

# The Syntheses, Crystal Structures and Photocatalytic Properties of a Series of Mercury Thioantimonates Directed by Transition Metal Complexes

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Supplementary Information

**Table S1.** Hydrogen bonds data for compound 1.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1D)...S(2)#2	0.90	2.86	3.641(5)	145.3
N(2)-H(2C)...S(2)#3	0.90	2.60	3.375(5)	144.5
N(2)-H(2D)...S(1)#1	0.90	2.75	3.564(5)	150.7
N(3)-H(3D)...S(2)#3	0.90	2.99	3.766(7)	146.0

Symmetric codes: #1  $-x+1/2, y+1/2, -z+1/2$ ; #2  $x-1/2, y-1/2, z$ ; #3  $-x+1/2, -y+1/2, -z+1$ .

**Table S2.** Selected hydrogen bonds data for compound **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(10)-H(10A)...S(2)	0.90	2.61	3.500(9)	172.6
N(10)-H(10B)...S(2)#2	0.90	2.66	3.446(8)	146.8
N(6)-H(6A)...Cl(1)#3	0.90	2.79	3.648(10)	159.6
N(2)-H(2A)...Cl(1)#4	0.90	2.77	3.580(8)	150.7
N(2)-H(2B)...S(2)#2	0.90	2.75	3.555(8)	148.9
N(2)-H(2B)...S(1)#4	0.90	3.00	3.672(7)	132.6
N(4)-H(4A)...Cl(1)	0.90	2.51	3.387(9)	166.3
N(4)-H(4B)...S(1)#4	0.90	2.74	3.561(9)	152.4
N(3)-H(3A)...Cl(1)#4	0.90	2.68	3.571(9)	172.4
N(3)-H(3B)...S(7)	0.90	2.84	3.711(9)	162.7
N(8)-H(8A)...Cl(1)#3	0.90	2.66	3.539(9)	166.8
N(8)-H(8B)...S(6)#1	0.90	2.62	3.457(8)	155.4
N(1)-H(1B)...S(7)	0.90	2.76	3.602(9)	156.6
N(12)-H(12A)...S(5)#1	0.90	3.00	3.886(11)	166.6
N(12)-H(12B)...S(4)#1	0.90	2.77	3.350(9)	123.1
N(12)-H(12B)...S(3)#1	0.90	2.99	3.845(10)	160.2
N(5)-H(5A)...S(2)	0.90	2.69	3.474(9)	146.7
N(5)-H(5A)...S(4)	0.90	2.93	3.426(8)	116.2
N(5)-H(5B)...S(6)#5	0.90	2.97	3.661(8)	135.3
N(11)-H(11A)...S(7)	0.90	2.98	3.765(13)	146.1
N(11)-H(11B)...S(3)#5	0.90	2.62	3.341(10)	137.1
N(9)-H(9B)...S(1)#6	0.90	2.86	3.745(10)	167.3
N(7)-H(7A)...S(7)	0.90	2.76	3.664(11)	177.8
N(7)-H(7B)...S(3)#1	0.90	2.54	3.370(9)	153.2

Symmetry transformations used to generate equivalent atoms: #1  $x, -y+1/2, z+1/2$ ; #2  $-x+1, -y+1, -z$ ; #3  $x-1, y, z$ ; #4  $-x+1, y+1/2, -z+1/2$ ; #5  $-x, -y+1, -z$ ; #6  $-x, y+1/2, -z+1/2$ .

**Table S3.** Hydrogen bonds data for compound **3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...S(5)	0.90	2.65	3.516(8)	161.3
N(2)-H(2B)...S(1)#2	0.90	2.66	3.491(8)	153.5
N(3)-H(3A)...S(3)#2	0.90	2.65	3.533(8)	166.1
N(4)-H(4A)...S(4)#3	0.90	2.96	3.483(6)	118.8
N(4)-H(4B)...S(5)#4	0.90	2.84	3.741(7)	176.3
N(5)-H(5A)...S(2)#3	0.90	2.62	3.492(8)	163.0
N(5)-H(5B)...S(2)#1	0.90	2.99	3.810(8)	152.8
N(6)-H(6A)...S(5)	0.90	2.86	3.684(7)	152.2
N(6)-H(6A)...S(4)	0.90	3.01	3.515(6)	117.0
N(6)-H(6B)...S(2)#1	0.90	2.69	3.584(6)	172.3

Symmetric codes: #1 -x+1, y+1/2, -z-1/2, #2 x-1, y, z, #3 x, -y-1/2, z+1/2, #4 -x+1, -y-1, -z.

