Four Co(II) coordination polymers based on 4,4'-(1H-1,2,4-triazol-1-yl)methylenebis(benzonic acid): Syntheses, structural diversity, magnetic properties, dye absorption and photocatalytic properties

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Table. S1 Selected Bond lengths [Å] and angles [°] for complexes **1-4**

Complex 1			
Co1-O4	1.935 (6)	Co3-O3^{iv}	2.055 (6)
Co1-O5	1.984 (5)	Co3-O12	2.054 (6)
Co1-O6	1.979 (7)	Co3-O13	2.354 (6)
Co1-N12^{i}	2.023 (6)	Co3-O14^{iii}	2.289 (6)
Co2-Co4^{ii}	2.9373 (12)	Co3-O15^{iii}	2.078 (6)
Co2-O1	1.992 (6)	Co3-C34^{iii}	2.507 (8)
Co2-O8^{ii}	2.051 (5)	Co3-N4^{iii}	2.05 (2)
Co2-O11^{ii}	2.078 (6)	Co4-Co2^{v}	2.9373 (12)
Co2-O16^{iii}	2.009 (5)	Co4-O2^{v}	2.042 (6)
Co2-N9	2.028 (7)	Co4-O9	2.053 (5)
Co4-O17^{vi}	2.036 (6)	Co4-O10	2.044 (6)
Co4-N1^{iii}	1.98 (4)	O3-Co3^{vii}	2.055 (5)
O4-Co1-O5	103.0 (3)	O3^{iv}-Co3-O13	96.4 (2)
O4-Co1-O6	116.5 (3)	O3^{iv}-Co3-O14^{iii}	150.3 (2)
O4-Co1-N12^{i}	122.3 (3)	O3^{iv}-Co3-O15^{iii}	90.8 (2)
O5-Co1-N12^{i}	94.9 (2)	O3^{iv}-Co3-C34^{iii}	120.3 (3)
O6-Co1-O5	98.4 (3)	O12-Co3-O3^{iv}	108.5 (2)

O6-Co1-N12^{i}	114.3 (3)	O12-Co3-O13	59.2 (2)
O1-Co2-Co4^{ii}	84.1 (2)	O12-Co3-O14^{iii}	100.0 (2)
O1-Co2-O8^{ii}	86.1 (2)	O12-Co3-O15^{iii}	148.0 (2)
O1-Co2-O11^{ii}	159.8 (3)	O12-Co3-C34^{iii}	126.5 (3)
O1-Co2-O16^{iii}	91.5 (2)	O13-Co3-C34^{iii}	93.2 (2)
O1-Co2-N9	106.3 (3)	O14^{iii}-Co3-O13	91.0 (2)
O8^{ii}-Co2-Co4^{ii}	79.69 (17)	O14^{iii}-Co3-C34^{iii}	30.2 (2)
O8^{ii}-Co2-O11^{ii}	88.5 (2)	O15^{iii}-Co3-O13	94.3 (2)
O11^{ii}-Co2-Co4^{ii}	75.77 (18)	O15^{iii}-Co3-O14^{iii}	59.9 (2)
O16^{iii}-Co2-Co4^{ii}	79.74 (18)	O15^{iii}-Co3-C34^{iii}	29.7 (2)
O16^{iii}-Co2-O8^{ii}	159.4 (3)	N4^{iii}-Co3-O3^{iv}	94.8 (7)
O16^{iii}-Co2-O11^{ii}	86.7 (3)	N4^{iii}-Co3-O12	95.1 (7)
O16^{iii}-Co2-N9	104.7 (3)	N4^{iii}-Co3-O13	154.1 (7)
N9-Co2-Co4^{ii}	168.32 (19)	N4^{iii}-Co3-O14^{iii}	90.7 (7)
N9-Co2-O8^{ii}	95.5 (2)	N4^{iii}-Co3-O15^{iii}	108.8 (7)
N9-Co2-O11^{ii}	93.6 (3)	N4^{iii}-Co3-C34^{iii}	101.1 (7)
O2^{v}-Co4-Co2^{v}	76.6 (2)	O17^{vi}-Co4-O9	160.3 (3)
O2^{v}-Co4-O9	87.2 (2)	O17^{vi}-Co4-O10	88.8 (2)
O2^{v}-Co4-O10	160.9 (3)	N1^{iii}-Co4-Co2^{v}	172.2 (12)
O9-Co4-Co2^{v}	80.56 (17)	N1^{iii}-Co4-O2^{v}	97.2 (12)
O10-Co4-Co2^{v}	84.32 (19)	N1^{iii}-Co4-O9	104.0 (8)
O10-Co4-O9	90.2 (2)	N1^{iii}-Co4-O10	101.8 (12)
O17^{vi}-Co4-Co2^{v}	79.77 (18)	N1^{iii}-Co4-O17^{vi}	95.5 (8)
O17^{vi}-Co4-O2^{v}	87.3 (3)		
Complex 2			
Co1-N1	2.034 (5)	Co1-O2	2.330 (7)
Co1-O4^{i}	2.024 (4)	Co1-N4^{ii}	2.053 (4)
Co1-O1	2.141 (8)		
N1-Co1-O1	96.4 (3)	O4^{i}-Co1-O1	141.0 (3)
N1-Co1-O2	154.0 (2)	O4^{i}-Co1-O2	92.0 (2)
N1-Co1-N4^{ii}	103.25 (19)	O4^{i}-Co1-N4^{ii}	94.07 (18)
O4^{i}-Co1-N1	110.67 (19)	O1-Co1-O2	57.7 (3)
N4^{ii}-Co1-O1	106.8 (2)	N4^{ii}-Co1-O2	86.9 (2)
Complex **3**			

