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A series of new lanthanoid thioantimonates: The rare example of organic-decorated cationic lanthanoid thioantimonate chains based on asymmetric dinuclear lanthanide complexes

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Table S1. Hydrogen bonds for **1** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1A...S4#1	0.90	2.85	3.646(3)	148.5
N2-H2...S2#2	0.91	2.42	3.316(3)	166.3
N3-H3...S2	0.91	2.70	3.372(3)	131.3
N4-H4A...S1#3	0.90	2.66	3.556(3)	173.3
N4-H4B...S3#4	0.90	2.63	3.475(3)	156.3
N5-H5A...S2#2	0.90	2.58	3.378(3)	147.6
N5-H5B...S3#4	0.90	2.65	3.518(3)	162.8
N6-H6...S4#1	0.91	2.48	3.368(3)	163.8
N7-H7...S1#3	0.91	2.55	3.432(3)	164.3
N8-H8A...S1	0.90	2.72	3.516(3)	148.0
N8-H8B...S4#5	0.90	2.53	3.379(3)	157.7

Symmetry transformations used to generate equivalent atoms: (#1) x,y-1,z; (#2) -x,y-1/2,-z+1/2; (#3) -x,-y+1,-z; (#4) -x-1/2,y-1/2,z; (#5) -x+1/2,y-1/2,z.

Table S2. Hydrogen bonds for **4** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1D...S7	0.90	2.91	3.696(7)	146.2
N2-H2C...S7#2	0.91	2.49	3.368(6)	161.7
N3-H3C...S3#3	0.91	2.99	3.630(6)	128.9
N4-H4C...Cl1	0.91	2.74	3.442(7)	134.6
N4-H4C...S1	0.91	2.89	3.367(6)	114.1
N5-H5C...S7#2	0.90	2.81	3.590(7)	145.7
N5-H5D...S5	0.90	2.65	3.419(7)	143.6
N6-H6C...S5	0.90	2.80	3.618(8)	150.9
N6-H6C...S4	0.90	3.01	3.641(7)	128.5
N6-H6D...Cl1#4	0.90	2.61	3.397(8)	146.0
N9-H9C...Cl1#4	0.91	2.42	3.319(8)	170.5
N10-H10C...S7	0.90	2.86	3.589(8)	139.3
N11-H11C...S6#5	0.90	2.73	3.456(7)	139.0
N12-H12C...S6	0.91	2.54	3.378(7)	153.4
N13-H13C...S4#1	0.91	2.48	3.385(7)	176.0
N14-H14C...S6#5	0.91	2.62	3.521(7)	170.1

N15-H15D...Cl1#4	0.90	2.96	3.561(7)	125.3
O1-H1W...S5	0.97(2)	2.47(5)	3.328(5)	148(6)
O2-H2W...S6#1	0.94(2)	2.51(4)	3.362(5)	151(7)
O2-H2W...S4#1	0.94(2)	2.85(7)	3.388(5)	117(6)

Symmetry transformations used to generate equivalent atoms: (#1) -*x*+1, -*y*, -*z*+1; (#2) -*x*+3/2, *y*+1/2, *z*; (#3) -*x*+1, *y*+1/2, -*z*+3/2; (#4) -*x*+1/2, *y*-1/2, *z*; (#5) *x*-1/2, -*y*+1/2, -*z*+1.

Table S3. Hydrogen bonds for **7** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O2-H2E...O3W	0.90	2.37	3.043(14)	132.0
N1-H1C...S4	0.90	2.55	3.434(3)	167.1
N1-H1D...S2#2	0.90	2.66	3.547(3)	170.8
N2-H2C...Cl1	0.91	2.41	3.279(4)	159.5
N3-H3C...S3	0.91	2.57	3.123(3)	120.1
N4-H4C...S1#1	0.91	2.55	3.415(4)	159.6
N6-H6C...S2#2	0.90	2.74	3.575(4)	154.5
N6-H6D...Cl1#3	0.90	2.54	3.378(3)	155.1
N5-H5D...S2	0.90	2.56	3.441(3)	166.5
N7-H7C...Cl1	0.91	2.59	3.399(4)	148.8
N8-H8C...O3W	0.91	2.39	3.138(14)	140.0
N8-H8C...S1#1	0.91	3.00	3.451(4)	112.2
N9-H9C...Cl1#3	0.91	2.51	3.398(3)	165.8
N10-H10C...S4#2	0.90	2.71	3.485(4)	144.6
N10-H10D...S3#1	0.90	2.59	3.476(3)	167.5
O3W-H3WA...Cl1#4	0.85	2.25	3.103(15)	176.8
O3W-H3WB...S1#1	0.85	2.25	3.103(13)	176.8
O1-H1...S(2)#2	0.96(4)	2.32(4)	3.221(3)	157(4)

