Supporting Information for

Novel lanthanoid thioantimonates: the first coexistence of different types of thioantimonate anions in the same framework

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Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1** and **2**.

1			
Sm(1)-N(5)	2.585(6)	Sm(2)-N(8)	2.53(3)
Sm(1)-N(1)	2.589(6)	Sm(2)-N(6)	2.54(4)
Sm(1)-N(3)	2.604(6)	Sm(2)-N(9)	2.55(2)
Sm(1)-N(2)	2.621(6)	Sm(2)-N(10)	2.63(4)
Sm(1)-N(4)	2.621(6)	Sm(2)-N(7)	2.64(2)
Sm(1)-S(4)	2.802(2)	Sm(2)-S(7)	2.800(2)
Sm(1)-S(3)	2.872(2)	Sm(2)-S(8)	2.852(2)
Sm(1)-S(1)	2.8787(19)	Sb(1)-S(1)	2.366(2)
Sb(3)-S(7)	2.383(2)	Sb(1)-S(3)	2.382(2)
Sb(3)-S(6)	2.4199(19)	Sb(1)-S(2)	2.474(2)
Sb(3)-S(5)	2.458(2)	Sb(2)-S(4)	2.376(2)
Sb(4)-S(8)	2.370(2)	Sb(2)-S(2)	2.463(2)
Sb(4)-S(9)	2.408(2)	Sb(2)-S(5)	2.510(2)
Sb(4)-S(9)#1	2.606(3)		
N(5)-Sm(1)-N(1)	70.4(2)	N(8)-Sm(2)-N(6)	129.3(7)
N(5)-Sm(1)-N(3)	131.2(2)	N(8)-Sm(2)-N(9)	61.1(7)
N(1)-Sm(1)-N(3)	104.3(2)	N(6)-Sm(2)-N(9)	139.3(10)
N(5)-Sm(1)-N(2)	135.7(2)	N(8)-Sm(2)-N(10)	100.6(11)
N(1)-Sm(1)-N(2)	65.7(2)	N(6)-Sm(2)-N(10)	74.9(12)
N(3)-Sm(1)-N(2)	67.3(2)	N(9)-Sm(2)-N(10)	64.4(7)
N(5)-Sm(1)-N(4)	65.0(2)	N(8)-Sm(2)-N(7)	67.4(5)
N(1)-Sm(1)-N(4)	78.4(2)	N(6)-Sm(2)-N(7)	62.0(7)
N(3)-Sm(1)-N(4)	66.4(2)	N(9)-Sm(2)-N(7)	108.2(8)
N(2)-Sm(1)-N(4)	109.7(2)	N(10)-Sm(2)-N(7)	80.7(10)
N(5)-Sm(1)-S(4)	75.31(18)	N(8)-Sm(2)-S(7)	152.2(4)
N(1)-Sm(1)-S(4)	81.90(17)	N(6)-Sm(2)-S(7)	78.2(6)
N(3)-Sm(1)-S(4)	153.48(15)	N(9)-Sm(2)-S(7)	96.4(5)
N(2)-Sm(1)-S(4)	93.25(15)	N(10)-Sm(2)-S(7)	81.7(9)
N(4)-Sm(1)-S(4)	139.64(18)	N(8)-Sm(2)-S(8)	86.2(6)
N(5)-Sm(1)-S(3)	76.86(16)	N(6)-Sm(2)-S(8)	75.8(9)
N(1)-Sm(1)-S(3)	145.66(15)	N(9)-Sm(2)-S(8)	142.1(4)
N(3)-Sm(1)-S(3)	89.45(15)	N(10)-Sm(2)-S(8)	146.8(7)
N(2)-Sm(1)-S(3)	147.33(14)	S(7)-Sm(2)-S(8)	107.16(8)
N(4)-Sm(1)-S(3)	78.75(16)	S(1)-Sb(1)-S(3)	98.03(7)

