5800	3.238(14)	126.00

Table S3 Hydrogen bonds of compound **2.**

D—H•••A	D—H(Å)	H•••A(Å)	D•••A(Å)	D—H•••A(°)
N1--H1C…O20	0.8900	2.0700	2.856(8)	147.00
N1--H1C…O14	0.8900	2.5800	3.066(9)	116.00
N1--H1D…O18	0.8900	2.2600	2.936(9)	132.00
N1--H1E…O4	0.8900	2.5400	3.207(9)	133.00
N1--H1E…O11	0.8900	2.5600	3.325(9)	145.00
N2--H2D…O6	0.8900	2.5000	3.095(8)	125.00
N3--H3C…O5	0.8900	2.2500	2.996(9)	141.00
N3--H3C…O27	0.8900	2.3700	3.090(8)	138.00
N3--H3D…O10	0.8900	2.1100	2.948(8)	156.00
N3--H3D…O13	0.8900	2.5200	3.134(8)	127.00
N4--H4C…O26	0.8900	2.5300	2.851(8)	102.00
N4--H4D…O14	0.8900	2.3800	2.921(8)	119.00
N4--H4D…O26	0.8900	2.3700	2.851(8)	114.00
N5--H5C…O17	0.8900	2.3700	3.016(9)	130.00
N6--H6E…O25	0.8900	1.9000	2.777(10)	166.00
N7--H7C…O28	0.8900	1.9900	2.882(9)	177.00
N7--H7D…O16	0.8900	2.1600	2.962(8)	150.00
N7--H7E…O11	0.8900	2.0400	2.894(8)	159.00
N8--H8C…O5	0.8900	2.1600	2.890(8)	139.00
N8--H8C…O27	0.8900	2.4300	3.194(8)	144.00
N8--H8D…O27	0.8900	2.0000	2.893(8)	176.00
N8--H8E…O1	0.8900	1.8500	2.717(8)	163.00
C5--H5A…O17	0.9700	2.5500	2.984(13)	107.00
C7--H7A…O1	0.9700	2.6000	3.250(9)	125.00
C8--H8A…O16	0.9700	2.3400	3.135(9)	138.00
C8--H8A…O19	0.9700	2.5100	3.101(9)	119.00
C8--H8B…O2	0.9700	2.5200	3.350(9)	143.00

Table S4 Hydrogen bonds of compound **3.**

D—H•••A	D—H(Å)	H•••A(Å)	D•••A(Å)	D—H•••A(°)
O1W--H1WA…O5	0.845(14)	2.057(14)	2.895(3)	171.5(13)
N1--H1D…O6	0.9000	2.5100	3.003(4)	115.00
N1--H1D…O10	0.9000	2.0300	2.890(3)	160.00
N1--H1E…O1	0.9000	2.4000	3.149(4)	141.00
N1--H1E…O2	0.9000	2.3700	3.023(3)	129.00
O1W--H1WB…O2	0.846(14)	2.549(15)	3.022(4)	116.5(15)

O1W--H1WB…O2	0.846(14)	2.086(15)	2.921(4)	168.9(16)
O1W--H1WC…O12	0.841(15)	2.015(14)	2.827(4)	162(2)
O2W--H2WA…O8	0.849(15)	2.070(15)	2.914(4)	173.6(13)
O2W--H2WB…O1	0.847(12)	2.098(18)	2.909(4)	160(2)
O2W--H2WC…O9	0.843(12)	2.51(2)	2.989(4)	117.4(14)
O2W--H2WC…O9	0.843(12)	2.214(10)	3.001(3)	156(2)