Symmetry transformations used to generate equivalent atoms: (#1) -*x*+1, *y*+1/2, -*z*+1/2; (#2) -*x*+1, -*y*+1, -*z*+1; (#3) -*x*, *y*+1/2, -*z*+1/2; (#4) -*x*, -*y*+1, -*z*.

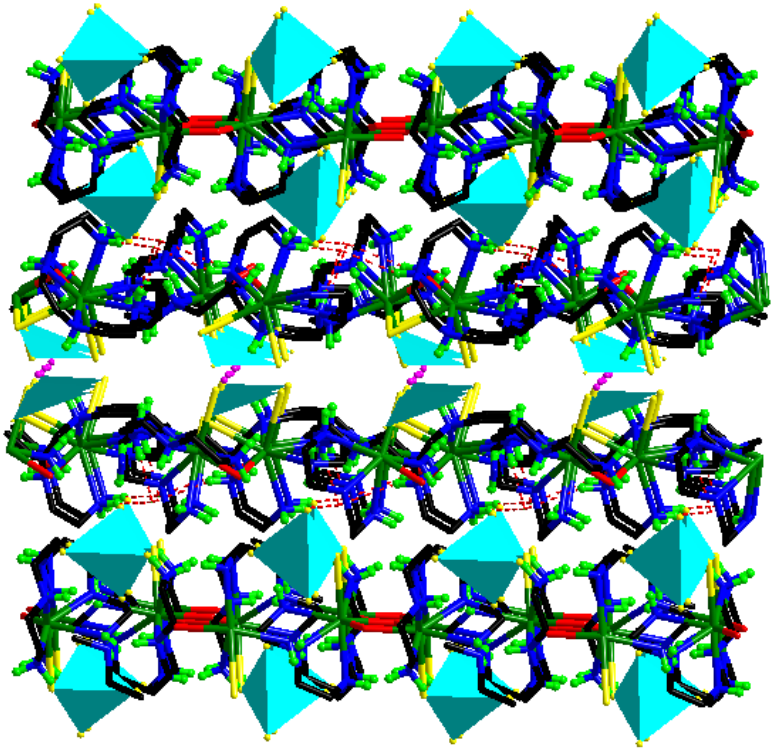

Figure S1 The 3-D H-bonding network structure in **4**(blue polyhedron: [SbS_3] and [SbS_4]).

