

Electronic Supplementary Information for

Solvothermal syntheses and characterizations of lanthanide(III)/SbS₄³⁻ complexes associated by dien ligand: A detailed study based on the lanthanide contraction effect

Weiwei Tang, Ruihong Chen, Jing Zhao, Wenqing Jiang, Yong Zhang and Dingxian Jia *

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, People's Republic of China.

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

Sb(1)–S(1)	2.325(3)	Sb(1)–S(2)	2.334(3)
Sb(1)–S(3)	2.320(3)	Sb(1)–S(4)	2.317(3)
Pr(1)–S(1)	3.064(3)	Pr(1)–S(2)	3.066(3)
Pr(1)–S(3)#1	3.202(3)		
Pr(1)–N(1)	2.704(8)	Pr(1)–N(2)	2.717(9)
Pr(1)–N(3)	2.704(8)	Pr(1)–N(4)	2.656(8)
Pr(1)–N(5)	2.682(9)	Pr(1)–N(6)	2.718(8)
S(1)–Sb(1)–S(2)	101.72(9)	S(1)–Sb(1)–S(3)	113.60(10)
S(1)–Sb(1)–S(4)	109.82(10)	S(2)–Sb(1)–S(3)	109.67(9)
S(2)–Sb(1)–S(4)	111.47(10)	S(3)–Sb(1)–S(4)	110.32(9)
Sb(1)–S(1)–Pr(1)	90.77(8)	Sb(1)–S(2)–Pr(1)	90.55(8)
Sb(1)–S(3)–Pr(1)#2	118.81(9)		
S(1)–Pr(1)–S(2)	72.24(7)	S(1)–Pr(1)–S(3)#1	137.57(7)
S(2)–Pr(1)–S(3)#1	131.32(7)	S(1)–Pr(1)–N(1)	75.5(2)
S(1)–Pr(1)–N(2)	138.5(2)	S(1)–Pr(1)–N(3)	133.7(2)
S(1)–Pr(1)–N(4)	78.1(2)	S(1)–Pr(1)–N(5)	70.0(2)
S(1)–Pr(1)–N(6)	91.78(19)	S(2)–Pr(1)–N(1)	76.44(19)
S(2)–Pr(1)–N(2)	91.00(19)	S(2)–Pr(1)–N(3)	67.8(2)
S(2)–Pr(1)–N(4)	79.0(2)	S(2)–Pr(1)–N(5)	131.1(2)
S(2)–Pr(1)–N(6)	146.97(18)	S(3)#1–Pr(1)–N(1)	137.3(2)
S(3)#1–Pr(1)–N(2)	81.9(2)	S(3)#1–Pr(1)–N(3)	65.6(2)
S(3)#1–Pr(1)–N(4)	74.5(2)	S(3)#1–Pr(1)–N(5)	69.0(2)
S(3)#1–Pr(1)–N(6)	79.83(18)	N(1)–Pr(1)–N(2)	63.6(3)
N(1)–Pr(1)–N(3)	115.4(3)	N(1)–Pr(1)–N(4)	148.2(3)
N(1)–Pr(1)–N(5)	121.1(3)	N(1)–Pr(1)–N(6)	71.5(3)
N(2)–Pr(1)–N(3)	65.1(3)	N(2)–Pr(1)–N(4)	136.9(3)
N(2)–Pr(1)–N(5)	137.8(3)	N(2)–Pr(1)–N(6)	82.1(3)
N(3)–Pr(1)–N(4)	72.3(3)	N(3)–Pr(1)–N(5)	123.1(3)
N(3)–Pr(1)–N(6)	134.5(3)	N(4)–Pr(1)–N(5)	63.9(3)
N(4)–Pr(1)–N(6)	126.9(3)	N(5)–Pr(1)–N(6)	63.7(2)
Symmetry transformations used to generate equivalent atoms: #1) x+1, y, z; #2) x–1, y, z.			