S(4)-Sm(1)-S(3)	99.74(8)	S(1)-Sb(1)-S(2)	98.10(8)
N(5)-Sm(1)-S(1)	142.23(16)	S(3)-Sb(1)-S(2)	100.62(8)
N(1)-Sm(1)-S(1)	136.54(16)	S(4)-Sb(2)-S(2)	103.71(8)
N(3)-Sm(1)-S(1)	75.15(15)	S(4)-Sb(2)-S(5)	96.66(8)
N(2)-Sm(1)-S(1)	74.99(15)	S(2)-Sb(2)-S(5)	92.60(7)
N(4)-Sm(1)-S(1)	134.33(17)	S(7)-Sb(3)-S(6)	96.63(7)
S(4)-Sm(1)-S(1)	82.69(6)	S(7)-Sb(3)-S(5)	105.69(9)
S(3)-Sm(1)-S(1)	77.10(7)	S(6)-Sb(3)-S(5)	95.79(8)
S(8)-Sb(4)-S(9)#1	97.59(8)	S(8)-Sb(4)-S(9)	103.78(9)
S(9)-Sb(4)-S(9)#1	85.90(8)		
2			
Eu(1)-O(1)	2.278(11)	Eu(2)-O(1)	2.272(11)
Eu(1)-N(5)	2.579(14)	Eu(2)-N(9)	2.576(14)
Eu(1)-N(1)	2.580(14)	Eu(2)-N(6)	2.597(14)
Eu(1)-N(4)	2.612(14)	Eu(2)-N(10)	2.597(14)
Eu(1)-N(2)	2.613(13)	Eu(2)-N(7)	2.602(13)
Eu(1)-N(3)	2.615(14)	Eu(2)-N(8)	2.616(13)
Eu(1)-S(1)	2.803(4)	Eu(2)-S(3)	2.799(4)
Eu(1)-S(2)	2.903(4)	Eu(2)-S(2)	2.927(4)
Eu(3)-O(2)	2.293(12)	Eu(4)-O(2)	2.282(11)
Eu(3)-N(15)	2.534(14)	Eu(4)-N(20)	2.557(17)
Eu(3)-N(11)	2.539(15)	Eu(4)-N(18)	2.582(15)
Eu(3)-N(12)	2.569(16)	Eu(4)-N(17)	2.592(16)
Eu(3)-N(14)	2.593(14)	Eu(4)-N(19)	2.608(16)
Eu(3)-N(13)	2.684(16)	Eu(4)-N(16)	2.613(16)
Eu(3)-S(5)	2.831(5)	Eu(4)-S(4)	2.824(6)
Eu(3)-S(6)	2.917(5)	Eu(4)-S(6)	2.892(5)
S(1)-Sb(2)	2.389(5)	S(6)-Sb(1)	2.437(6)
S(2)-Sb(2)	2.420(4)	Sb(3)-S(8)	2.321(4)
S(3)-Sb(2)	2.395(4)	Sb(3)-S(10)	2.321(4)
S(4)-Sb(1)	2.360(6)	Sb(3)-S(7)	2.321(4)
S(5)-Sb(1)	2.378(6)	Sb(3)-S(9)	2.321(4)
O(1)-Eu(1)-N(5)	79.7(4)	O(1)-Eu(2)-N(9)	96.2(4)
O(1)-Eu(1)-N(1)	78.3(5)	O(1)-Eu(2)-N(6)	78.7(4)
N(5)-Eu(1)-N(1)	70.8(5)	N(9)-Eu(2)-N(6)	139.0(4)
O(1)-Eu(1)-N(4)	143.8(4)	O(1)-Eu(2)-N(10)	81.4(4)
N(5)-Eu(1)-N(4)	66.4(4)	N(9)-Eu(2)-N(10)	66.1(5)
N(1)-Eu(1)-N(4)	78.7(5)	N(6)-Eu(2)-N(10)	73.0(5)
O(1)-Eu(1)-N(2)	90.2(4)	O(1)-Eu(2)-N(7)	143.1(4)
N(5)-Eu(1)-N(2)	136.6(5)	N(9)-Eu(2)-N(7)	102.3(5)
N(1)-Eu(1)-N(2)	65.8(4)	N(6)-Eu(2)-N(7)	66.4(4)
N(4)-Eu(1)-N(2)	105.3(5)	N(10)-Eu(2)-N(7)	77.6(4)
O(1)-Eu(1)-N(3)	149.2(4)	O(1)-Eu(2)-N(8)	149.5(4)

