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Two novel 3D metal-organic frameworks based on two tetrahedral ligands: syntheses, structures, photoluminescence and photocatalytic properties

Jiao Guo, Jin Yang*, Ying-Ying Liu and Jian-Fang Ma*

Key Lab of Polyoxometalate Science, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

* Correspondence authors

E-mail: yangjinnenu@yahoo.com.cn (J. Yang)

E-mail: jianfangma@yahoo.com.cn (J.-F. Ma)

Fax: +86-431-85098620 (J.-F. Ma)

Table S1 Selected bond distances (Å) and angles (°) for **1**

Co(1)-N(1)	2.026(5)	Co(1)-O(1)	2.351(4)
Co(1)-O(2)	2.040(4)	Co(1)-O(8)#3	2.302(4)
Co(1)-O(9)#3	2.046(4)	Co(1)-N(8)#4	2.050(5)
Co(2)-O(11)	1.84(3)	Co(2)-O(11')	2.066(17)
Co(2)-N(6)#1	1.997(5)	Co(2)-N(4)#2	2.027(5)
Co(2)-O(6)#5	1.995(4)		
N(1)-Co(1)-O(1)	86.18(19)	O(2)-Co(1)-O(1)	58.90(16)
N(1)-Co(1)-O(2)	99.41(19)	O(2)-Co(1)-O(9)#3	112.85(18)
N(1)-Co(1)-O(9)#3	95.08(19)	O(9)#3-Co(1)-O(1)	171.73(17)
O(2)-Co(1)-O(8)#3	89.92(16)	N(1)-Co(1)-O(8)#3	155.28(18)
O(8)#3-Co(1)-O(1)	118.00(17)	O(9)#3-Co(1)-O(8)#3	60.24(17)
O(2)-Co(1)-N(8)#4	140.3(2)	N(1)-Co(1)-N(8)#4	97.7(2)
O(9)#3-Co(1)-N(8)#4	100.90(18)	N(8)#4-Co(1)-O(8)#3	89.19(18)
N(8)#4-Co(1)-O(1)	87.01(18)	O(11)-Co(2)-N(6)#1	109.6(7)
N(6)#1-Co(2)-O(11')	124.6(6)	N(4)#2-Co(2)-O(11')	103.8(7)
O(11)-Co(2)-N(4)#2	103.5(8)	N(6)#1-Co(2)-N(4)#2	113.6(2)
O(11)-Co(2)-O(6)#5	116.7(6)	O(6)#5-Co(2)-O(11')	98.1(5)
O(6)#5-Co(2)-N(6)#1	115.2(2)	O(6)#5-Co(2)-N(4)#2	97.2(2)

Symmetry codes for **1**: #1 -x+3, -y+1, -z+1; #2 x, -y+1/2, z-1/2; #3 x, y-1, z; #4 x-1, y, z; #5 -x+1, y+1/2, -z+1/2.

Table S2 Selected bond distances (Å) and angles (°) for **2**

Cd(1)-N(1)	2.328(5)	Cd(1)-O(2)	2.289(4)
Cd(1)-N(4)#2	2.262(5)	Cd(1)-O(2)#3	2.378(4)
Cd(1)-O(6)#4	2.335(6)	Cd(1)-O(5)#4	2.474(6)
O(2)-Cd(1)-N(1)	94.38(17)	N(4)#2-Cd(1)-N(1)	102.04(19)
N(4)#2-Cd(1)-O(2)	119.29(18)	O(2)-Cd(1)-O(2)#3	78.40(15)
N(1)-Cd(1)-O(2)#3	169.92(17)	N(4)#2-Cd(1)-O(2)#3	87.71(18)

N(1)-Cd(1)-O(6)#4	89.1(2)	O(2)-Cd(1)-O(6)#4	146.0(2)
O(2)-Cd(1)-O(5)#4	93.07(19)	N(1)-Cd(1)-O(5)#4	84.35(19)
N(4)#2-Cd(1)-O(5)#4	146.0(2)	N(4)#2-Cd(1)-O(6)#4	92.8(2)
O(6)#4-Cd(1)-O(2)#3	93.01(19)	O(2)#3-Cd(1)-O(5)#4	88.98(17)
O(6)#4-Cd(1)-O(5)#4	53.6(2)		

Symmetry codes for 2: #1 -x+1, y, -z+1/2; #2 -x+1, -y+1, -z+1; #3 -x, -y+1, -z+1; #4 x-1, y-1, z.