Table S2. Selected bond lengths (Å) and angles (°) for **1b**

Sb(1)–S(1)	2.324(2)	Sb(1)–S(2)	2.334(2)
Sb(1)–S(3)	2.320(2)	Sb(1)–S(4)	2.317(2)
Nd(1)–S(1)	3.017(2)	Nd(1)–S(2)	3.025(2)
Nd(1)–S(3)#1	3.203(2)		
Nd(1)–N(1)	2.633(7)	Nd(1)–N(2)	2.662(7)
Nd(1)–N(3)	2.641(7)	Nd(1)–N(4)	2.653(7)
Nd(1)–N(5)	2.625(7)	Nd(1)–N(6)	2.601(7)
S(1)–Sb(1)–S(2)	100.80(8)	S(1)–Sb(1)–S(3)	114.13(8)
S(1)–Sb(1)–S(4)	109.94(8)	S(2)–Sb(1)–S(3)	110.01(8)
S(2)–Sb(1)–S(4)	111.58(8)	S(3)–Sb(1)–S(4)	110.10(8)
Sb(1)–S(1)–Nd(1)	91.06(7)	Sb(1)–S(2)–Nd(1)	90.68(7)
Sb(1)–S(3)–Nd(1)#2	119.59(8)		
S(1)–Nd(1)–S(2)	72.87(6)	S(1)–Nd(1)–S(3)#1	137.42(6)
S(2)–Nd(1)–S(3)#1	131.87(6)	S(1)–Nd(1)–N(1)	134.02(17)
S(1)–Nd(1)–N(2)	139.43(19)	S(1)–Nd(1)–N(3)	75.15(18)
S(1)–Nd(1)–N(4)	92.42(17)	S(1)–Nd(1)–N(5)	70.39(18)
S(1)–Nd(1)–N(6)	77.46(19)	S(2)–Nd(1)–N(1)	68.35(17)
S(2)–Nd(1)–N(2)	91.68(17)	S(2)–Nd(1)–N(3)	76.35(16)
S(2)–Nd(1)–N(4)	147.01(16)	S(2)–Nd(1)–N(5)	131.91(17)
S(2)–Nd(1)–N(6)	78.18(18)	S(3)#1–Nd(1)–N(1)	65.10(17)
S(3)#1–Nd(1)–N(2)	80.59(18)	S(3)#1–Nd(1)–N(3)	136.88(17)
S(3)#1–Nd(1)–N(4)	78.71(16)	S(3)#1–Nd(1)–N(5)	68.25(18)
S(3)#1–Nd(1)–N(6)	76.18(19)	N(1)–Nd(1)–N(2)	66.1(3)
N(1)–Nd(1)–N(3)	117.0(2)	N(1)–Nd(1)–N(4)	133.5(2)
N(1)–Nd(1)–N(5)	121.3(2)	N(1)–Nd(1)–N(6)	71.3(2)
N(2)–Nd(1)–N(3)	64.7(3)	N(2)–Nd(1)–N(4)	80.5(2)
N(2)–Nd(1)–N(5)	136.3(2)	N(2)–Nd(1)–N(6)	137.0(3)
N(3)–Nd(1)–N(4)	71.3(2)	N(3)–Nd(1)–N(5)	121.2(2)
N(3)–Nd(1)–N(6)	146.9(3)	N(4)–Nd(1)–N(5)	64.4(2)
N(4)–Nd(1)–N(6)	128.3(2)	N(5)–Nd(1)–N(6)	64.5(2)
Symmetry transformations used to generate equivalent atoms: #1) x+1, y, z; #2) x–1, y, z.			