Co1-O3^{i}	2.123 (5)	Co1-C30^{ii}	2.500 (8)
Co1-O4^{i}	2.153 (5)	Co2-O1^{iii}	2.105 (5)
Co1-O5^{ii}	2.195 (5)	Co2-O2^{iii}	2.222 (5)
Co1-O6^{ii}	2.150 (5)	Co2-O7^{iv}	2.135 (5)
Co1-N3	2.072 (6)	Co2-O8^{iv}	2.216 (5)
Co1-N4	2.055 (6)	Co2-N7	2.085 (6)
Co2-N8	2.105 (6)	O1-Co2^{iii}	2.105 (5)
O3^{i}-Co1-O4^{i}	61.54 (19)	O1^{iii}-Co2-O2^{iii}	60.53 (18)
O3^{i}-Co1-O5^{ii}	153.0 (2)	O1^{iii}-Co2-O7^{iv}	147.1 (2)
O3^{i}-Co1-O6^{ii}	97.1 (2)	O1^{iii}-Co2-O8^{iv}	94.8 (2)
O3^{i}-Co1-C15^{i}	30.5 (2)	O1^{iii}-Co2-C1^{iv}	122.1 (2)
O3^{i}-Co1-C30^{ii}	125.0 (3)	O1^{iii}-Co2-C16^{iii}	30.1 (2)
O4^{i}-Co1-O5^{ii}	100.9 (2)	O2^{iii}-Co2-C1^{iv}	91.1 (2)
O4^{i}-Co1-C15^{i}	31.1 (2)	O2^{iii}-Co2-C16^{iii}	30.5 (2)
O4^{i}-Co1-C30^{ii}	93.8 (2)	O7^{iv}-Co2-O2^{iii}	95.5 (2)
O5^{ii}-Co1-C15^{i}	129.5 (2)	O7^{iv}-Co2-O8^{iv}	60.4 (2)
O5^{ii}-Co1-C30^{ii}	30.5 (2)	O7^{iv}-Co2-C1^{iv}	29.5 (2)
O6^{ii}-Co1-O4^{i}	89.1 (2)	O7^{iv}-Co2-C16^{iii}	123.1 (2)
O6^{ii}-Co1-O5^{ii}	60.3 (2)	O8^{iv}-Co2-O2^{iii}	89.3 (2)
O6^{ii}-Co1-C15^{i}	94.2 (2)	O8^{iv}-Co2-C1^{iv}	31.0 (2)
O6^{ii}-Co1-C30^{ii}	30.0 (2)	O8^{iv}-Co2-C16^{iii}	92.7 (2)
N3-Co1-O3^{i}	101.4 (2)	N7-Co2-O1^{iii}	103.2 (2)
N3-Co1-O4^{i}	85.8 (2)	N7-Co2-O2^{iii}	163.7 (2)
N3-Co1-O5^{ii}	97.2 (2)	N7-Co2-O7^{iv}	99.5 (2)
N3-Co1-O6^{ii}	155.5 (2)	N7-Co2-O8^{iv}	92.6 (2)
N3-Co1-C15^{i}	93.7 (2)	N7-Co2-N8	97.3 (2)
N3-Co1-C30^{ii}	126.6 (3)	N7-Co2-C1^{iv}	98.8 (2)
N4-Co1-O3^{i}	102.8 (2)	N7-Co2-C16^{iii}	133.3 (2)
N4-Co1-O4^{i}	164.2 (2)	N8-Co2-O1^{iii}	101.1 (2)
N4-Co1-O5^{ii}	94.5 (2)	N8-Co2-O2^{iii}	86.5 (2)
N4-Co1-O6^{ii}	95.6 (2)	N8-Co2-O7^{iv}	99.3 (2)
N4-Co1-N3	95.8 (3)	N8-Co2-O8^{iv}	158.8 (2)
N4-Co1-C15^{i}	133.2 (2)	C15^{i}-Co1-C30^{ii}	112.5 (2)