**Table S4.** Selected hydrogen bonds data for compound **4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4A)...S(4)#1	0.90	2.75	3.624(6)	164.2
N(4)-H(4A)...S(1)	0.90	2.99	3.468(6)	115.4
N(4)-H(4B)...S(4)	0.90	2.69	3.530(5)	156.8
N(6)-H(6C)...S(3)#2	0.90	2.75	3.646(6)	172.8
N(6)-H(6D)...S(1)	0.90	2.80	3.517(6)	137.6
N(5)-H(5A)...S(3)#3	0.91	2.70	3.524(6)	150.3
N(1)-H(1A)...S(1)	0.90	2.53	3.288(6)	142.4
N(1)-H(1B)...S(1)#2	0.90	2.57	3.452(6)	167.7
N(3)-H(3A)...S(1)#2	0.90	2.86	3.589(7)	139.2
N(3)-H(3A)...S(3)#2	0.90	2.93	3.605(7)	133.5

Symmetric codes: #1 -x+1, y-1/2, -z+3/2; #2 -x, -y+1, -z+1; #3 -x, y-1/2, -z+1/2.

**Table S5.** The hydrogen bonds data for compounds **5-7**.

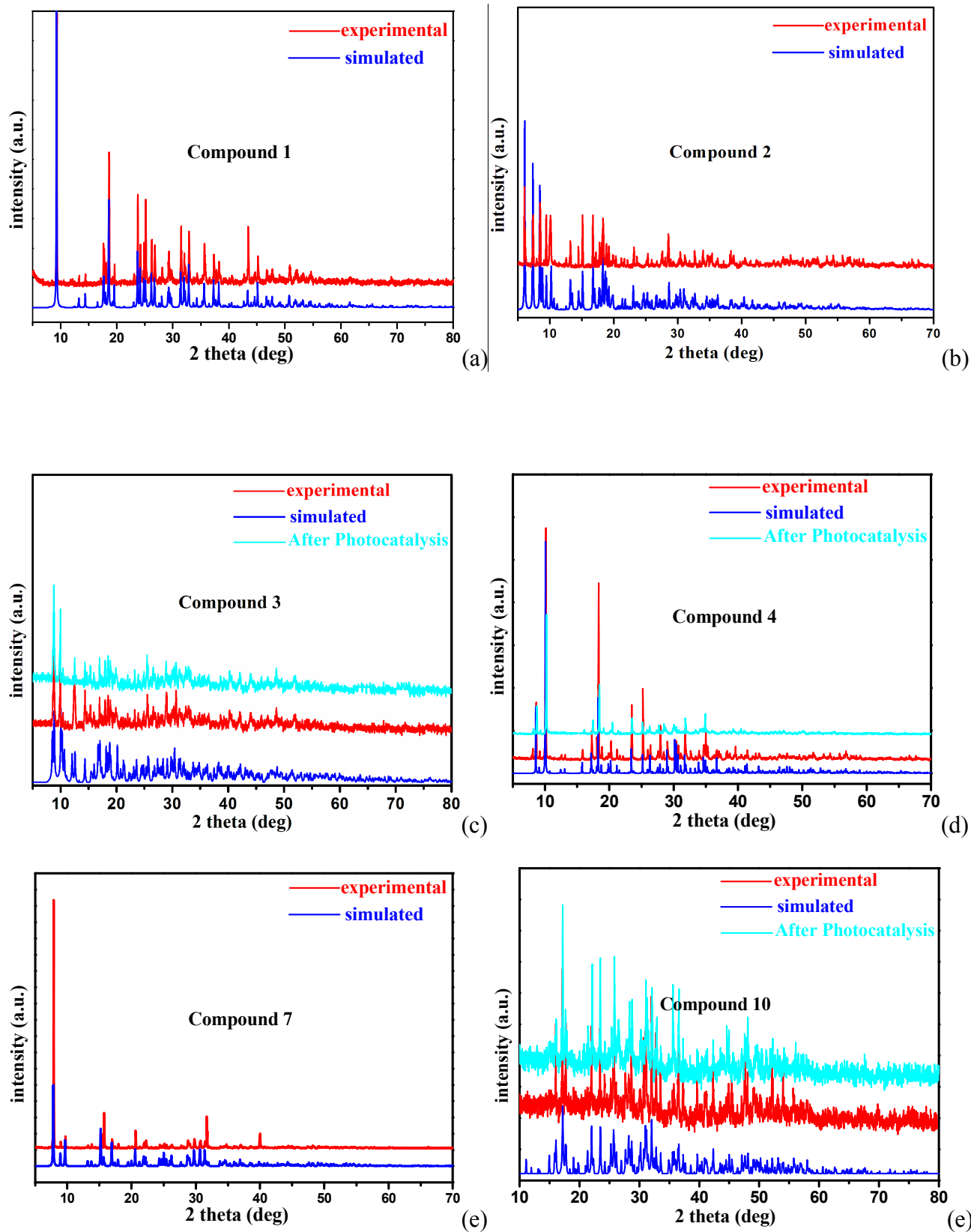
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
<b>5</b>				
N(4)-H(4C)...S(4)#2	0.90	2.65	3.499(10)	158.2
N(4)-H(4C)...S(1)	0.90	2.94	3.479(9)	119.8
N(4)-H(4D)...S(5)#3	0.90	2.93	3.589(9)	131.3
N(3)-H(3C)...S(3)#4	0.90	2.77	3.580(10)	149.8
N(3)-H(3D)...S(2)#1	0.90	2.75	3.591(10)	156.5
N(2)-H(2C)...S(3)#3	0.90	2.82	3.657(11)	155.3
<b>6</b>				
N(3)-H(3C)...S(2)#1	0.90	2.71	3.536(6)	153.9
N(3)-H(3D)...S(3)#2	0.90	2.69	3.518(6)	152.7
N(2)-H(2D)...S(3)#3	0.90	2.81	3.634(7)	153.3
N(4)-H(4D)...S(4)	0.90	2.67	3.498(6)	153.1
N(4)-H(4D)...S(1)	0.90	2.84	3.429(6)	124.2
<b>7</b>				
N(3)-H(3C)...S(2)#1	0.90	2.70	3.531(5)	153.7
N(3)-H(3D)...S(3)#2	0.90	2.69	3.511(5)	152.7
N(4)-H(4C)...S(5)#3	0.90	2.87	3.636(5)	143.2
N(4)-H(4D)...S(4)#1	0.90	2.67	3.498(5)	152.7
N(4)-H(4D)...S(1)	0.90	2.83	3.426(4)	124.5
N(2)-H(2D)...S(3)#3	0.90	2.82	3.641(5)	152.9

