Electronic Supplementary Material (ESI) for Dalton Transactions.

$[Mn_2Ga_4Sn_4S_{20}]^{8-}$ T3 Supertetrahedral Nanocluster Directed by a Series of Transition Metal Complexes

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

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(3)-H(3A)...S(1)#1	0.90	2.69	3.557(6)	163.0
N(3)-H(3B)...S(2)	0.90	2.87	3.631(6)	143.5
N(1)-H(1A)...S(4)#2	0.90	2.76	3.557(6)	148.5
N(4)-H(4B)...S(5)#2	0.90	2.48	3.372(6)	170.3
N(2)-H(2A)...S(1)#1	0.90	2.69	3.541(6)	158.4
N(5)-H(5A)...S(2)	0.90	2.73	3.515(5)	146.7
O(1)-H(2)...S(5)	0.853(10)	2.51(3)	3.344(17)	167(12)

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

Table S2. Hydrogen bonds data for compound **2**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(12)-H(12C)...S(1)#2	0.91	2.83	3.551(2)	136.6
N(11)-H(11C)...S(10)#1	0.90	2.86	3.538(2)	133.3
N(11)-H(11D)...S(4)#1	0.90	2.79	3.5876(18)	148.9
N(10)-H(10C)...S(3)#3	0.90	2.79	3.586(3)	148.0
N(10)-H(10D)...S(3)#4	0.90	2.58	3.436(2)	158.1
N(5)-H(5C)...S(1)#5	0.90	2.87	3.657(3)	146.4
N(5)-H(5D)...S(2)#6	0.90	2.57	3.414(2)	157.3

N(8)-H(8C)...S(3)#3	0.90	2.68	3.548(2)	163.5
N(4)-H(4C)...S(8)	0.90	2.81	3.572(2)	142.8
N(4)-H(4D)...O(1)	0.90	2.55	3.241(6)	134.1
N(6)-H(6C)...S(8)#7	0.91	2.54	3.352(2)	149.3
N(7)-H(7D)...S(5)#4	0.90	2.61	3.492(2)	165.9
N(3)-H(3C)...O(1)	0.90	2.40	3.086(6)	133.5
N(3)-H(3D)...S(9)	0.90	3.00	3.776(4)	145.3

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

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

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(4)-H(4C)...S(1)#1	0.91	2.67	3.526(5)	157.4
N(3)-H(3C)...S(5)#2	0.90	2.81	3.657(6)	157.8
N(3)-H(3D)...S(3)	0.90	2.99	3.636(7)	130.6
N(2)-H(2C)...S(1)#3	0.91	2.88	3.647(5)	143.1
N(1)-H(1C)...S(3)	0.90	2.80	3.400(5)	125.7
N(1)-H(1D)...S(4)#2	0.90	2.70	3.478(6)	144.8

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

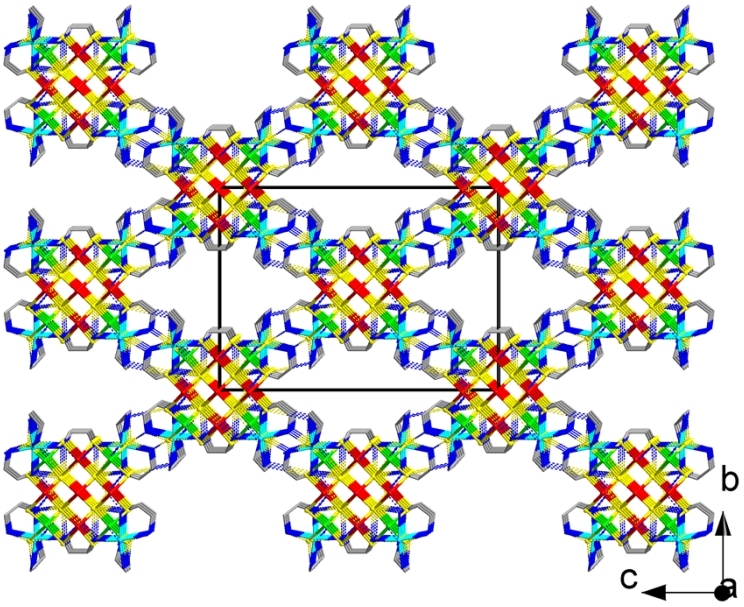


Fig. S1. The 3D H-bonding network of compound **1**. The N-H···S hydrogen bonds are showed as dotted line.