N4-Co1-C30^{ii}	97.8 (2)		
Complex 4			
Co1-O4	2.170 (2)	Co2-O1^{ii}	2.062 (3)
Co1-O4^{i}	2.170 (2)	Co2-O1	2.061 (3)
Co1-O5^{i}	2.058 (2)	Co2-N3^{iii}	2.183 (3)
Co1-O5	2.058 (2)	Co2-N3^{iv}	2.183 (3)
Co1-N4^{i}	2.104 (3)	Co2-N7^{v}	2.144 (3)
Co1-N4	2.104 (3)	Co2-N7^{vi}	2.144 (3)
O4-Co1-O4^{i}	180.0	O1-Co2-O1^{ii}	87.76 (17)
O5-Co1-O4^{i}	92.96 (9)	O1-Co2-N3^{iii}	90.73 (11)
O5^{i}-Co1-O4^{i}	87.04 (9)	O1-Co2-N3^{iv}	85.13 (11)
O5-Co1-O4	87.04 (9)	O1^{ii}-Co2-N3^{iii}	85.13 (11)
O5^{i}-Co1-O4	92.96 (9)	O1^{ii}-Co2-N3^{iv}	90.73 (11)
O5-Co1-O5^{i}	180.0	O1-Co2-N7^{v}	178.45 (12)
O5-Co1-N4^{i}	88.38 (11)	O1^{ii}-Co2-N7^{v}	93.17 (12)
O5^{i}-Co1-N4^{i}	91.62 (11)	O1-Co2-N7^{vi}	93.17 (12)
O5^{i}-Co1-N4	88.37 (11)	O1^{ii}-Co2-N7^{vi}	178.45 (12)
O5-Co1-N4	91.63 (11)	N3^{iii}-Co2-N3^{iv}	174.26 (16)
N4-Co1-O4^{i}	90.88 (10)	N7^{v}-Co2-N3^{iv}	93.62 (11)
N4-Co1-O4	89.12 (10)	N7^{vi}-Co2-N3^{iii}	93.62 (11)
N4^{i}-Co1-O4^{i}	89.12 (10)	N7^{v}-Co2-N3^{iii}	90.58 (11)
N4^{i}-Co1-O4	90.88 (10)	N7^{vi}-Co2-N3^{iv}	90.58 (11)
N4-Co1-N4^{i}	180.0	N7^{v}-Co2-N7^{vi}	85.92 (15)

Symmetry codes for **1**: (i) *x*, *y*, *z*-1; (ii) *x*-2, *y*, *z*; (iii) *x*, *y*, *z*+1; (iv) -*x*+1, *y*-1/2, -*z*+1; (v) *x*+2, *y*, *z*; (vi) *x*+2, *y*, *z*+1; (vii) -*x*+1, *y*+1/2, -*z*+1; (viii) *x*-2, *y*, *z*-1.

Symmetry codes for **2**: (i) *x*+1/2, *y*+1/2, *z*; (ii) *x*, -*y*+1, *z*-1/2.

Symmetry codes for **3**: (i) -*x*+2, -*y*+1, -*z*+2; (ii) *x*+1, *y*, *z*; (iii) -*x*+1, -*y*, -*z*+1; (iv) *x*-1, *y*, *z*.

