Electronic Supplementary Material (ESI) for RSC Advances.

Extended Structural Materials Composed of Transition-Metal-Substituted Arsenicniobates and Their Photocatalytic Activity

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Table S1. Bond valence sum calculations of compound **1.**[S1,S2]

Bonds	Bond length (Å)	BVS	Bonds	Bond length (Å)	BVS
V(1)-O(14)	1.617(9)	1.570	V(2)-O(33)	1.623(9)	1.545
V(1)-O(8)	1.920(8)	0.691	V(2)-O(19)	1.924(8)	0.685
V(1)-O(6)	1.923(8)	0.687	V(2)-O(26)	1.927(8)	0.679
V(1)-O(16)	2.025(8)	0.521	V(2)-O(13)	1.986(9)	0.579
V(1)-O(3)	2.041(8)	0.499	V(2)-O(37)	2.030(9)	0.514
$\boldsymbol{V}_{V_{(1)}} = 3.968$			$\boldsymbol{V}_{V_{(2)}} = 4.002$		
V(3)-O(41)	1.620(9)	1.558	V(4)-O(34)	1.618(9)	1.566
V(3)-O(24)	1.903(9)	0.725	V(4)-O(10)	1.923(8)	0.725
V(3)-O(2)	1.915(8)	0.702	V(4)-O(5)	1.936(8)	0.702
V(3)-O(22)	2.005(8)	0.550	V(4)-O(12)	2.005(9)	0.550
V(3)-O(9)	2.027(8)	0.519	V(4)-O(7)	2.017(9)	0.519
$\boldsymbol{V}_{V_{(3)}} = 4.054$			$\boldsymbol{V}_{V_{(4)}} = 4.062$		

Table S2. Bond valence sum calculations of compound **2.**[S1,S2]

Bonds	Bond length (Å)	BVS	Bonds	Bond length (Å)	BVS
V(1)-O(13)	1.633(8)	1.501	V(2)-O(9)	1.644(9)	1.460
V(1)-O(10)	1.955(10)	0.630	V(2)-O(12)#1	1.957(11)	0.627
V(1)-O(6)	1.978(10)	0.592	V(2)-O(15)	1.969(11)	0.607
V(1)-O(2)	1.981(9)	0.587	V(2)-O(7)	1.995(11)	0.565
V(1)-O(8)	1.992(10)	0.570	V(2)-O(3)#1	2.001(9)	0.556
V(1)-O(22)#1	2.444(13)	0.168	V(2)-O(21)#1	2.420(13)	0.179
V(1)-O(24)	2.461(14)	0.160			
$\boldsymbol{V}_{V_{(1)}} = 4.208$			$\boldsymbol{V}_{V_{(2)}} = 3.994$		
V(3)-O(16)	1.627(10)	1.529	V(4)-O(1)	1.617(9)	1.570
V(3)-O(10)	1.946(11)	0.645	V(4)-O(2)	1.945(9)	0.647
V(3)-O(6)	1.947(10)	0.644	V(4)-O(3)	1.954(9)	0.632
V(3)-O(7)	1.950(9)	0.638	V(4)-O(8)	1.956(10)	0.628
V(3)-O(15)	1.951(12)	0.637	V(4)-O(12)	1.960(11)	0.621
$\boldsymbol{V}_{V_{(3)}} = 4.093$			$\boldsymbol{V}_{V_{(4)}} = 4.098$		

S1. The valence sum calculations are performed on a program of bond valence calculator, version 2.00 February **1993**, written by C. Hormillosa, with assistance from S. Healy, distributed by I. D. Brown.

S2. Brown, I. D.; Altermatt, D. *Acta Crystallogr.* **1985**, B41, 244.