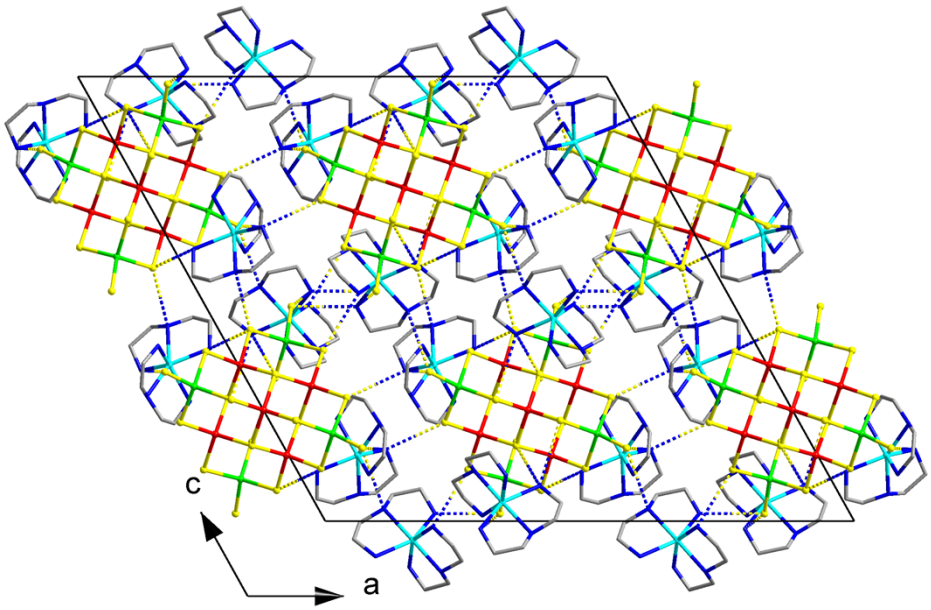


Fig. S2. View of the $[Mn(dien)_2]^{2+}$ complex (a), and the 3D H-bonding network of compound **2** (b). The N-H···S hydrogen bonds are showed as dotted line.

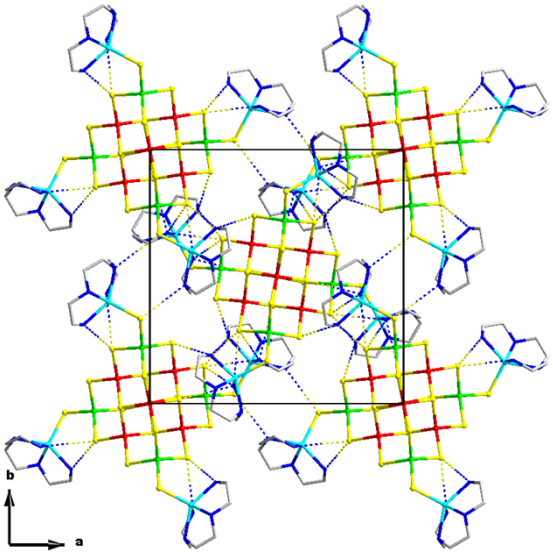
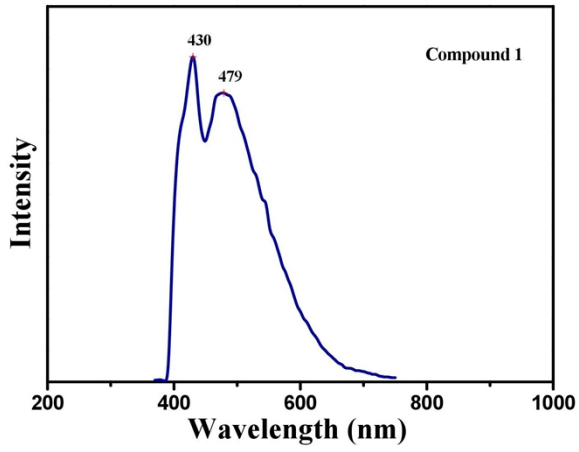
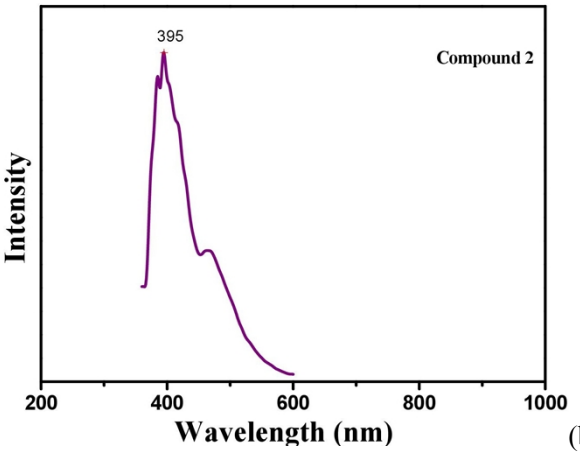