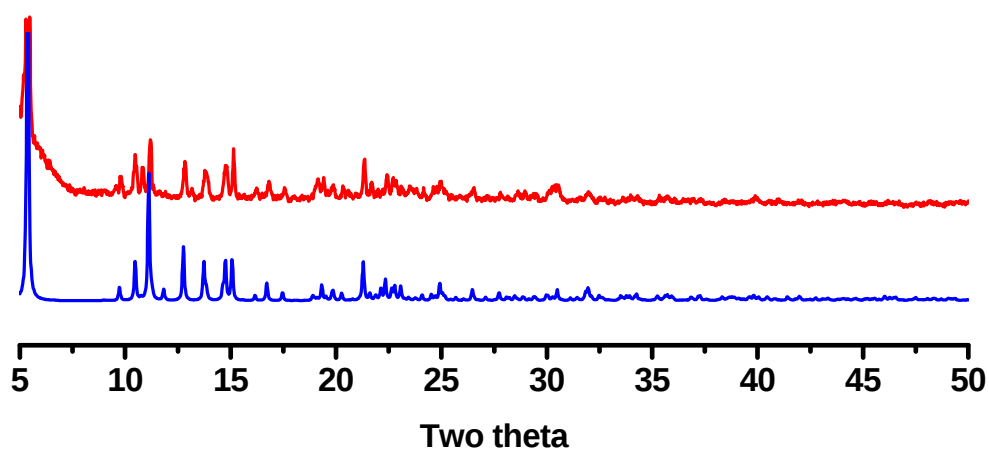
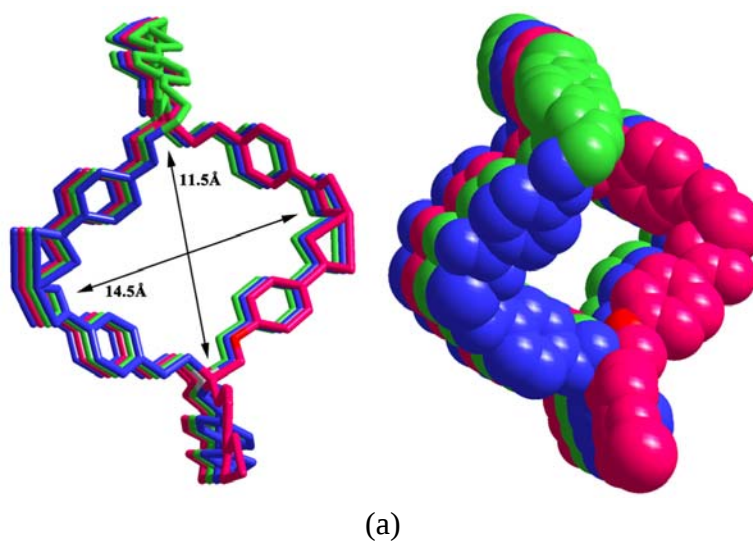
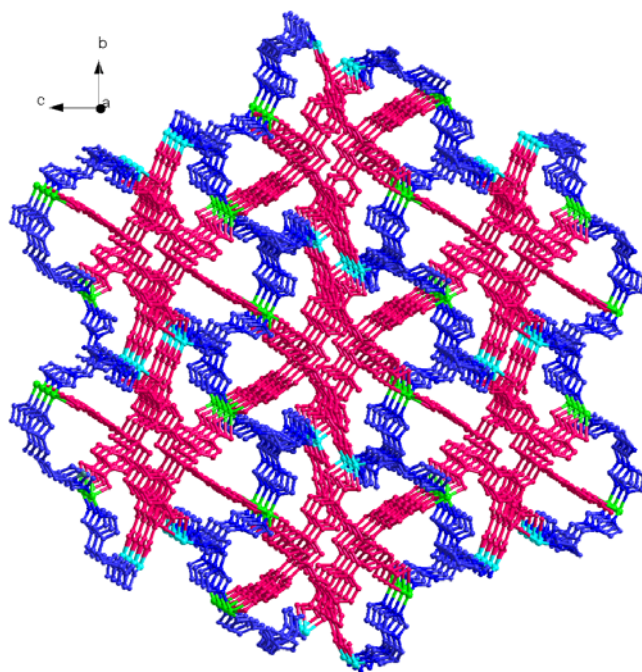


Fig. S1 The simulated (blue) and experimental (red) XRD patterns for compound 2.