N(5)-Eu(1)-N(3)	131.1(4)	N(9)-Eu(2)-N(8)	65.3(4)
N(1)-Eu(1)-N(3)	107.9(5)	N(6)-Eu(2)-N(8)	131.3(4)
N(4)-Eu(1)-N(3)	65.6(4)	N(10)-Eu(2)-N(8)	109.7(5)
N(2)-Eu(1)-N(3)	66.8(4)	N(7)-Eu(2)-N(8)	67.1(4)
O(1)-Eu(1)-S(1)	105.0(3)	O(1)-Eu(2)-S(3)	102.9(3)
N(5)-Eu(1)-S(1)	76.3(3)	N(9)-Eu(2)-S(3)	143.0(3)
N(1)-Eu(1)-S(1)	145.8(3)	N(6)-Eu(2)-S(3)	76.4(3)
N(4)-Eu(1)-S(1)	79.8(3)	N(10)-Eu(2)-S(3)	147.6(3)
N(2)-Eu(1)-S(1)	146.6(3)	N(7)-Eu(2)-S(3)	80.7(3)
N(3)-Eu(1)-S(1)	86.8(3)	N(8)-Eu(2)-S(3)	83.0(3)
O(1)-Eu(1)-S(2)	72.7(3)	O(1)-Eu(2)-S(2)	72.2(3)
N(5)-Eu(1)-S(2)	136.1(3)	N(9)-Eu(2)-S(2)	77.8(3)
N(1)-Eu(1)-S(2)	132.7(4)	N(6)-Eu(2)-S(2)	135.7(3)
N(4)-Eu(1)-S(2)	142.0(3)	N(10)-Eu(2)-S(2)	132.2(3)
N(2)-Eu(1)-S(2)	77.7(3)	N(7)-Eu(2)-S(2)	142.7(3)
N(3)-Eu(1)-S(2)	82.2(3)	N(8)-Eu(2)-S(2)	79.9(3)
S(1)-Eu(1)-S(2)	78.80(12)	S(3)-Eu(2)-S(2)	78.33(12)
O(2)-Eu(3)-N(15)	80.6(4)	O(2)-Eu(4)-N(20)	80.7(5)
O(2)-Eu(3)-N(11)	78.0(4)	O(2)-Eu(4)-N(18)	147.2(5)
N(15)-Eu(3)-N(11)	78.6(5)	N(20)-Eu(4)-N(18)	131.7(5)
O(2)-Eu(3)-N(12)	105.4(5)	O(2)-Eu(4)-N(17)	86.6(5)
N(15)-Eu(3)-N(12)	142.1(5)	N(20)-Eu(4)-N(17)	140.7(6)
N(11)-Eu(3)-N(12)	66.7(5)	N(18)-Eu(4)-N(17)	65.3(5)
O(2)-Eu(3)-N(14)	142.9(5)	O(2)-Eu(4)-N(19)	140.5(5)
N(15)-Eu(3)-N(14)	67.5(5)	N(20)-Eu(4)-N(19)	65.6(5)
N(11)-Eu(3)-N(14)	77.5(5)	N(18)-Eu(4)-N(19)	67.7(5)
N(12)-Eu(3)-N(14)	89.8(5)	N(17)-Eu(4)-N(19)	106.2(5)
O(2)-Eu(3)-N(13)	151.4(5)	O(2)-Eu(4)-N(16)	78.1(5)
N(15)-Eu(3)-N(13)	123.4(5)	N(20)-Eu(4)-N(16)	73.2(6)
N(11)-Eu(3)-N(13)	119.1(5)	N(18)-Eu(4)-N(16)	104.4(5)
N(12)-Eu(3)-N(13)	66.5(5)	N(17)-Eu(4)-N(16)	67.7(5)
N(14)-Eu(3)-N(13)	65.8(5)	N(19)-Eu(4)-N(16)	73.1(5)
O(2)-Eu(3)-S(5)	98.0(3)	O(2)-Eu(4)-S(4)	114.3(3)
N(15)-Eu(3)-S(5)	74.2(4)	N(20)-Eu(4)-S(4)	78.1(4)
N(11)-Eu(3)-S(5)	152.8(3)	N(18)-Eu(4)-S(4)	82.0(4)
N(12)-Eu(3)-S(5)	138.9(4)	N(17)-Eu(4)-S(4)	140.3(4)
N(14)-Eu(3)-S(5)	91.3(4)	N(19)-Eu(4)-S(4)	79.4(4)
N(13)-Eu(3)-S(5)	76.7(4)	N(16)-Eu(4)-S(4)	146.4(4)
O(2)-Eu(3)-S(6)	72.3(3)	O(2)-Eu(4)-S(6)	72.9(3)
N(15)-Eu(3)-S(6)	138.3(3)	N(20)-Eu(4)-S(6)	133.0(4)
N(11)-Eu(3)-S(6)	124.0(3)	N(18)-Eu(4)-S(6)	83.7(4)
N(12)-Eu(3)-S(6)	76.9(4)	N(17)-Eu(4)-S(6)	76.3(4)
N(14)-Eu(3)-S(6)	144.8(4)	N(19)-Eu(4)-S(6)	145.9(4)