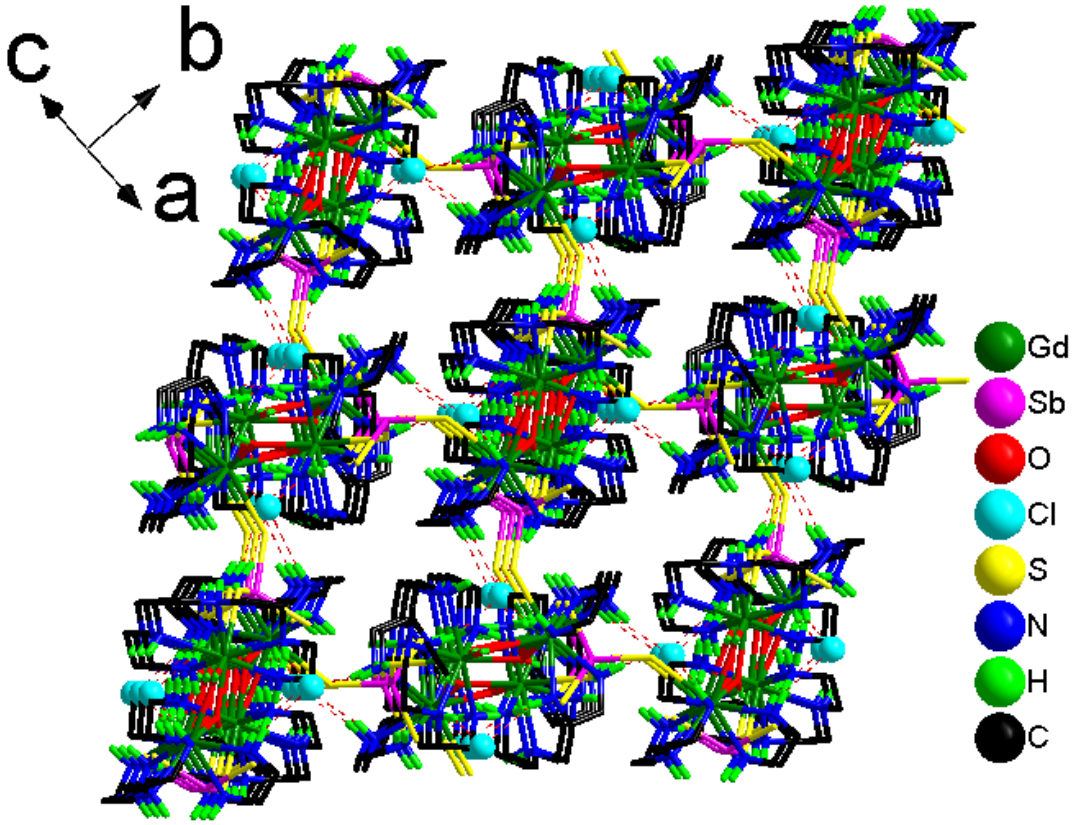

Figure S2 The 3-D H-bonding network structure in **7**.

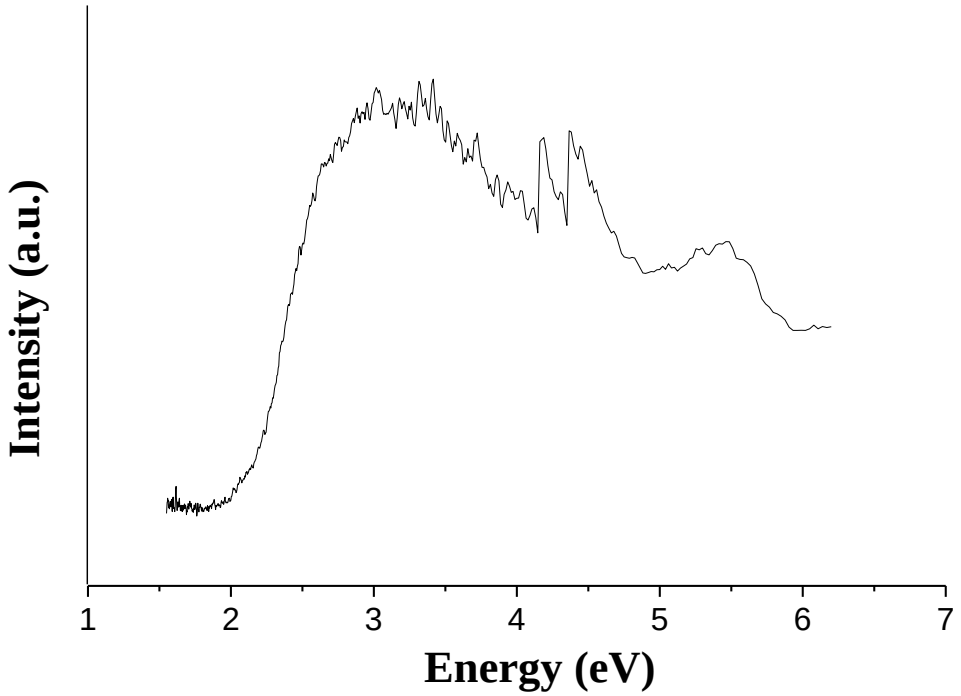

Figure S3 Optical absorption spectrum of **2**.