(b)

Fig. S2 (a) The quadrilateral nanotube with a $11.5 \text{ \AA} \times 14.5 \text{ \AA}$ free aperture. (b) The 3D framework of compound 1.

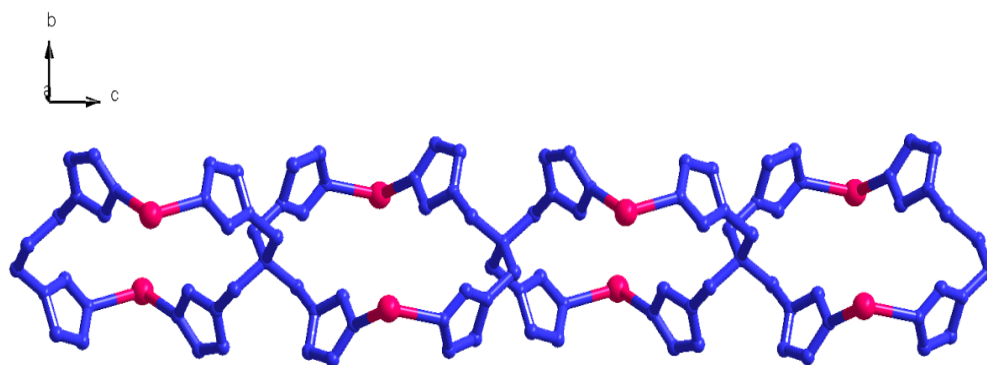


Fig. S3 View of the 1D chain constructed by the L2 ligands and Cd(II) atoms.

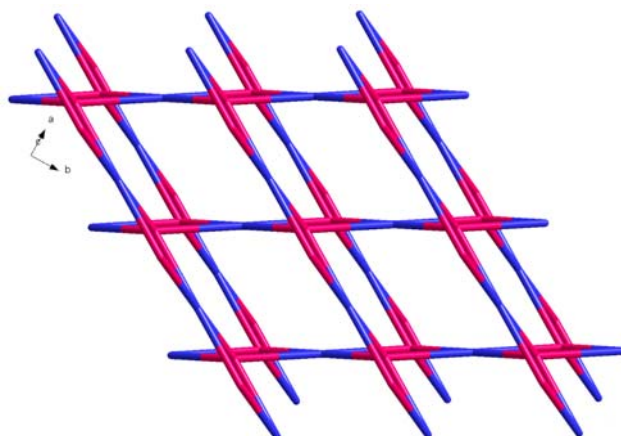


Fig. S4 Schematic representation of the 3D framework constructed by the L1 anions and Cd(II) atoms.

