**Supplementary Material (ESI) for CrystEngComm**
This journal is © The Royal Society of Chemistry

# pH, solvent and metal ions induced octamolybdate-based metal–organic complexes decorated by pyridyl-carboxylate ligand containing amide group †

**Xiuli Wang,* Danna Liu, Hongyan Lin, Guocheng Liu, Xiang Wang, Mao Le, Xing Rong**

*Department of Chemistry, Bohai University, Jinzhou, 121000, P. R. China*

**Table S1** Selected bond distances (Å) and angles (°) for compounds **1–3**.

| | | | |
|---|---|---|---|
| Compound **1** | | | |
| Cu(1)-O(5)#1 | 1.942(3) | O(1)-Cu(1)-O(16)#3 | 86.88(11) |
| Cu(1)-N(6)#1 | 1.961(3) | N(1)-Cu(1)-O(16)#3 | 87.41 |
| Cu(1)-N(1) | 1.981(3) | O(5)#1-Cu(1)-O(16)#3 | 94.49 |
| Cu(1)-O(1) | 1.984(2) | O(3)#2-Cu(1)-O(16)#3 | 167.77 |
| Cu(1)-O(3)#2 | 2.342(3) | N(6)#1-Cu(1)- O(16)#3 | 91.72 |
| Cu(1)-O(16) #3 | 2.655(3) | N(2)#2-Cu(2)- O(1W)#2 | 89.95 |
| Cu(2)-O(2)#2 | 2.002(2) | O(1W)-Cu(2)- O(1W)#2 | 180 |
| Cu(2)-O(2) | 2.002(2) | O(2)#2-Cu(2)-O(2) | 180 |
| Cu(2)-N(2)#2 | 2.016(3) | O(2)#2-Cu(2)-N(2)#2 | 86.64(12) |
| Cu(2)-N(2) | 2.016(3) | N(2)-Cu(2)- O(1W) | 90.05 |
| Cu(2)-O(1W) | 2.453(3) | O(2)#2-Cu(2)- O(1W) | 79.26(12) |
| Cu(2)-O(1W)#2 | 2.453(3) | O(2)-Cu(2)-N(2) | 86.64(12) |
| O(5)#1-Cu(1)-N(6)#1 | 83.93(11) | N(2)#2-Cu(2)-N(2) | 180 |
| O(5)#1-Cu(1)-N(1) | 97.64(11) | O(2)#2-Cu(2)-O(2) | 180 |
| N(6)#1-Cu(1)-N(1) | 178.26(13) | O(2)-Cu(2)-N(2)#2 | 93.36(12) |
| O(5)#1-Cu(1)-O(1) | 178.41(12) | O(2)#2-Cu(2)-N(2) | 93.36(12) |
| N(6)#1-Cu(1)-O(1) | 95.25(11) | O(2)-Cu(2)- O(1W) | 79.26(11) |
| N(1)-Cu(1)-O(1) | 83.19(11) | N(2)#2-Cu(2)- O(1W) | 90.05(11) |
| O(5)#1-Cu(1)-O(3)#2 | 97.42(11) | O(1W)#2-Cu(2)- O(1W) | 180.00(11) |
| N(6)#1-Cu(1)-O(3)#2 | 92.23(11) | N(2)-Cu(2)- O(1W)#2 | 89.95(11) |
| N(1)-Cu(1)-O(3)#2 | 88.31(11) | O(2)#2-Cu(2)- O(1W)#2 | 79.26(11) |
| O(1)-Cu(1)-O(3)#2 | 81.24(10) | O(2)-Cu(2)- O(1W)#2 | 100.74(12) |
| Symmetry code for **1**: #1 x–1, y+1, z; #2 –x+1, –y–1, –z+1; #3 x, 1 + y, z. | | | |
| Compound **2** | | | |
| Cu(1)-O(1W)#2 | 1.976(3) | O(21)#4-Cu(1)-O(1) | 88.09(12) |
| Cu(1)-O(1W) | 1.976(3) | O(1W)#2-Cu(1)-O(1)#2 | 89.13(12) |
| Cu(1)-O(21)#3 | 1.985(3) | O(1W)-Cu(1)-O(1)#2 | 90.87(12) |
| Cu(1)-O(21)#4 | 1.985(3) | O(21)#3-Cu(1)-O(1)#2 | 88.09(12) |
| Cu(1)-O(1) | 2.390(3) | O(21)#4-Cu(1)-O(1)#2 | 91.91(12) |
| Cu(1)-O(1)#2 | 2.390(3) | O(1)-Cu(1)-O(1)#2 | 180 |
| Cu(2)- N(1) | 1.961(3) | O(18)-Cu(2)-O(18)#3 | 180 |
| Cu(2)-O(18) | 1.943(3) | O(18)-Cu(2)-N(1)#3 | 96.66(13) |