N(13)-Eu(3)-S(6)	79.1(3)	N(16)-Eu(4)-S(6)	134.6(4)
S(5)-Eu(3)-S(6)	78.82(16)	S(4)-Eu(4)-S(6)	78.39(17)
S(4)-Sb(1)-S(5)	103.0(2)	S(8)-Sb(3)-S(10)	105.5(4)
S(4)-Sb(1)-S(6)	97.72(18)	S(8)-Sb(3)-S(7)	108.1(4)
S(5)-Sb(1)-S(6)	98.55(17)	S(10)-Sb(3)-S(7)	114.5(5)
S(1)-Sb(2)-S(3)	103.14(17)	S(8)-Sb(3)-S(9)	110.3(3)
S(1)-Sb(2)-S(2)	97.73(14)	S(10)-Sb(3)-S(9)	109.5(5)
S(3)-Sb(2)-S(2)	97.39(14)	S(7)-Sb(3)-S(9)	109.0(3)

Symmetry transformations used to generate equivalent atoms: (#1) -*x*+2, -*y*+2, -*z*+2.

Table S2. Hydrogen bonds for **1** [Å and deg].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N1-H1B···S4#1	0.90	2.55	3.400(7)	157.6
N5-H5B···S4#1	0.90	2.54	3.432(8)	172.6
N6-H6B···S7#2	0.90	2.81	3.67(4)	160.9
N8-H8C···S9	0.91	2.60	3.41(3)	149.5
N10-H10B···S7#2	0.90	2.65	3.55(4)	170.7

Symmetry transformations used to generate equivalent atoms: (#1) -x+1,-y+2,-z+1; (#2) -x+1,-y+1,-z+1.