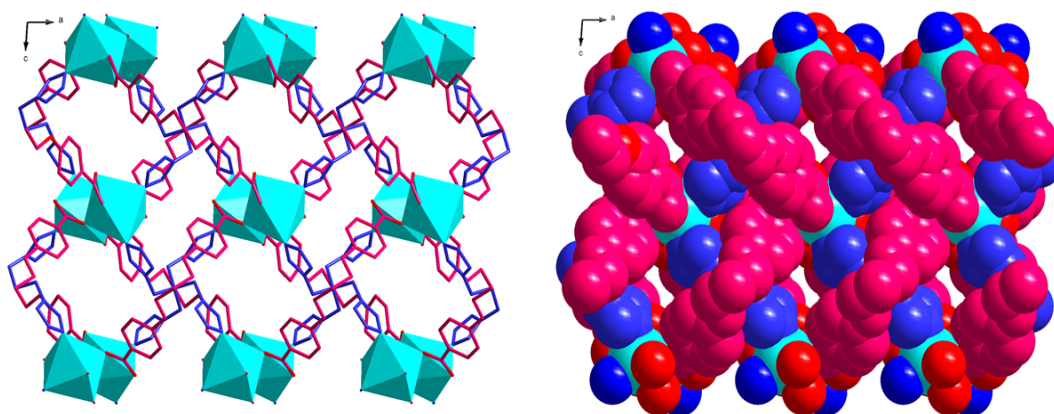
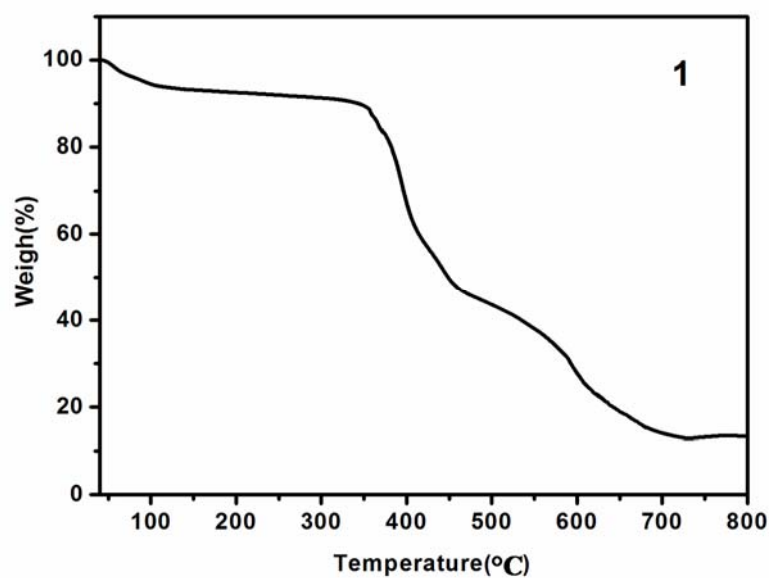


Fig. S5 The 3D framework with channels in the structure of **2** along the *b* axis.



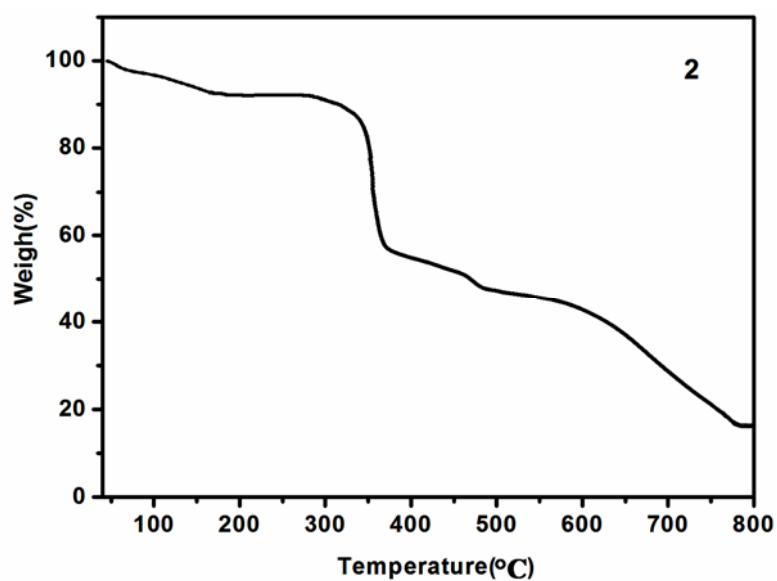


Fig. S6 The TGA curves of compounds **1** and **2**.