| | | | |
|---|---|---|---|
| Cu(2)-O(18)#3 | 1.943(3) | O(18)#3-Cu(2)-N(1)#3 | 83.34(13) |
| Cu(2)-N(1)#3 | 1.961(3) | O(18)-Cu(2)-N(1) | 83.34(13) |
| Cu(2)-O2 | 2.611(3) | O(18)#3-Cu(2)-N(1) | 96.66(13) |
| Cu(2)-O2#3 | 2.611(3) | N(1)#3-Cu(2)-N(1) | 180 |
| O(1W)#2-Cu(1)-O(1W) | 179.999(2) | N(1)-Cu(2)-O(2) | 93.96(12) |
| O(1W)#2-Cu(1)-O(21)#3 | 93.99(13) | N(1)#3-Cu(2)-O(2) | 86.04(12) |
| O(1W)-Cu(1)-O(21)#3 | 86.01(13) | O(18)-Cu(2)-O(2) | 100.76(12) |
| O(1W)#2-Cu(1)-O(21)#4 | 86.01(13) | O(18)#3-Cu(2)-O(2) | 79.25(12) |
| O(1W)-Cu(1)-O(21)#4 | 93.99(13) | N(1)-Cu(2)-O(2)#3 | 86.04(12) |
| O(21)#3-Cu(1)-O(21)#4 | 179.998(1) | N(1)#3-Cu(2)-O(2)#3 | 93.96(12) |
| O(1W)#2-Cu(1)-O(1) | 90.87(12) | O(18)-Cu(2)-O(2)#3 | 79.24(12) |
| O(1W)-Cu(1)-O(1) | 89.13(12) | O(18)#3-Cu(2)-O(2)#3 | 100.76(12) |
| O(21)#3-Cu(1)-O(1) | 91.91(12) | O(2)-Cu(2)-O(2)#3 | 180 |
| Symmetry code for **2**: #2 –x–2, –y, –z+2; #3 –x–1, –y, –z + 2; #4 x–1, y, z | | | |
| Compound **3** | | | |
| Co(1)-O(1) | 2.040(3) | N(2)-Co(1)-N(1) | 89.42(12) |
| Co(1)-O(2) | 2.050(3) | O(1)-Co(1)-O(10)#2 | 90.09(11) |
| Co(1)-O(1W) | 2.120(3) | O(2)-Co(1)-O(10)#2 | 91.81(11) |
| Co(1)-N(2) | 2.130(3) | O(1W)-Co(1)-O(10)#2 | 88.96(12) |
| Co(1)-N(1) | 2.133(3) | N(2)-Co(1)-O(10)#2 | 92.25(11) |
| Co(1)-O(10)#2 | 2.160(3) | N(1)-Co(1)-O(10)#2 | 168.16(12) |
| Co(2)-O(3W)#3 | 2.081(4) | O(3W)#3-Co(2)-O(3W) | 180 |
| Co(2)-O(3W) | 2.081(4) | O(3W)#3-Co(2)-O(4W)#3 | 87.90(17) |
| Co(2)-O(4W)#3 | 2.097(3) | O(3W)-Co(2)-O(4W)#3 | 92.10(17) |
| Co(2)-O(4W) | 2.097(3) | O(3W)#3-Co(2)-O(4W) | 92.10(17) |
| Co(2)-O(2W)#3 | 2.110(4) | O(3W)-Co(2)-O(4W) | 87.90(17) |
| Co(2)-O(2W) | 2.110(4) | O(4W)#3-Co(2)-O(4W) | 180 |
| O(1)-Co(1)-O(2) | 173.51(12) | O(3W)#3-Co(2)-O(2W)#3 | 91.7(2) |
| O(1)-Co(1)-O(1W) | 94.34(13) | O(3W)-Co(2)-O(2W)#3 | 88.3(2) |
| O(2)-Co(1)-O(1W) | 91.89(12) | O(4W)#3-Co(2)-O(2W)#3 | 88.64(14) |
| O(1)-Co(1)-N(2) | 95.70(12) | O(4W)-Co(2)-O(2W)#3 | 91.36(14) |
| O(2)-Co(1)-N(2) | 78.04(11) | O(3W)#3-Co(2)-O(2W) | 88.3(2) |
| O(1W)-Co(1)-N(2) | 169.88(13) | O(3W)-Co(2)-O(2W) | 91.7(2) |
| O(1)-Co(1)-N(1) | 78.08(13) | O(3W)#3-Co(2)-O(2W)#3 | 91.7(2) |
| O(2)-Co(1)-N(1) | 100.00(13) | O(3W)-Co(2)-O(2W)#3 | 88.3(2) |
| O(1W)-Co(1)-N(1) | 91.45(13) | O(4W)#3-Co(2)-O(2W)#3 | 88.64(14) |
| Symmetry code for **3** #2 x + 1, y, z; #3 –x, –y, –z. | | | |