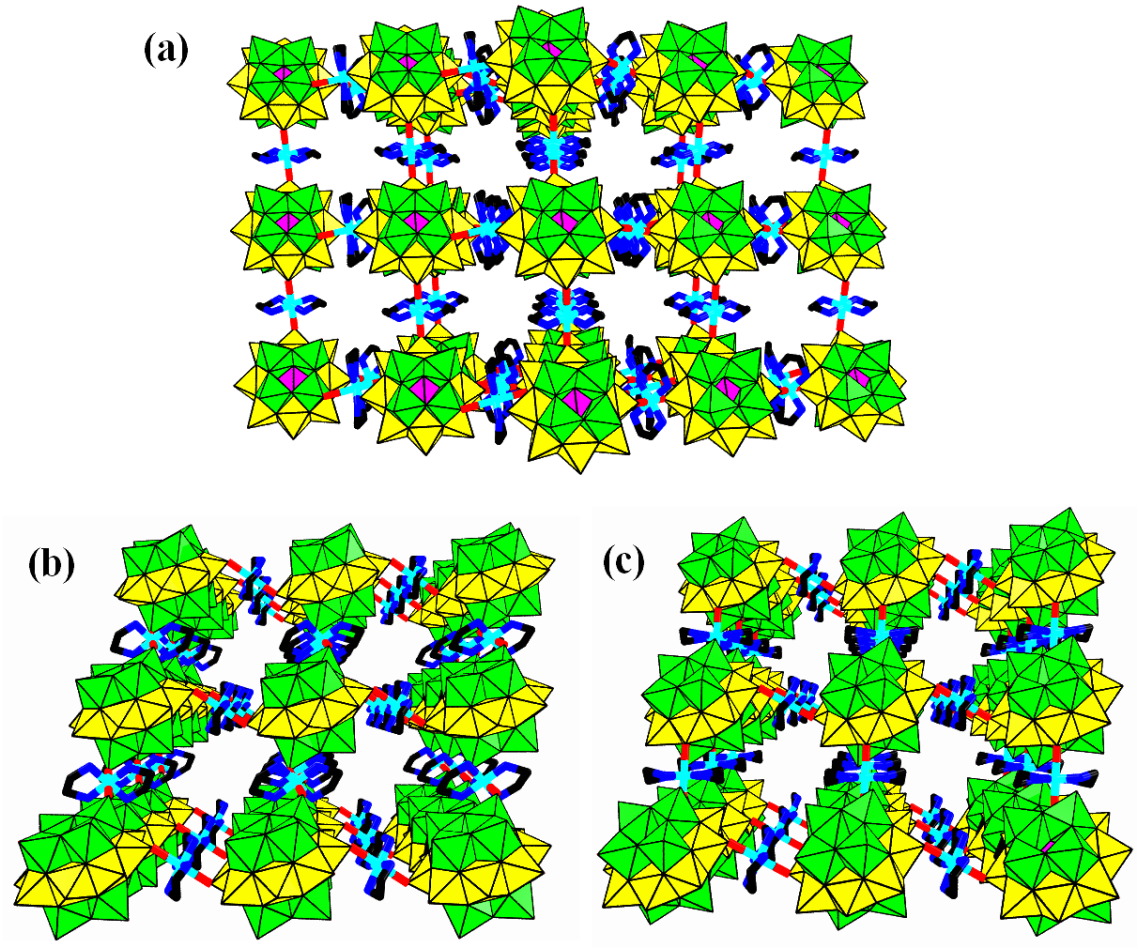

Fig. S1. 3D framework of compound **2** view along [100] (a), [010] (b), [-110] (c).

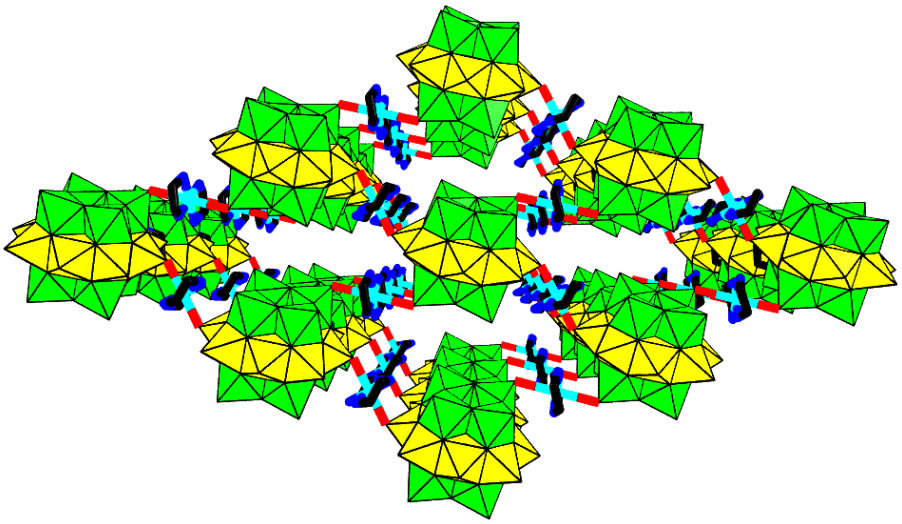

Fig. S2. 3D framework of compound **2** view along [001].