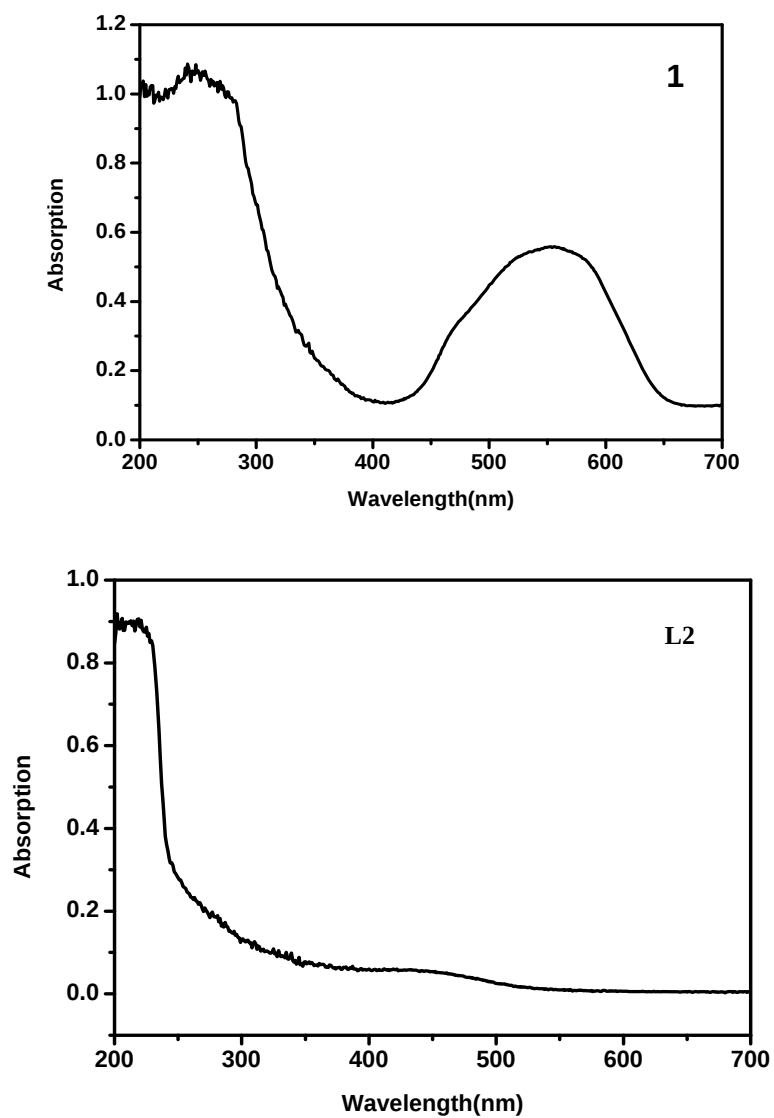


Fig. S7 UV-Vis absorption spectra of ligands H_4L1 and $L2$.