**Table S2.** Selected hydrogen–bonding geometry (Å, º) for compounds **1–3**.

| | D–H···A | D–H | H···A | D···A | D–H···A |
|---|---|---|---|---|---|
| Compound **1** | C(24)–H(24A)···O(6) | 0.93 | 2.38 | 3.3036 | 170 |
| Compound **2** | C(8)–H(8A)···O(5) | 0.93 | 2.47 | 3.1204 | 127 |
| Compound **3** | N(5)–H(5B)···O(5) | 0.86 | 1.95 | 2.7812 | 163 |

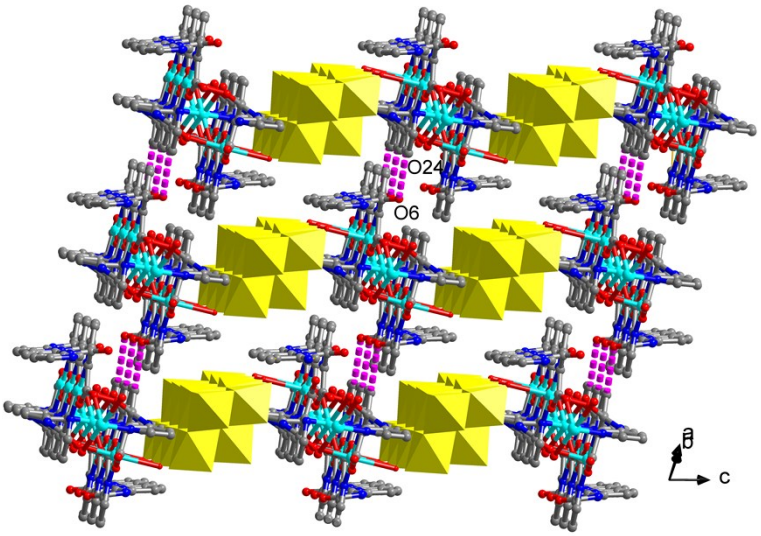


**Fig. S1** The 3D supramolecular structure in **1**.

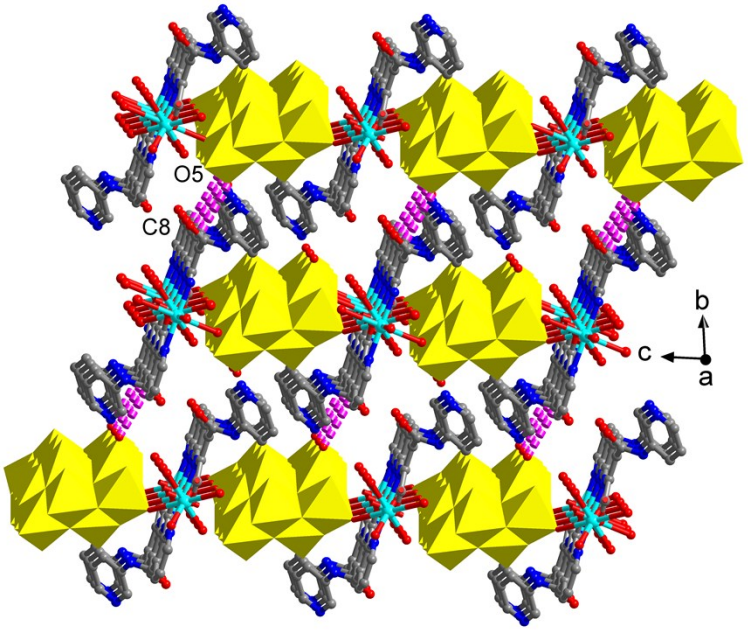