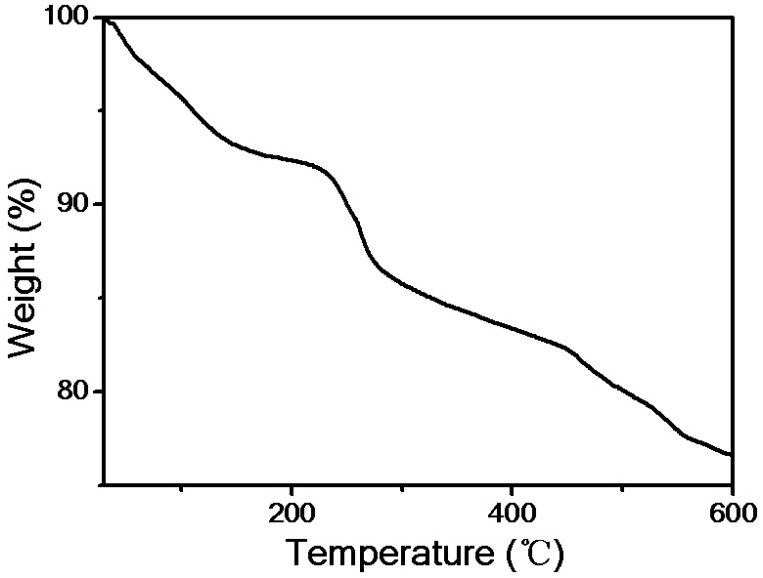

Fig. S3. TG curve for compound **1**.

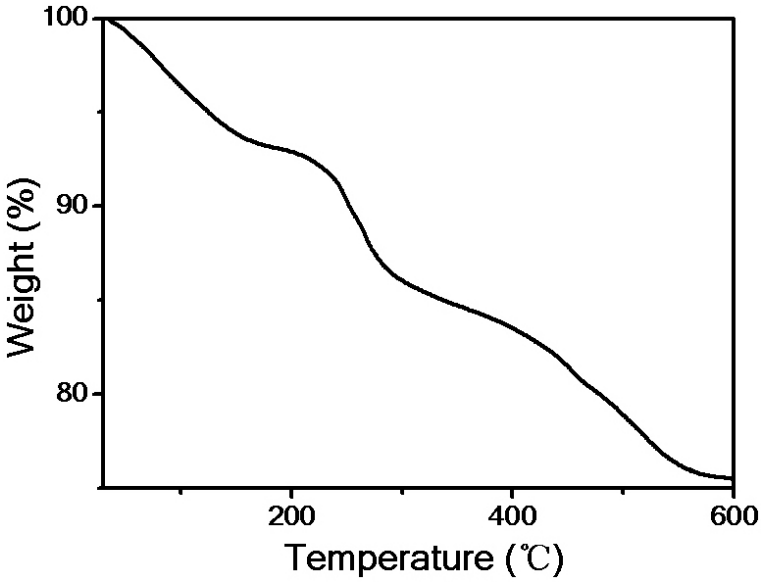

Fig. S4. TG curve for compound **2**.