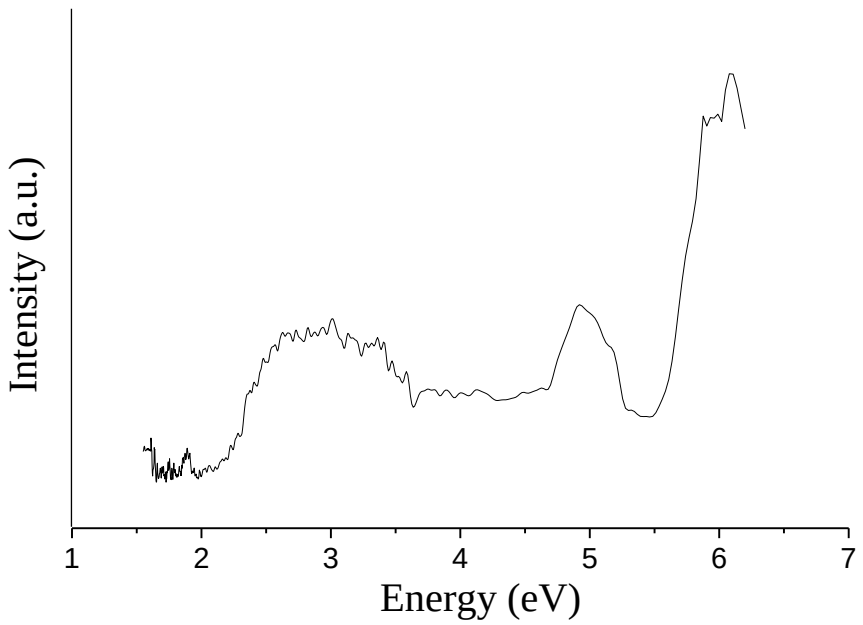

Figure S4 Optical absorption spectrum of **3**.

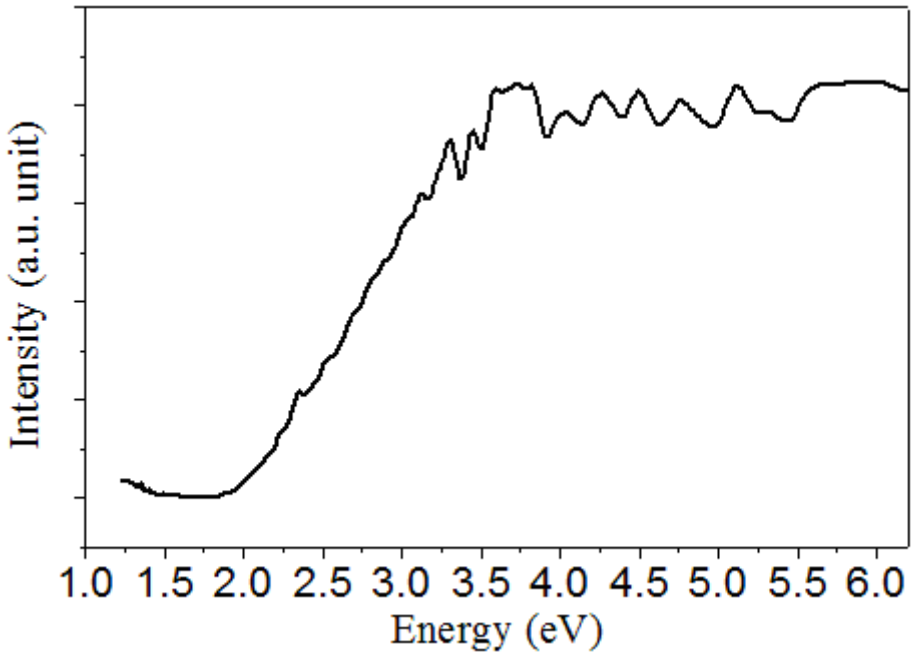

Figure S5 Solid-state optical absorption spectrum of **5**.