Table S5 Hydrogen bonds of compound **4.**

D—H•••A	D—H(Å)	H•••A(Å)	D•••A(Å)	D—H•••A(°)
N3A--H3AA…O10	0.9000	2.5800	2.99(2)	109.00
N3A--H3AA…O11	0.9000	2.3300	3.09(2)	142.00
N1--H1A…O3	0.9000	2.1800	2.870(10)	133.00
N1--H1A…O5	0.9000	2.2600	3.037(10)	145.00
N1--H1B…O11	0.9000	1.9100	2.788(11)	166.00
N3--H3AB…O10	1.4000	2.1200	2.880(14)	108.00
N2--H2A…O9	0.9000	1.8700	2.767(10)	173.00
N2--H2B…O1	0.9000	2.5200	3.204(9)	133.00
N2--H2B…O12	0.9000	1.9500	2.827(10)	163.00
N3--H3A…O2	0.9000	2.0300	2.781(12)	141.00
N3--H3B…O10	0.9000	2.0200	2.880(14)	159.00
C2--H2D…O9	0.9600	2.4500	3.263(13)	142.00
C2--H2E…O11	0.9600	2.5000	3.402(12)	156.00
C5--H5B…O6	0.9600	2.4900	3.411(13)	162.00
C5--H5C…O6	0.9600	2.2900	3.174(13)	152.00
C6--H6A…O8	0.9600	2.5100	3.226(13)	131.00
C6--H6B…O2	0.9600	2.3900	3.168(13)	138.00
C6--H6C…O11	0.9600	2.2200	3.138(13)	158.00

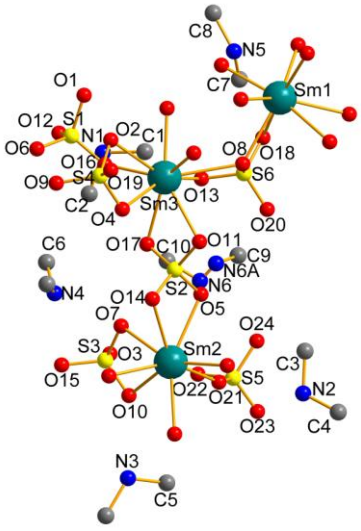

Fig. S1 ORTEP view of the $[(CH_3)_2NH_2]_9[Sm_5(SO_4)_{12}]$ **1** structure

showing the atom labeling scheme.

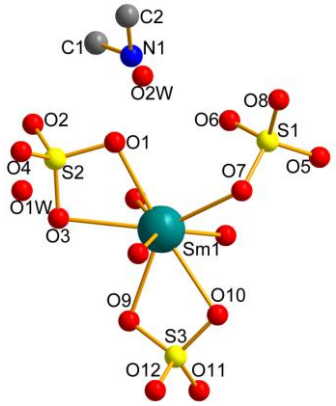

Fig. S2 ORTEP view of the $[H_3O]_2[(CH_3)_2NH_2][Sm(SO_4)_3]$ **3** structure showing the atom labeling scheme.

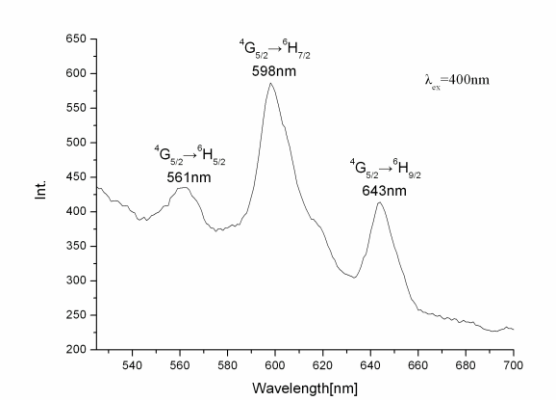

Fig. S3 The photoluminescence spectra of compound **1**. The excitation wavelength is 400 nm, and spectrum is taken at room temperature.

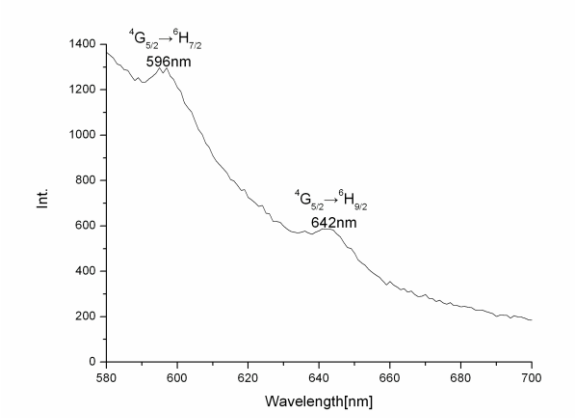

Fig. S4 The photoluminescence spectra of compound **2**. The excitation

wavelength is 400 nm, and spectrum is taken at room temperature.