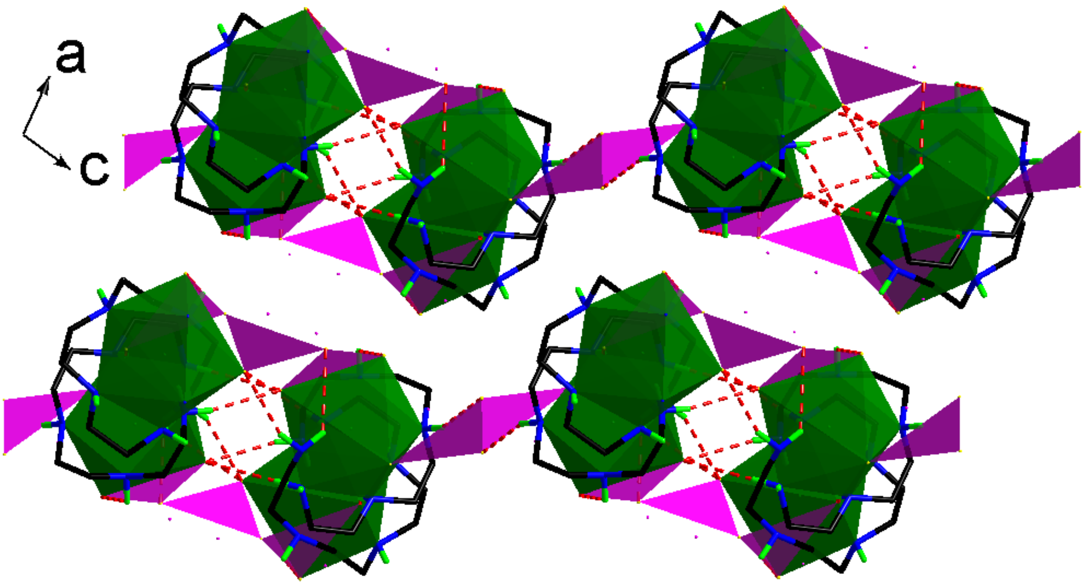

Fig. S1 View of the stacking mode for the layers in **1**.

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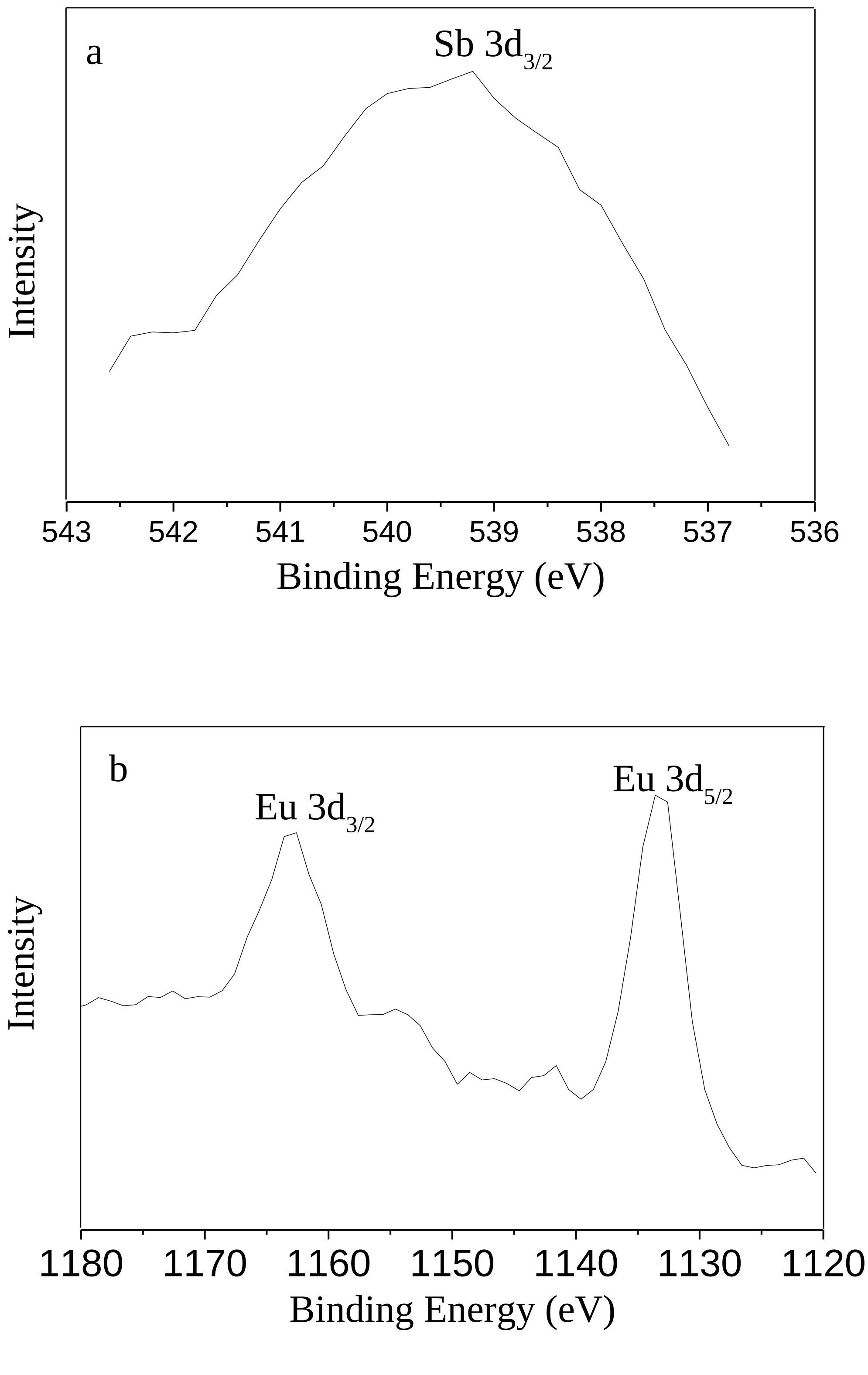