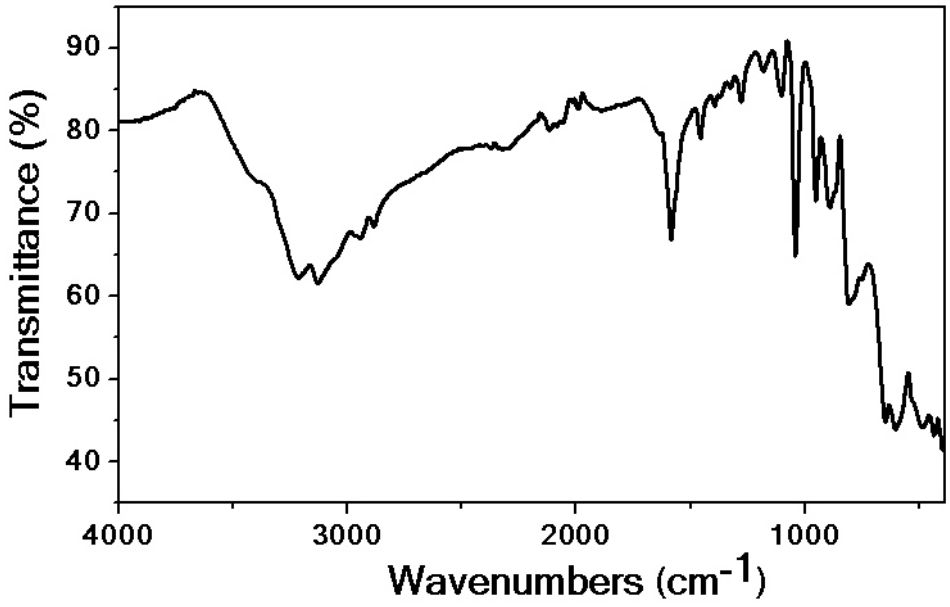

Fig. S5. IR spectrum of compound **1**.

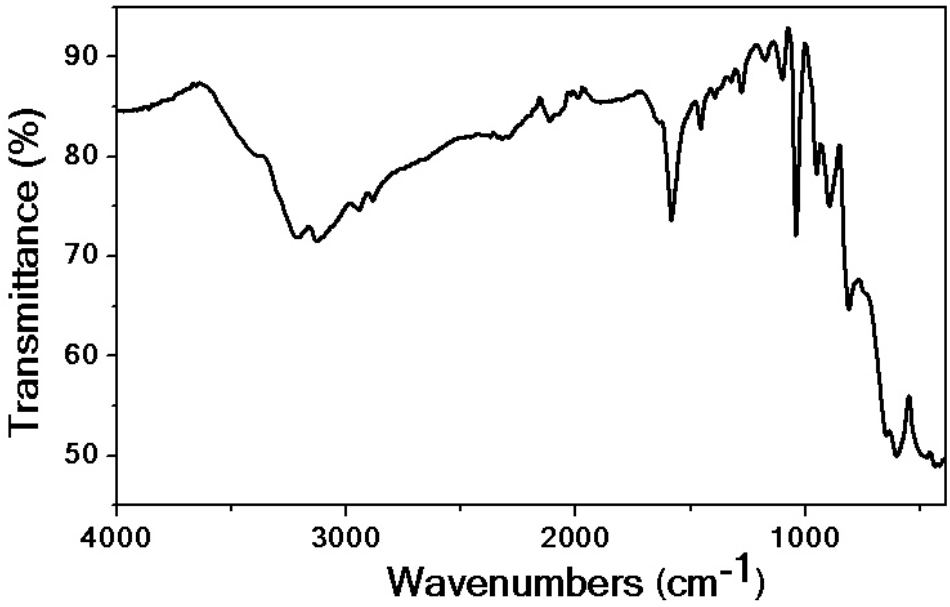

Fig. S6. IR spectrum of compound **2**.

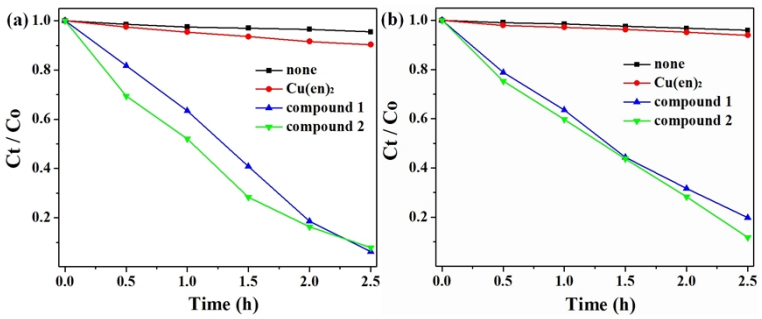

Fig. S7. Plots of C_t/C_0 of MB (a) and RhB (b) versus irradiation time under UV light in the presence of compounds **1** and **2**, the precursors $Cu(en)_2$ as well as in the absence of catalyst.