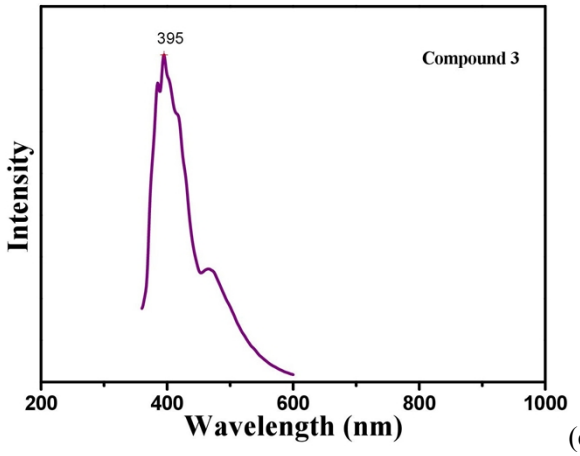
Fig S3. The 3D H-bonding network of compound **3** (b).The N-H···S hydrogen bonds are showed as dotted line.



(a)



(b)



(c)

Fig. S4. Photoluminescent emission spectra of the title compounds.

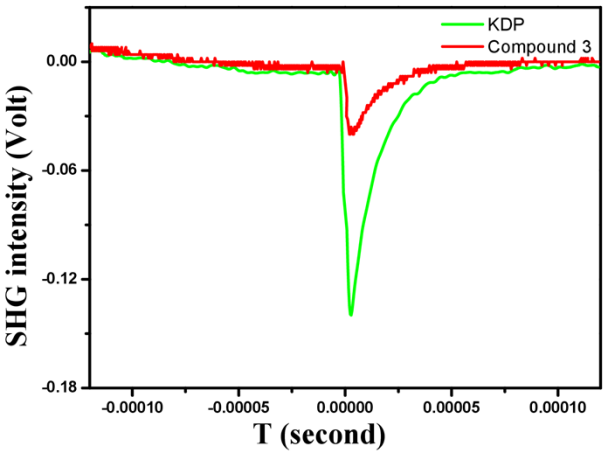
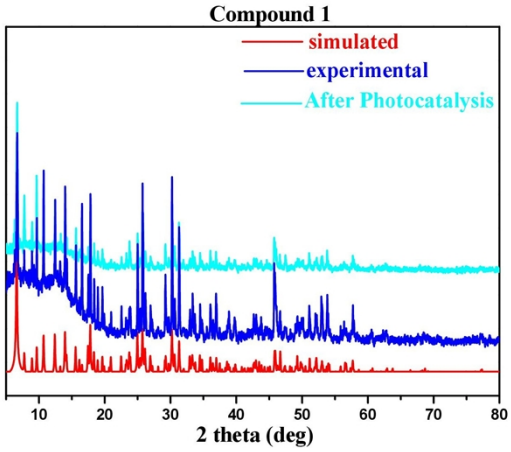
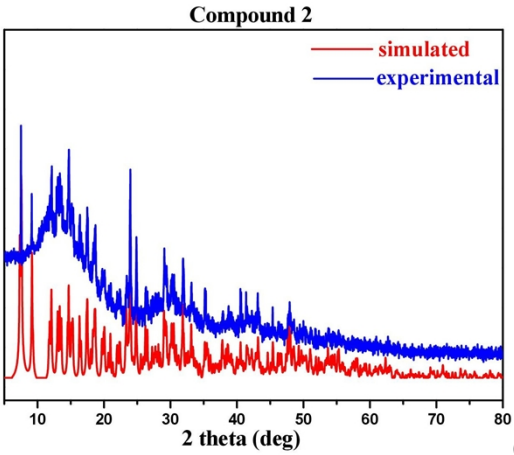


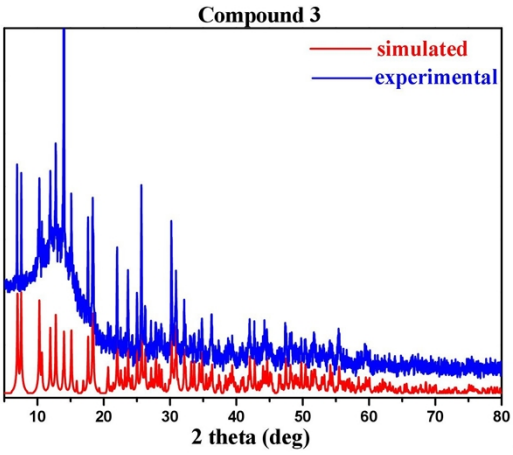
Fig. S5. SHG responses of compound **3** (red) and KDP (green) at 1.064 μm.



(a)



(b)



(c)

Fig. S6. Experimental and simulated XRD powder patterns for **1** (a), **2** (b) and **3** (b) as well as the experimental XRD powder pattern after the visible photocatalysis for **1**.