**Fig. S2** The 3D supramolecular structure in **2**.

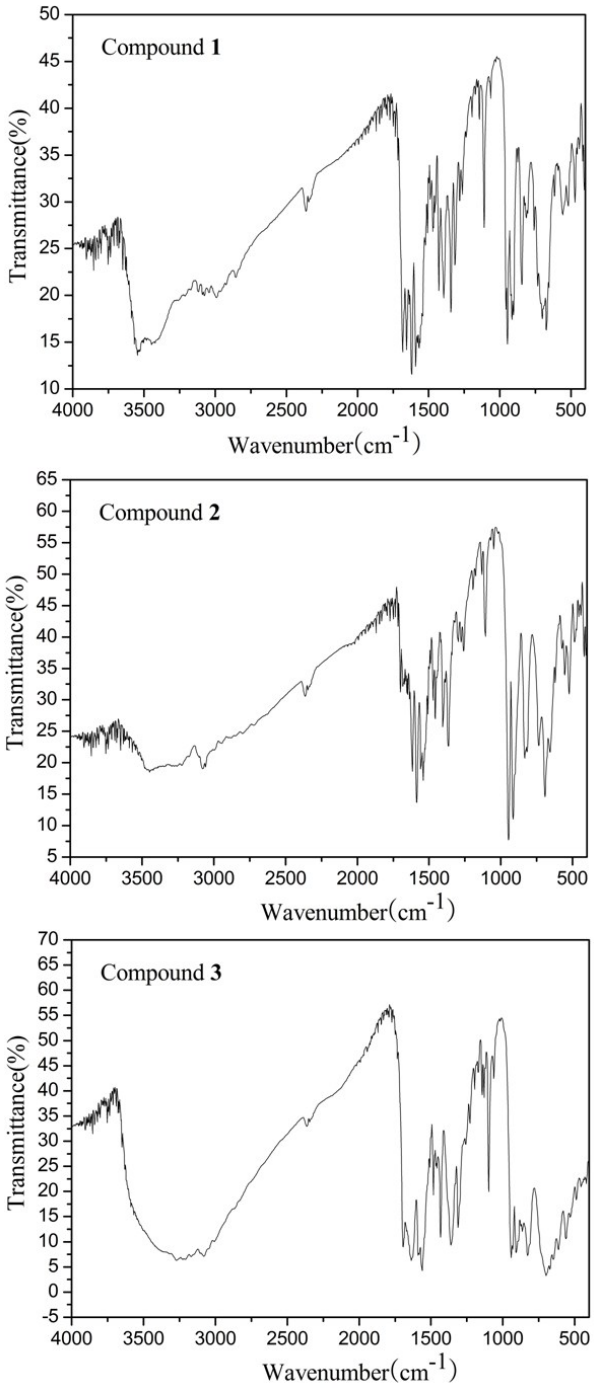


**Fig. S3.** The IR spectra of compounds **1-3**.

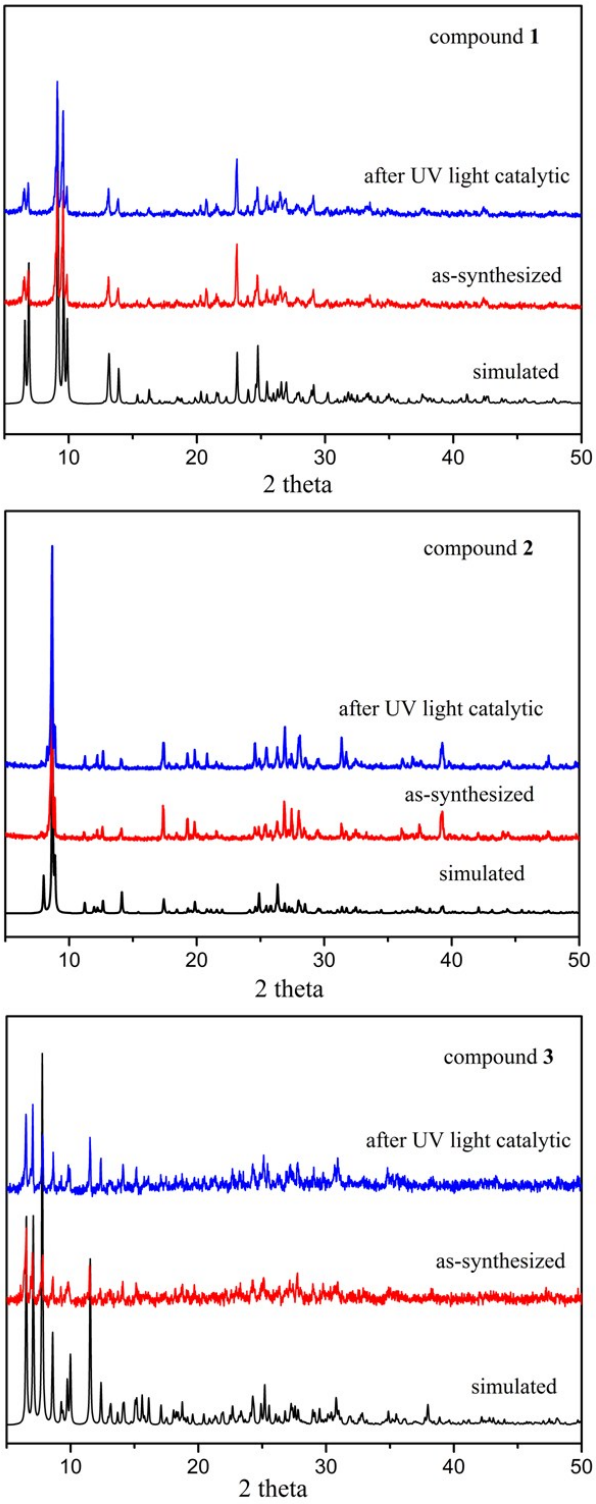


**Fig. S4.** The PXRD of compounds **1–3**.

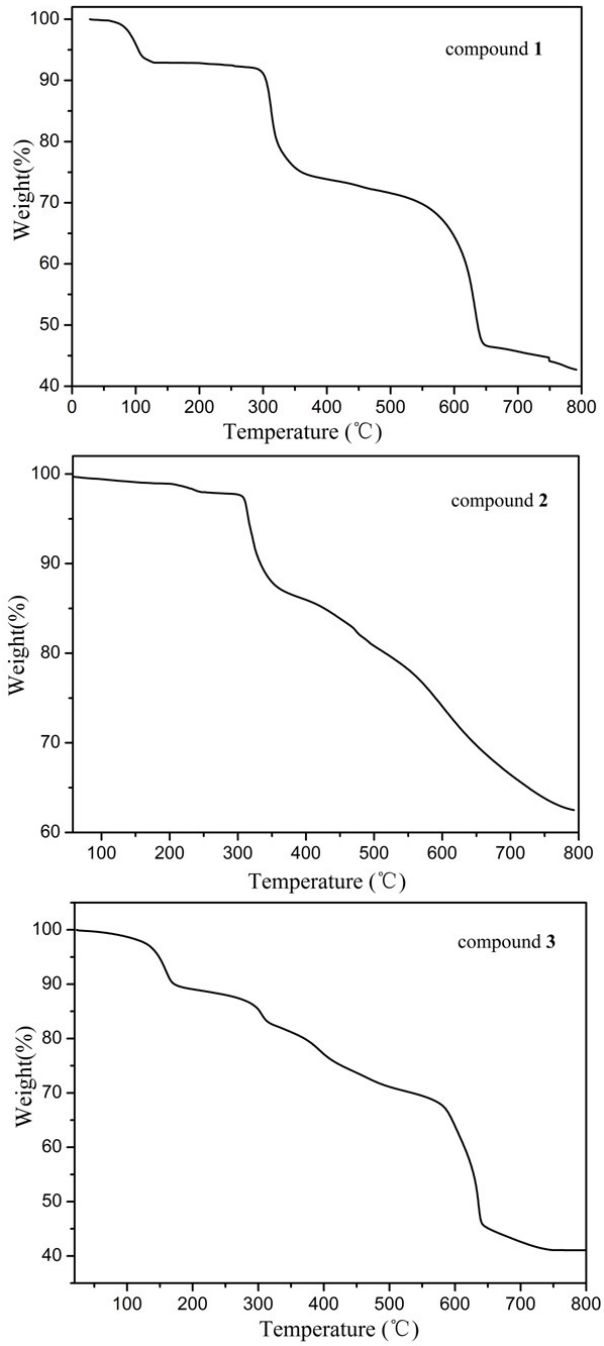