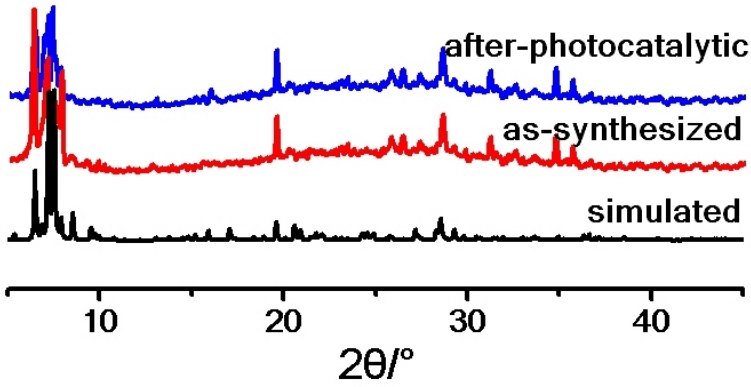

Fig. S8. The PXRD patterns of compound **1**.

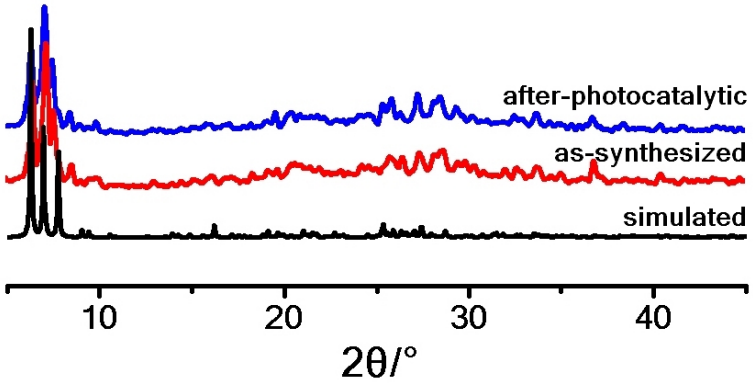

Fig. S9. The PXRD patterns of compound **2**.

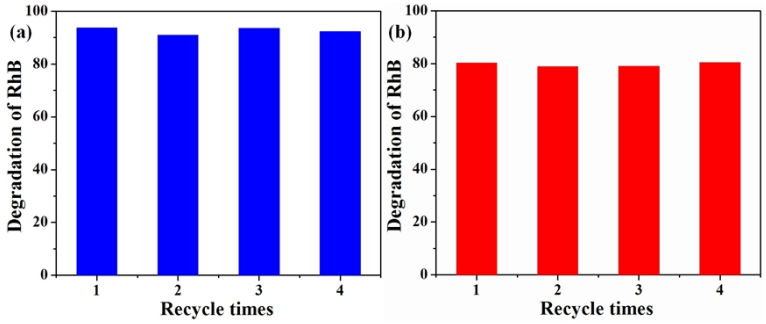

Fig. S10. Four recycles of photocatalytic degradation of MB (a) RhB (b) with compound **1**.

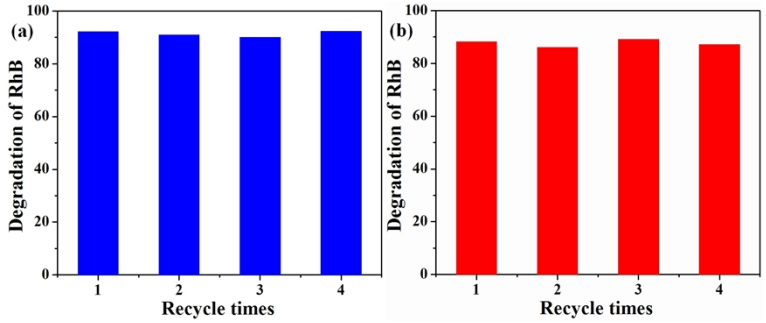

Fig. S11. Four cycles of photocatalytic degradation of MB (a) RhB (b) with compound **2**.