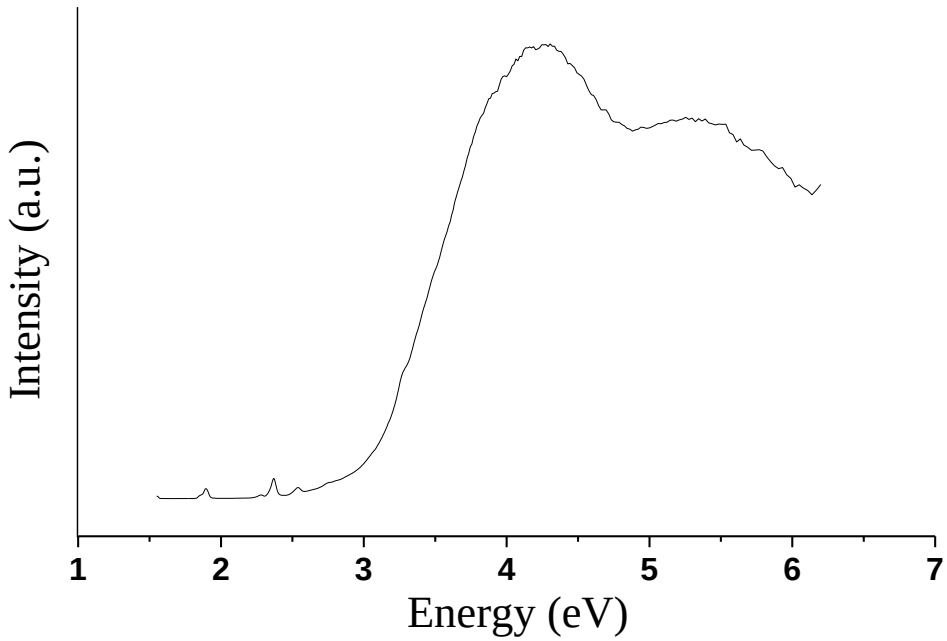

Figure S6 Solid-state optical absorption spectrum of **6**.

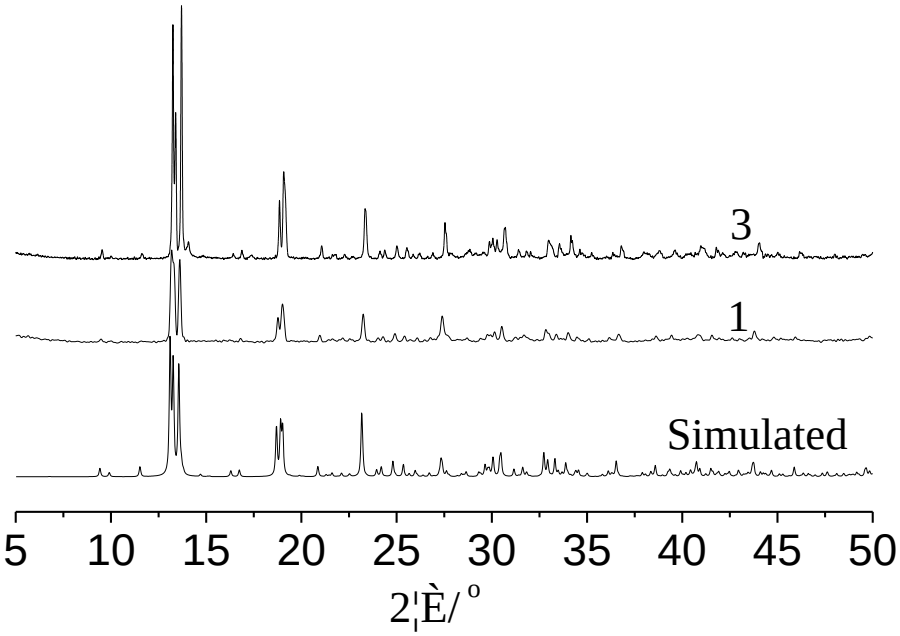

Figure S7 Simulated and experimental powder XRD patterns of **1** and **3**.