**Fig. S5.** The TG curves of compounds **1–3**.

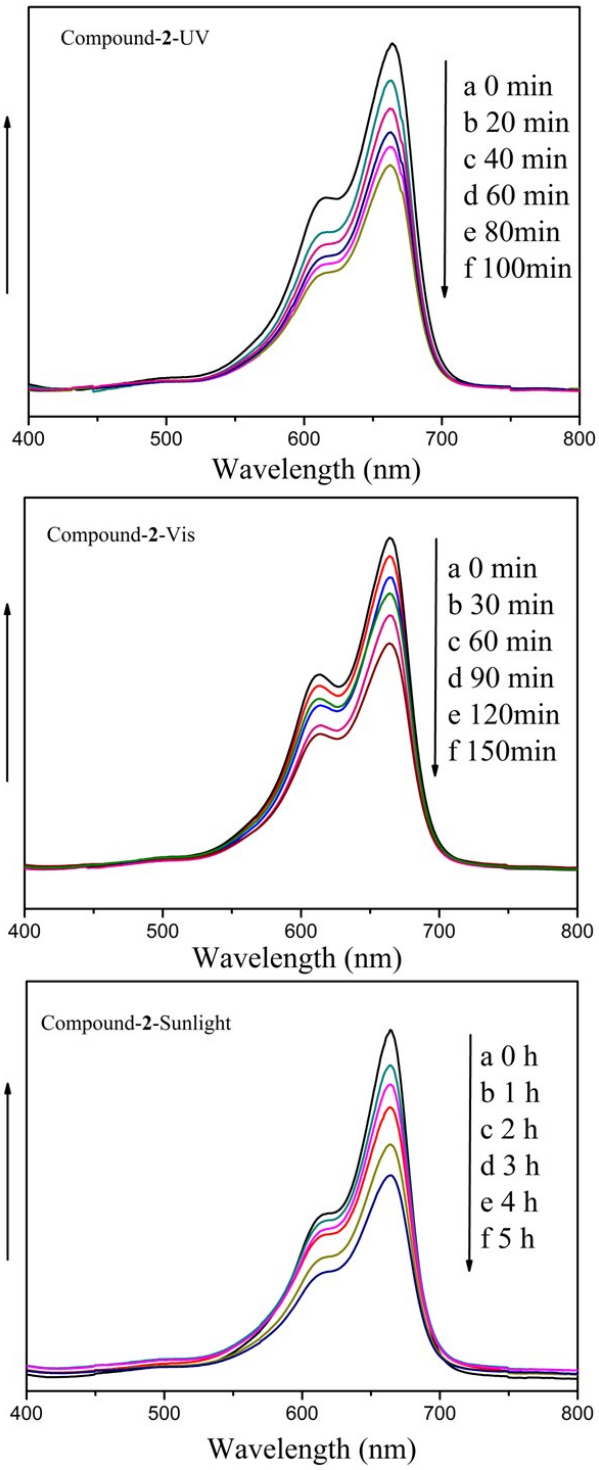


**Fig. S6.** Absorption spectra of the MB solution during the decomposition reaction under UV (a), visible (b) and sunlight (c) irradiation in the presence of the compound **2**.