Fig. S2 XPS spectrum of Sb $3d_{3/2}$.

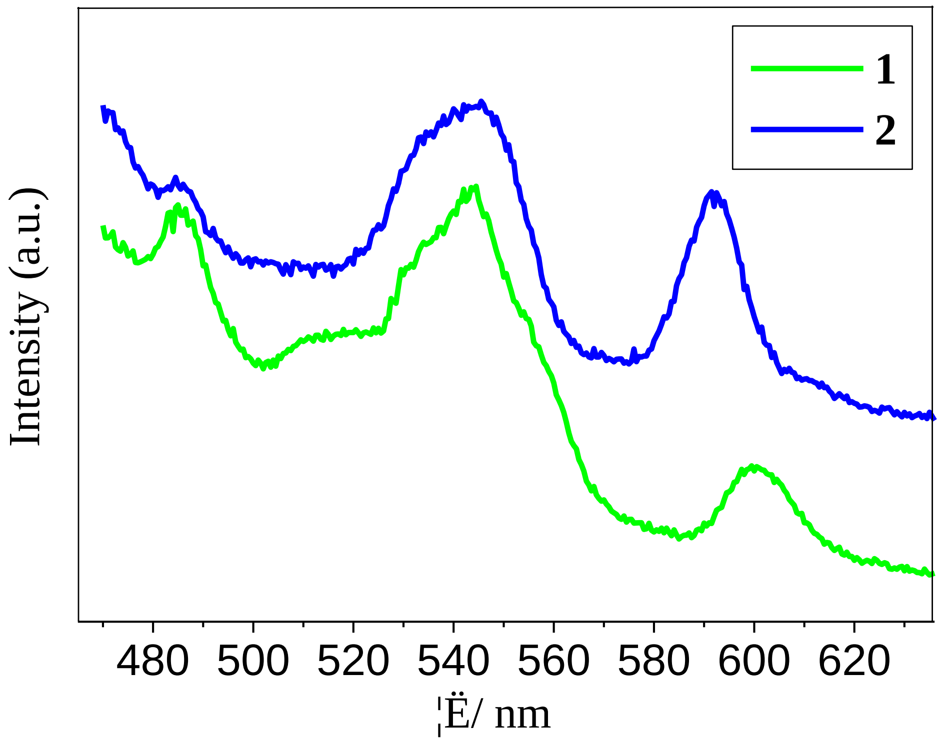

Fig. S3 Solid-state luminescence of **1** and **2** at room temperature.