Table S3. Selected bond lengths (Å) and angles (°) for **1c**

Sb(1)–S(1)	2.334(2)	Sb(1)–S(2)	2.320(2)
Sb(1)–S(3)	2.321(2)	Sb(1)–S(4)	2.319(2)
Sm(1)–S(1)	3.006(2)	Sm(1)–S(2)	2.995(2)
Sm(1)–S(3)#1	3.248(2)		
Sm(1)–N(1)	2.609(8)	Sm(1)–N(2)	2.630(7)
Sm(1)–N(3)	2.616(7)	Sm(1)–N(4)	2.585(7)
Sm(1)–N(5)	2.598(7)	Sm(1)–N(6)	2.623(7)
S(1)–Sb(1)–S(2)	100.70(8)	S(1)–Sb(1)–S(3)	110.29(8)
S(1)–Sb(1)–S(4)	111.50(8)	S(2)–Sb(1)–S(3)	114.32(9)
S(2)–Sb(1)–S(4)	109.75(9)	S(3)–Sb(1)–S(4)	110.00(8)
Sb(1)–S(1)–Sm(1)	90.59(7)	Sb(1)–S(2)–Sm(1)	91.11(7)
Sb(1)–S(3)–Sm(1)#2	119.40(9)		
S(1)–Sm(1)–S(2)	73.33(6)	S(1)–Sm(1)–S(3)#1	131.94(6)
S(2)–Sm(1)–S(3)#1	137.22(6)	S(1)–Sm(1)–N(1)	68.5(2)
S(1)–Sm(1)–N(2)	91.98(17)	S(1)–Sm(1)–N(3)	76.34(17)
S(1)–Sm(1)–N(4)	77.60(17)	S(1)–Sm(1)–N(5)	132.66(17)
S(1)–Sm(1)–N(6)	147.01(16)	S(2)–Sm(1)–N(1)	134.1(2)
S(2)–Sm(1)–N(2)	139.77(19)	S(2)–Sm(1)–N(3)	74.97(18)
S(2)–Sm(1)–N(4)	77.43(19)	S(2)–Sm(1)–N(5)	71.19(18)
S(2)–Sm(1)–N(6)	92.67(17)	S(3)#1–Sm(1)–N(1)	64.8(2)
S(3)#1–Sm(1)–N(2)	80.17(18)	S(3)#1–Sm(1)–N(3)	136.88(17)
S(3)#1–Sm(1)–N(4)	76.75(19)	S(3)#1–Sm(1)–N(5)	67.13(18)
S(3)#1–Sm(1)–N(6)	78.35(16)	N(1)–Sm(1)–N(2)	66.8(3)
N(1)–Sm(1)–N(3)	117.9(3)	N(1)–Sm(1)–N(4)	70.4(3)
N(1)–Sm(1)–N(5)	119.7(3)	N(1)–Sm(1)–N(6)	133.1(3)
N(2)–Sm(1)–N(3)	65.1(3)	N(2)–Sm(1)–N(4)	136.8(3)
N(2)–Sm(1)–N(5)	135.2(2)	N(2)–Sm(1)–N(6)	79.6(2)
N(3)–Sm(1)–N(4)	146.4(2)	N(3)–Sm(1)–N(5)	121.8(2)
N(3)–Sm(1)–N(6)	71.1(2)	N(4)–Sm(1)–N(5)	64.9(2)
N(4)–Sm(1)–N(6)	129.3(2)	N(5)–Sm(1)–N(6)	64.8(2)
Symmetry transformations used to generate equivalent atoms: #1) x–1, y, z; #2) x+1, y, z.			

Table S4. Selected bond lengths (Å) and angles (°) for **2a**

Sb(1)–S(1)	2.3503(18)	Sb(1)–S(2)	2.3098(18)
Eu(1)–S(1)	2.8415(18)	Eu(1)–N(1)	2.570(5)
Eu(1)–N(2)	2.581(6)	Eu(1)–N(3)	2.605(5)
S(2)–Sb(1)–S(1)	107.69(7)	S(1)–Sb(1)–S(1)#1	104.17(9)
S(2)#1–Sb(1)–S(1)	110.78(7)	S(2)#1–Sb(1)–S(2)	115.19(10)
Sb(1)–S(1)–Eu(1)	87.18(6)	S(1)#1–Eu(1)–S(1)	81.47(7)
N(1)–Eu(1)–S(1)#1	152.95(13)	N(2)–Eu(1)–S(1)#1	138.95(13)
N(1)–Eu(1)–S(1)	90.83(14)	N(2)–Eu(1)–S(1)	83.90(14)
N(3)–Eu(1)–S(1)	80.46(14)	N(3)–Eu(1)–S(1)#1	73.87(13)
N(1)–Eu(1)–N(1)#1	106.7(3)	N(2)–Eu(1)–N(2)#1	129.4(3)
N(1)–Eu(1)–N(2)	64.76(17)	N(2)–Eu(1)–N(3)#1	131.11(19)
N(1)–Eu(1)–N(2)#1	85.17(19)	N(2)–Eu(1)–N(3)	65.96(17)
N(1)–Eu(1)–N(3)#1	72.49(18)	N(1)–Eu(1)–N(3)	130.58(17)
N(3)#1–Eu(1)–N(3)	146.0(3)		
Symmetry transformations used to generate equivalent atoms: #1) $-x+1, y, -z+1/2$.			