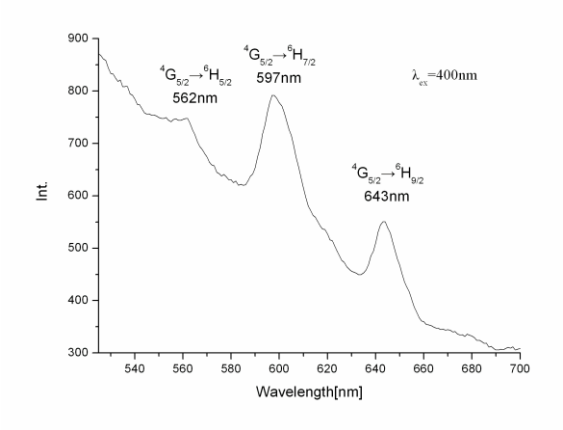

Fig. S5 The photoluminescence spectra of compound **4**. The excitation wavelength is 400 nm, and spectrum is taken at room temperature.

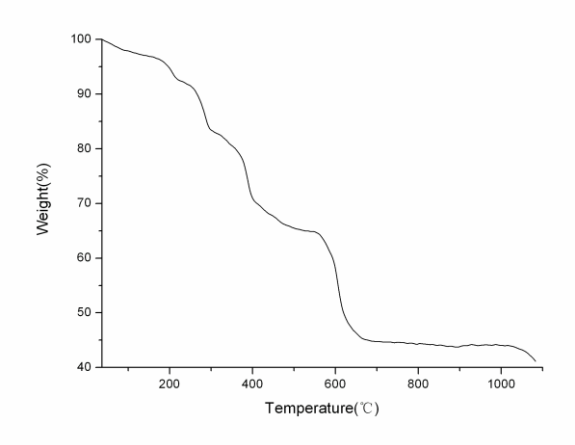

Fig. S6 TG curve of compound **1**.

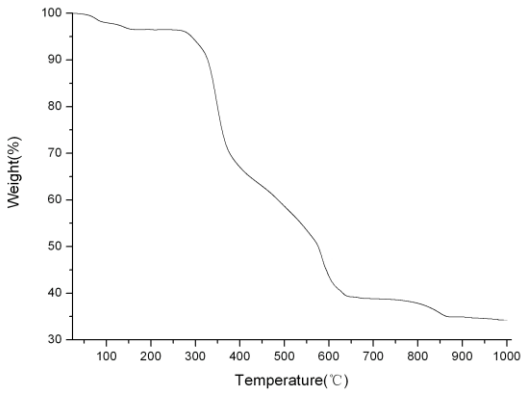

Fig. S7 TG curve of compound **2**.

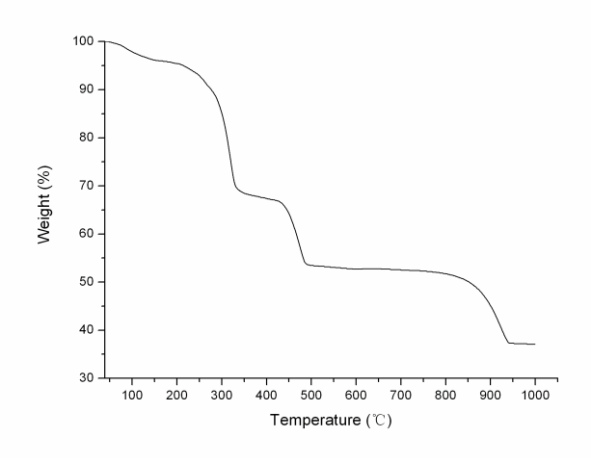

Fig. S8 TG curve of compound **3**.

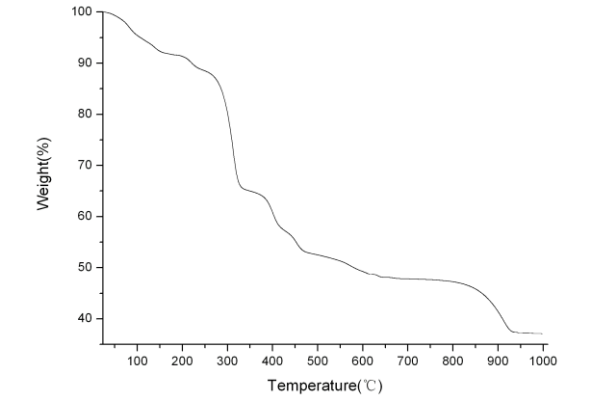

Fig. S9 TG curve of compound **4**.