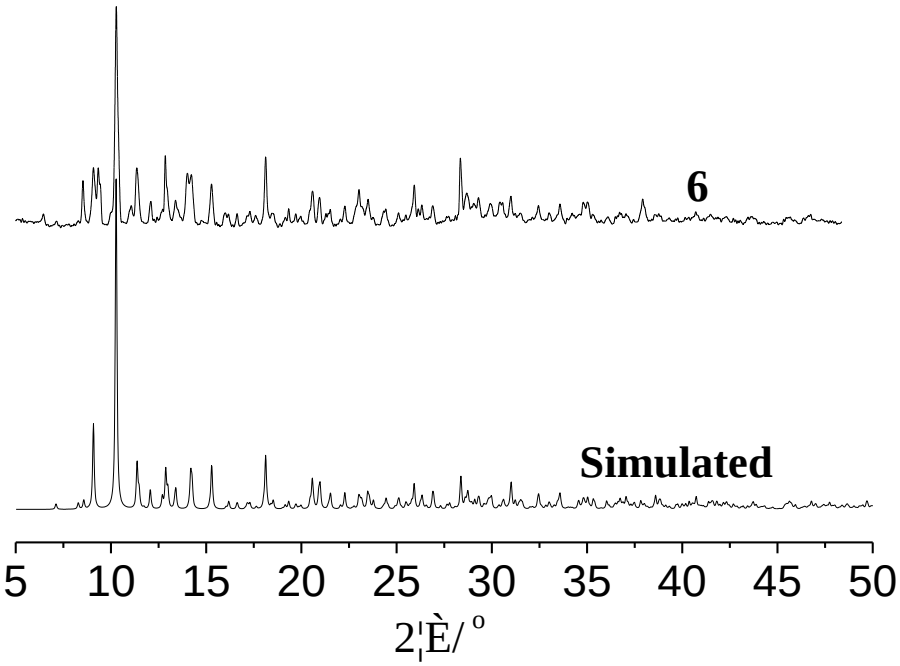

Figure S8 Simulated and experimental powder XRD patterns of **6**.

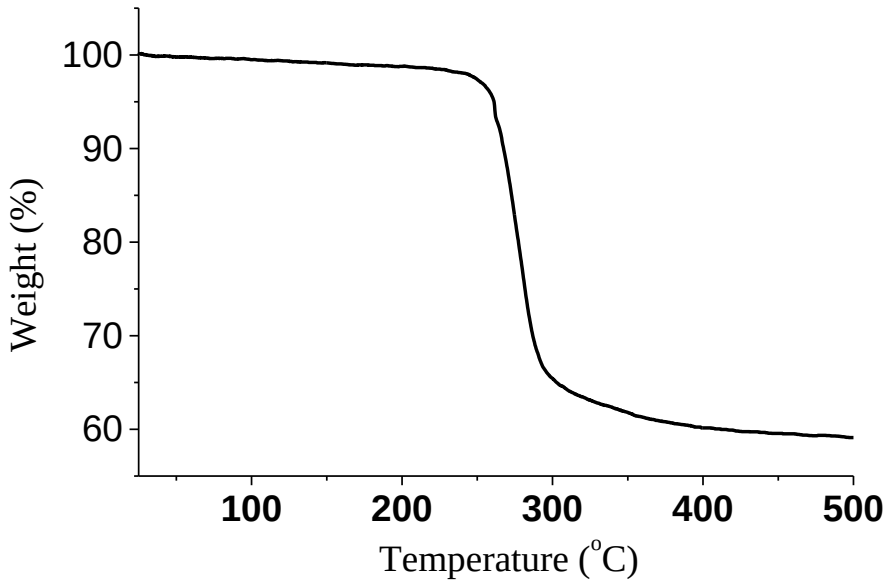

Figure S9 TG curves of **5**.

The thermal stabilities of **5** are investigated under a N_2 atmosphere with a heating rate of 10 °C·min^{-1}. Their TG curves show that one-step weight losses (38.23 %) occur in the range of 25-450 °C, assigned to the removal of the H_2O molecules and decomposition of organic species (calcd. 37.66 %).