Symmetric codes: #1 -x,-y,-z+1, #2 -x+1,-y,-z+1, #3 -x+1,-y+1,-z+1, #4 -x,-y+1,-z+1 for **5**; #1 -x+1,-y+1,-z+1, #2 -x+1,-y,-z+1, #3 -x,-y,-z+1 for **6**; #1 -x+1,-y+1,-z+1, #2 -x+1,-y,-z+1, #3 -x,-y,-z+1 for **7**.

**Table S6.** Selected hydrogen bonds data for compounds **8-10**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
<b>8</b>				
N(1)-H(1C)...S(5)#3	0.91	2.67	3.538(5)	158.8
N(2)-H(2C)...S(2)#2	0.90	2.75	3.391(5)	129.2
N(2)-H(2D)...S(3)#1	0.90	2.73	3.552(5)	152.6
N(3)-H(3C)...S(3)#4	0.90	2.75	3.642(5)	170.3
N(3)-H(3D)...S(5)#5	0.90	2.83	3.653(5)	152.0
<b>9</b>				
N(3)-H(3C)...S(5)#3	0.91	2.68	3.543(6)	159.5
N(2)-H(2C)...S(2)#2	0.90	2.76	3.404(6)	129.2
N(2)-H(2D)...S(3)#1	0.90	2.73	3.547(6)	152.3
N(1)-H(1C)...S(3)#4	0.90	2.75	3.641(6)	169.9
N(1)-H(1D)...S(5)#5	0.90	2.84	3.654(7)	151.6
<b>10</b>				
N(3)-H(3C)...S(5)#3	0.91	2.67	3.538(6)	159.4
N(2)-H(2C)...S(5)#3	0.90	2.78	3.607(7)	153.7
N(2)-H(2D)...S(3)#4	0.90	2.72	3.611(6)	168.5
N(1)-H(1C)...S(3)#1	0.90	2.76	3.565(6)	149.2
N(1)-H(1D)...S(2)#2	0.90	2.78	3.407(6)	127.7

Symmetric codes: #1 -x+1,-y,-z, #2 -x+1,y-1/2,-z+1/2, #3 -x,y-1/2,-z-1/2, #4 x-1,y-1,z, #5 x,-y-1/2,z+1/2 for **8**; #1 -x, -y-1, -z, #2 -x, y-1/2, -z+1/2, #3 -x-1, y-1/2, -z-1/2, #4 x-1, y-1, z, #5 x, -y-3/2, z+1/2 for **9**; #1 -x+1,-y+2,-z, #2 -x+1,y+1/2,-z+1/2, #3 x,-y+5/2,z+1/2, #4 x-1,y+1, z for **10**.



**Figure S1.** Experimental and simulated XRD powder pattern for compounds **1** (a), **2** (b), **3** (b), **4** (c), **7** (d) and **10** (e) before and after the visible photocatalysis.