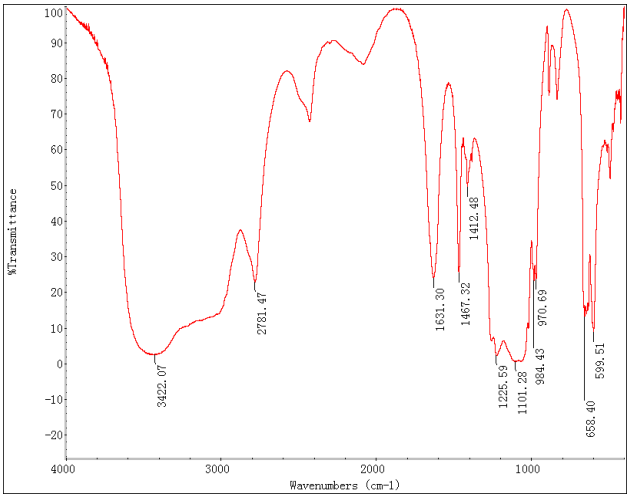

Fig. S10 IR of compound **1**.

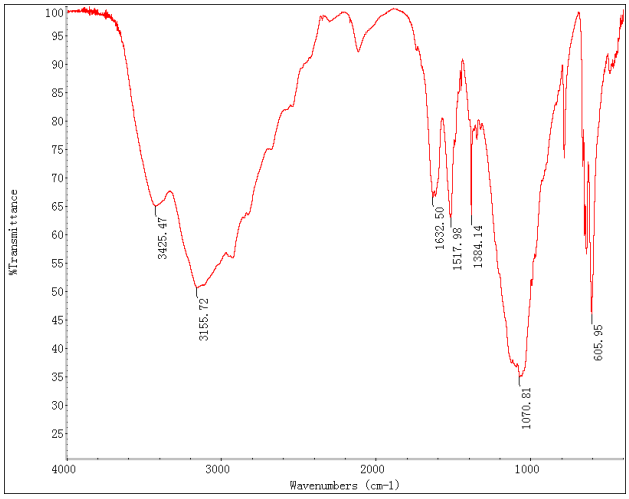

Fig. S11 IR of compound **2**.

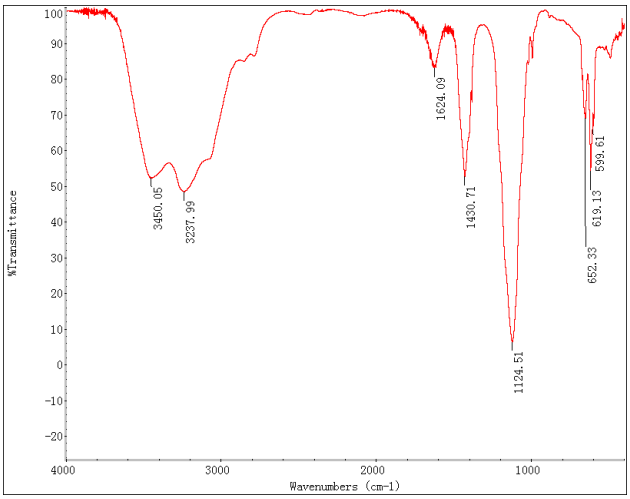

Fig. S12 IR of compound **3**.

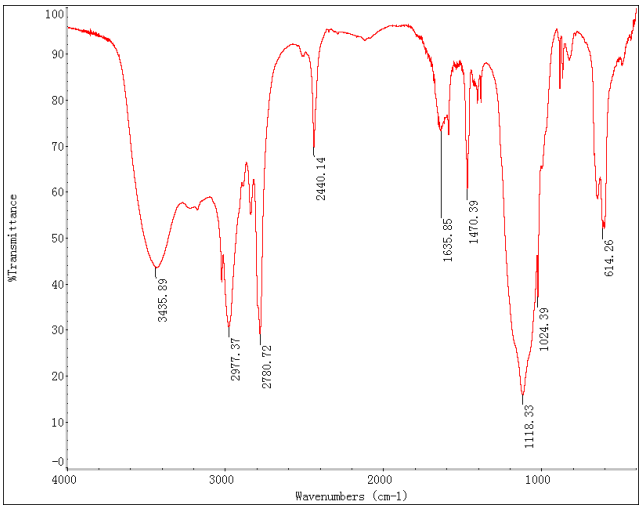

Fig. S13 IR of compound **4**.