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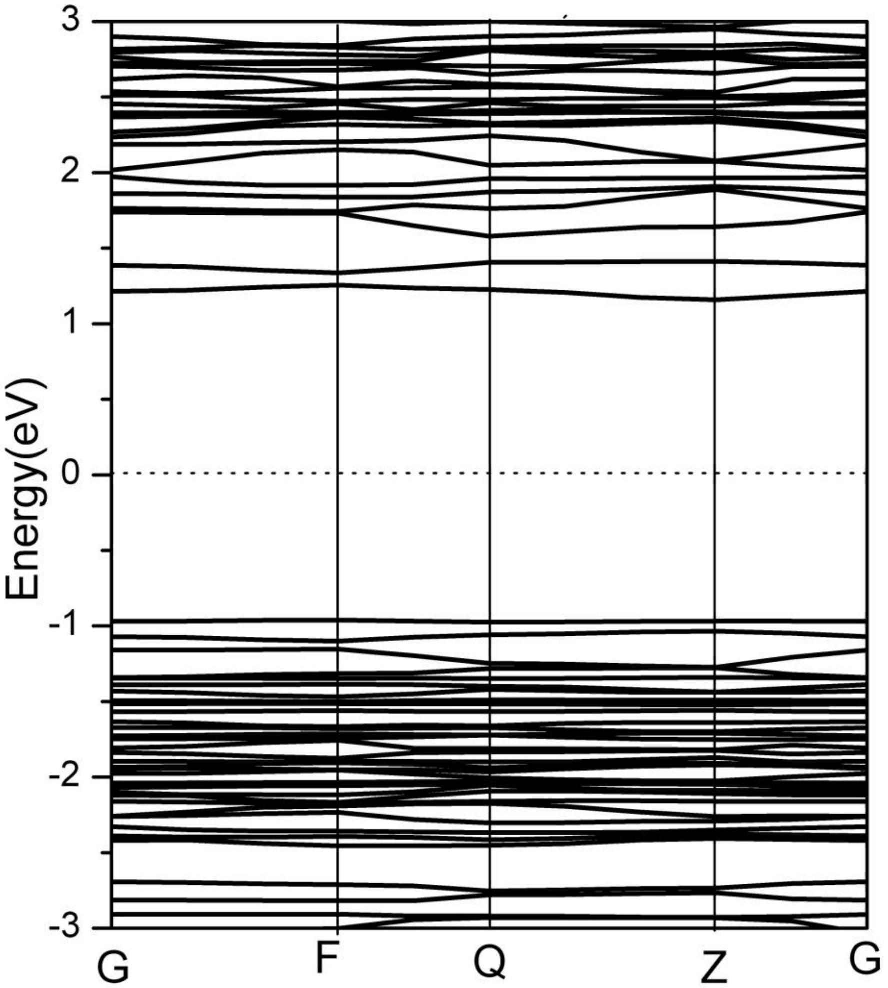

Fig. S4 Band structure of **1**. The Fermi level is set at 0 eV.

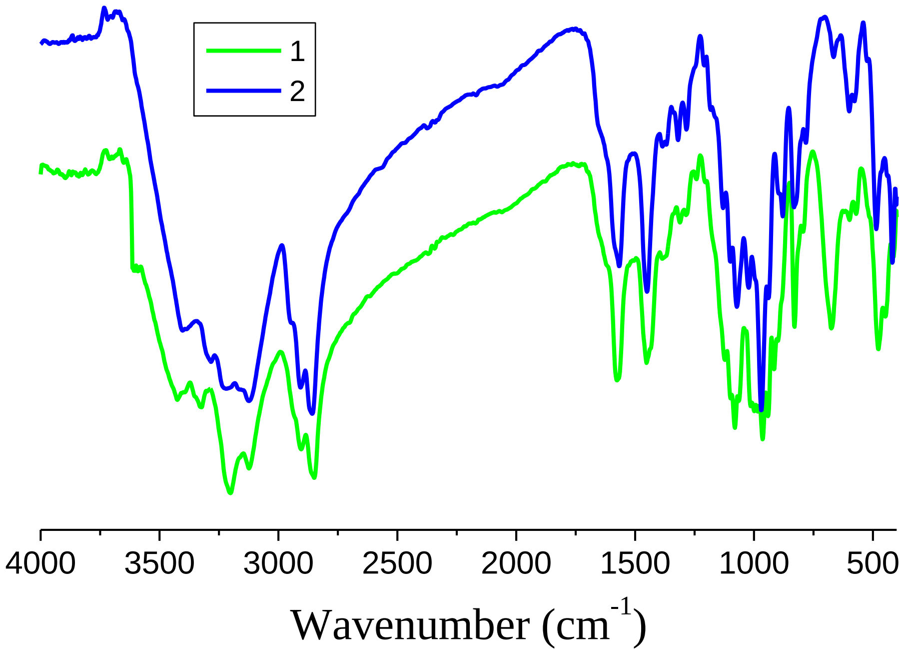

Fig. S5 IR spectra of **1** and **2**.