Table S5. Selected bond lengths (Å) and angles (°) for **2b**

Sb(1)–S(1)	2.3489(11)	Sb(1)–S(2)	2.3112(12)
Dy(1)–S(1)	2.8132(12)	Dy(1)–N(1)	2.581(3)
Dy(1)–N(2)	2.537(4)	Dy(1)–N(3)	2.533(4)
S(2)#1–Sb(1)–S(2)	114.89(7)	S(1)–Sb(1)–S(1)#1	103.63(6)
S(2)#1–Sb(1)–S(1)	111.01(4)	S(2)–Sb(1)–S(1)	107.87(4)
Sb(1)–S(1)–Dy(1)	87.17(4)	S(1)#1–Dy(1)–S(1)	82.03(5)
N(1)–Dy(1)–S(1)#1	73.80(9)	N(2)–Dy(1)–S(1)#1	139.61(9)
N(1)–Dy(1)–S(1)	79.80(9)	N(2)–Dy(1)–S(1)	84.71(10)
N(3)–Dy(1)–S(1)	91.67(10)	N(3)–Dy(1)–S(1)#1	152.48(9)
N(1)–Dy(1)–N(1)#1	144.82(18)	N(3)–Dy(1)–N(3)#1	105.26(19)
N(2)–Dy(1)–N(2)#1	127.3(2)	N(3)–Dy(1)–N(2)	65.45(12)
N(2)–Dy(1)–N(1)	66.35(12)	N(3)#1–Dy(1)–N(2)	82.94(13)
N(2)#1–Dy(1)–N(1)	132.01(12)	N(3)–Dy(1)–N(1)	131.59(12)
N(3)#1–Dy(1)–N(1)	72.72(12)		
Symmetry transformations used to generate equivalent atoms: #1) $-x+1, y, -z+3/2$.			

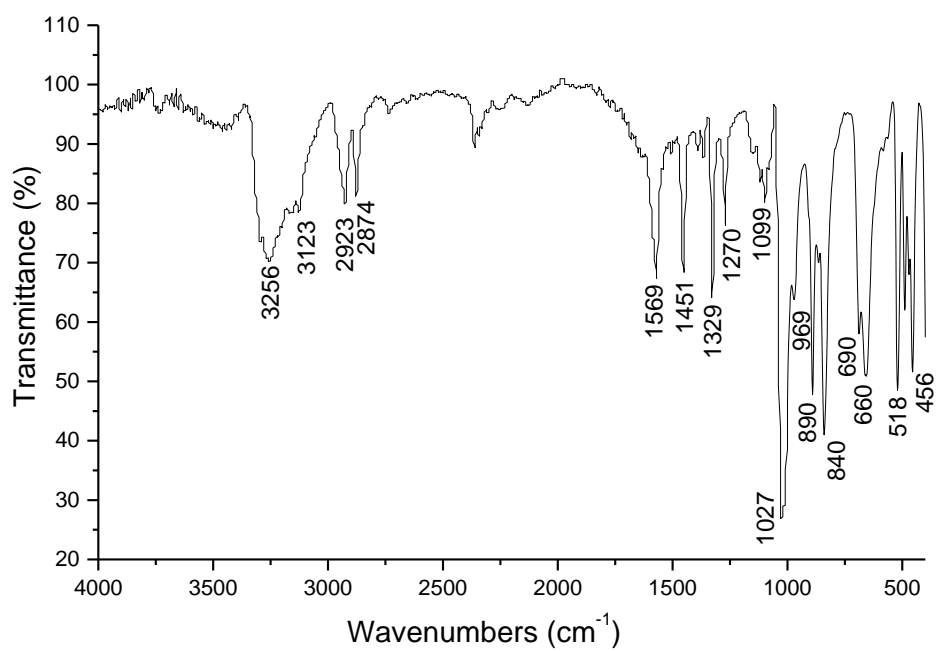


Fig. S1 IR spectra of complex **1a**.