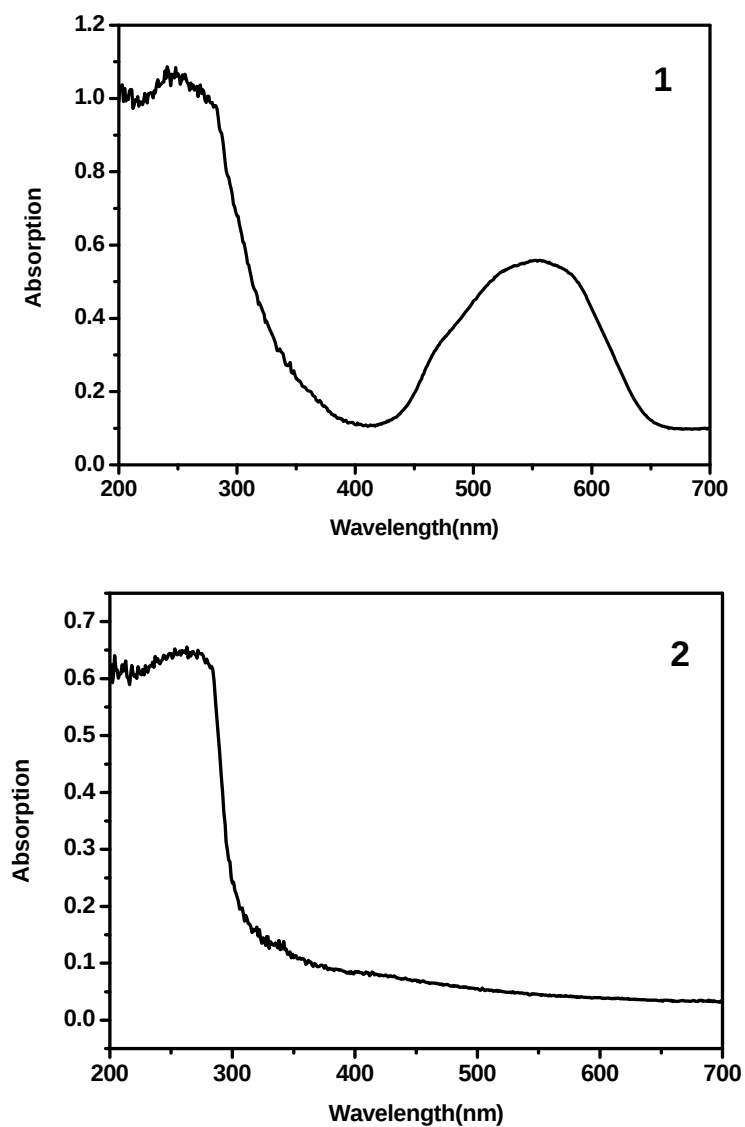
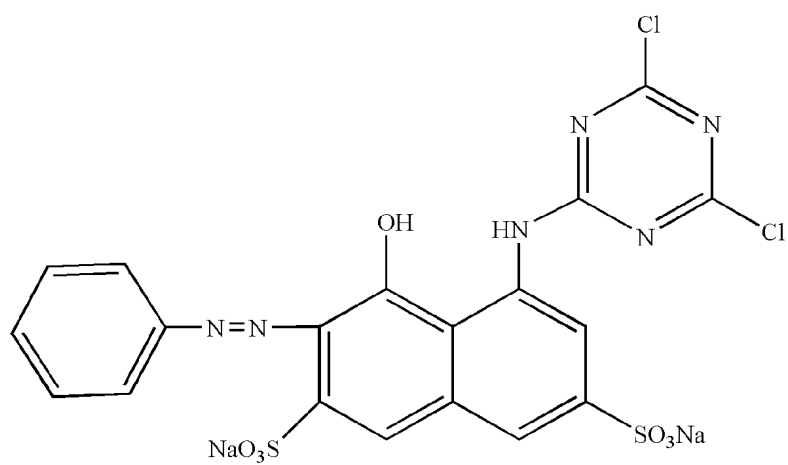
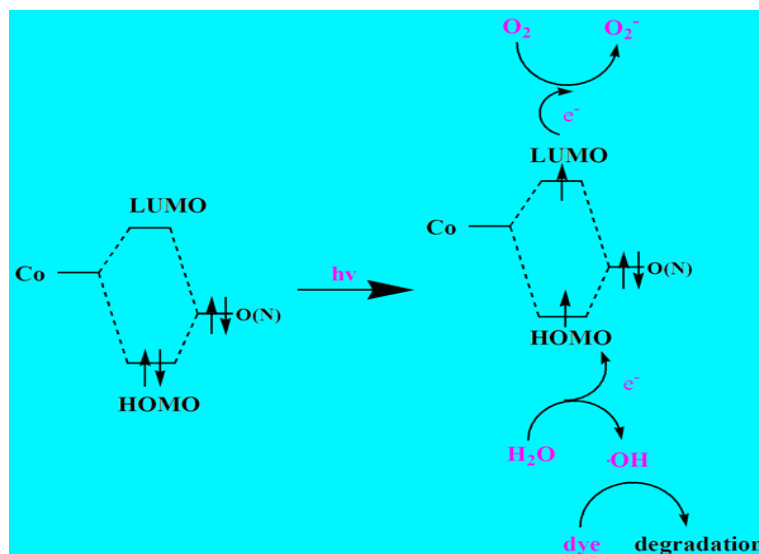


Fig. S8 UV-Vis absorption spectra of compounds **1** and **2**.



Scheme S1 Molecular structure of **X3B**



Scheme S2 A simplified explanation of photocatalytic effect of dye on compound **1**

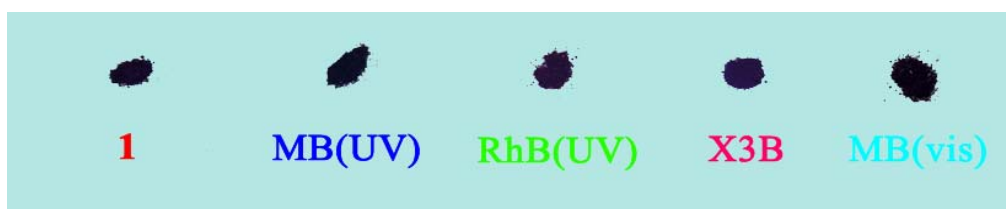


Fig. S9 The colors of compound **1** before a photocatalysis process (red), **1** after a photocatalysis process (**MB(UV)**) (blue), **1** after a photocatalysis process (**RhB**) (green), **1** after a photocatalysis process (**X3B**) (pink) and **1** after a photocatalysis process (**MB(vis)**) (cyan).