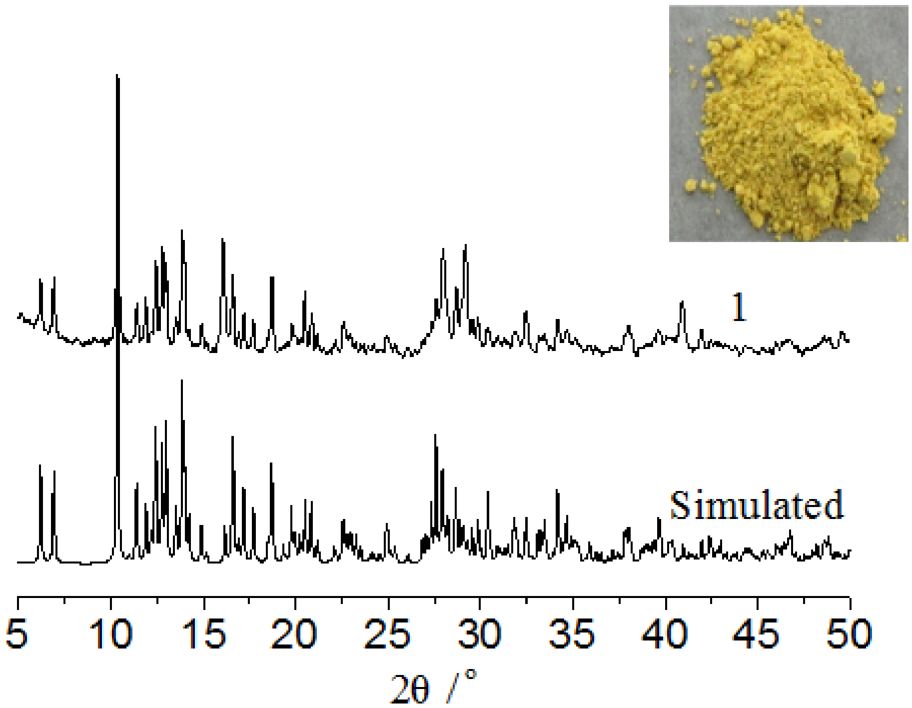

Fig. 6 Simulated and experimental powder XRD patterns of **1**.

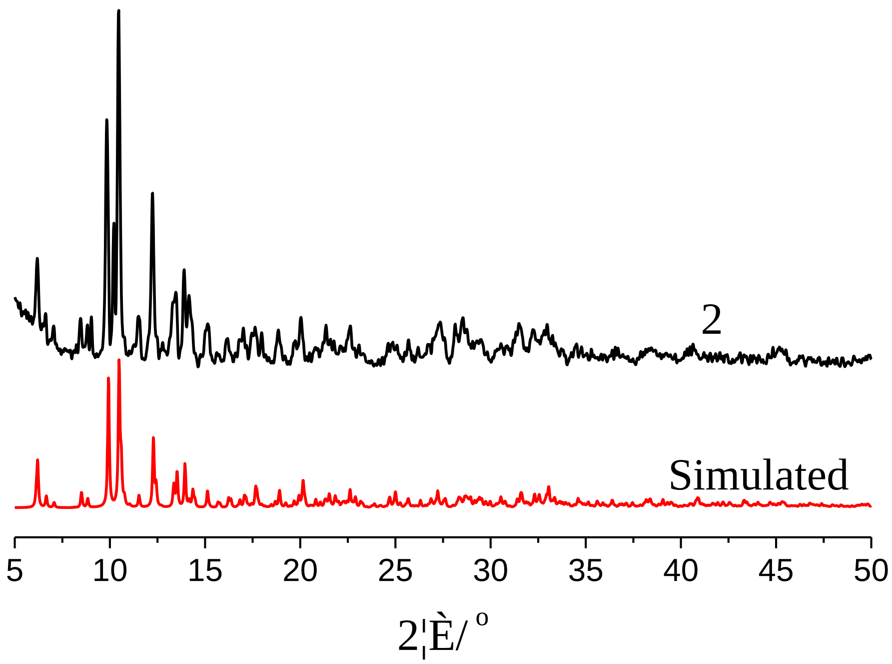

Fig. 7 Simulated and experimental powder XRD patterns of **2**.