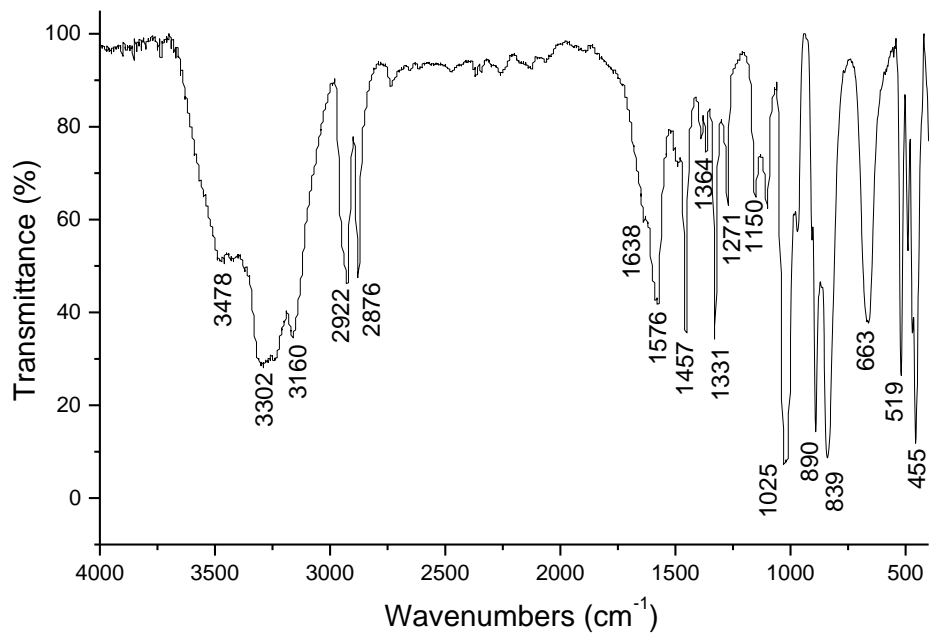


Fig. S2 IR spectra of complex **2a**.

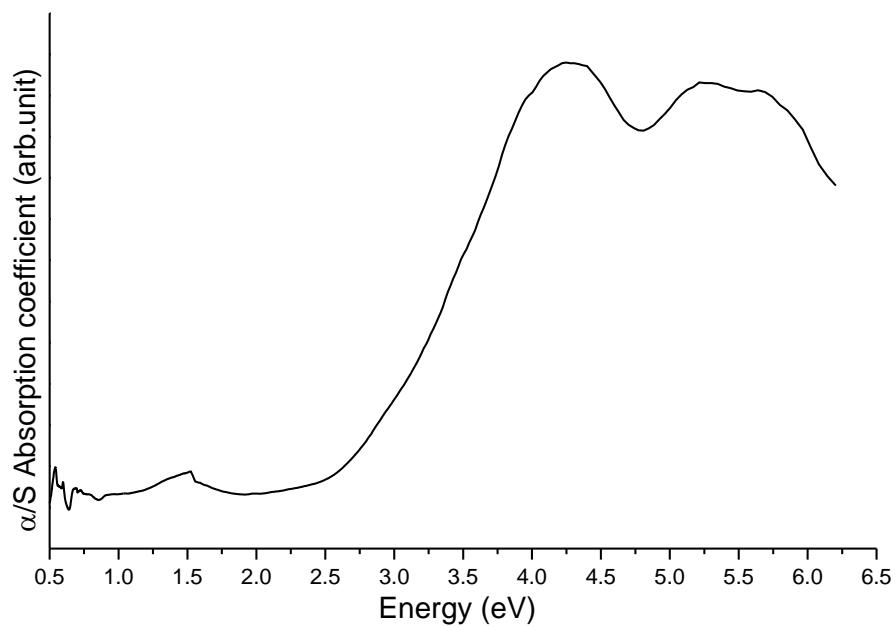


Fig. S3 Optical absorption spectra of **1b**.