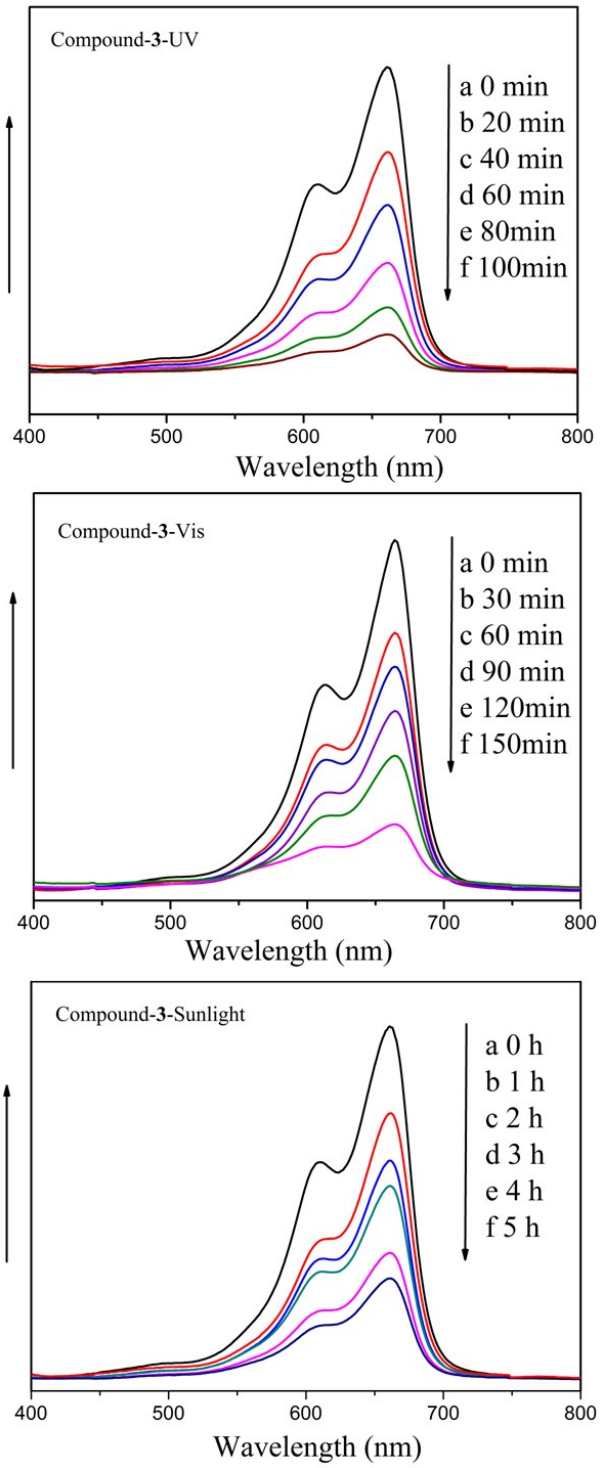


**Fig. S7.** Absorption spectra of the MB solution during the decomposition reaction under UV (a), visible (b) and sunlight (c) irradiation in the presence of the compound **3**.