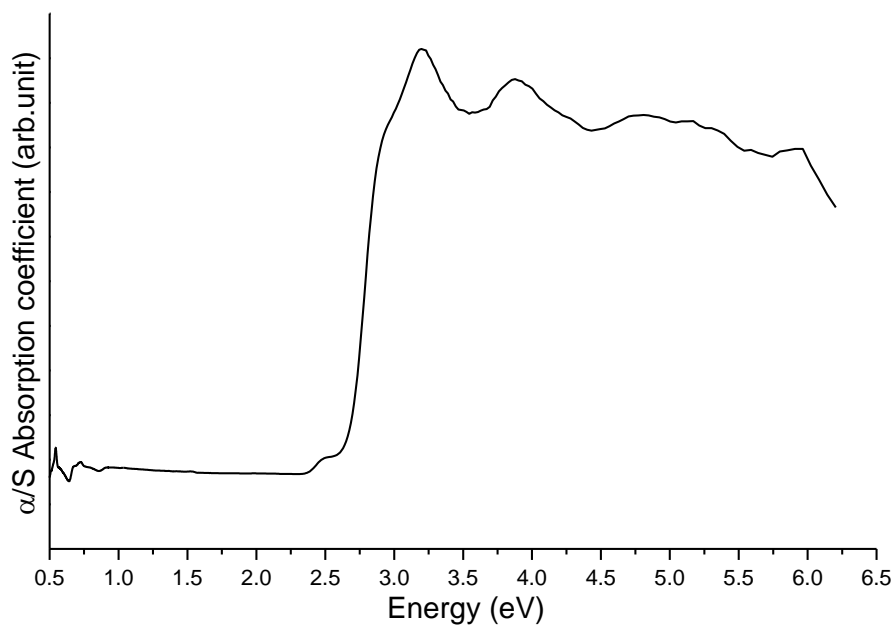


Fig. S4 Optical absorption spectra of **1c**.

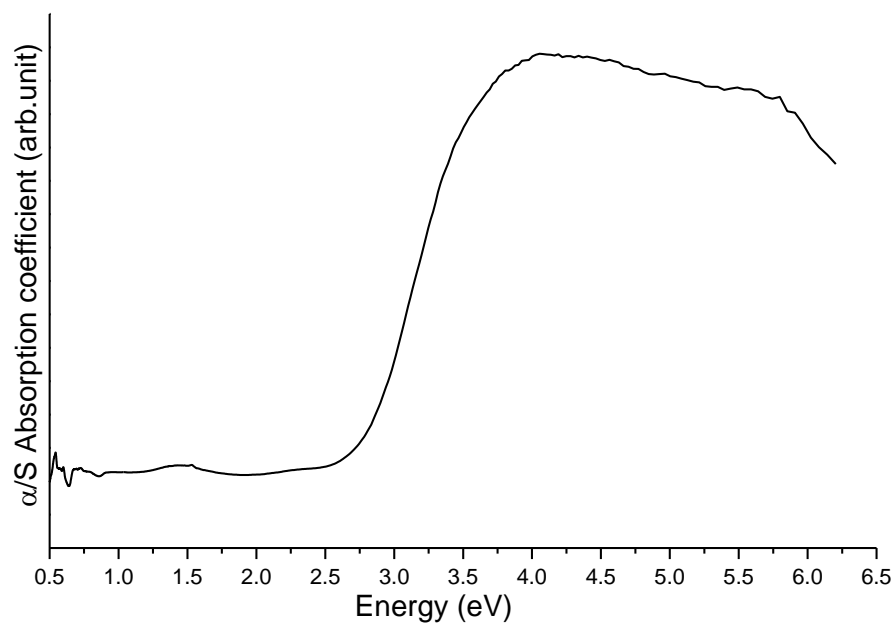


Fig. S5 Optical absorption spectra of **2b**.