Symmetry codes for **4**: (i) -*x*+3/2, -*y*+3/2, -*z*; (ii) -*x*+1, *y*, -*z*-1/2; (iii) -*x*+1, -*y*+1, -*z*; (iv) *x*, -*y*+1, *z*-1/2; (v) *x*-1/2, -*y*+1/2, *z*-3/2; (vi) -*x*+3/2, -*y*+1/2, -*z*+1.

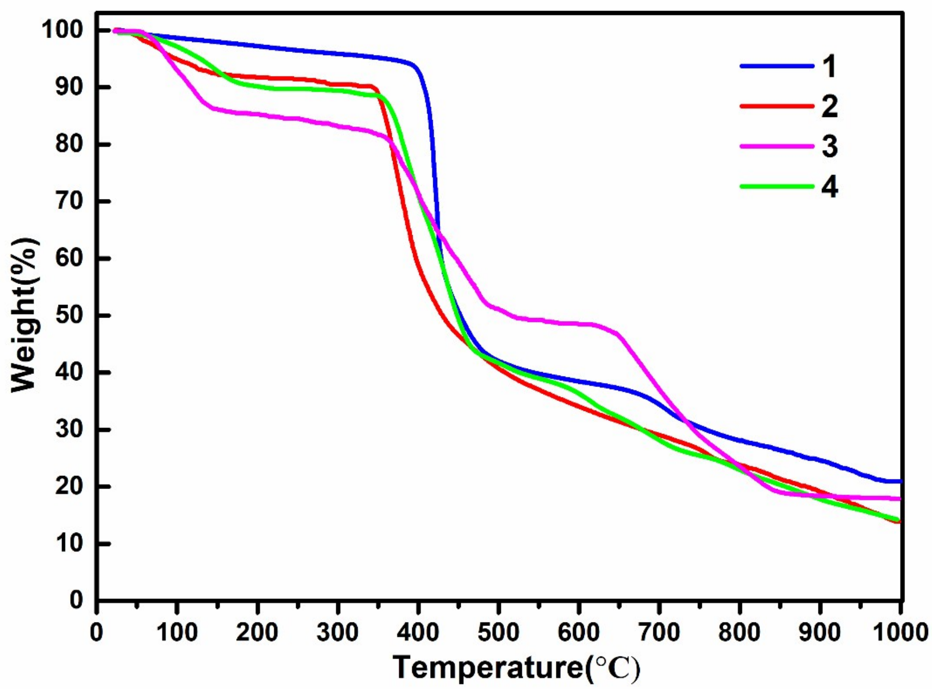


Figure. S1 TG curve of complexes **1-4**

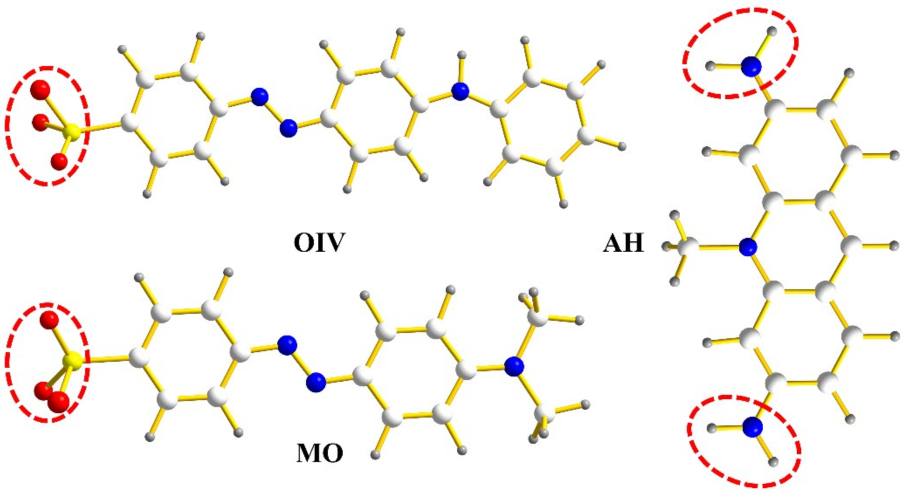


Figure. S2 The different structures and sizes of three organic dyes.

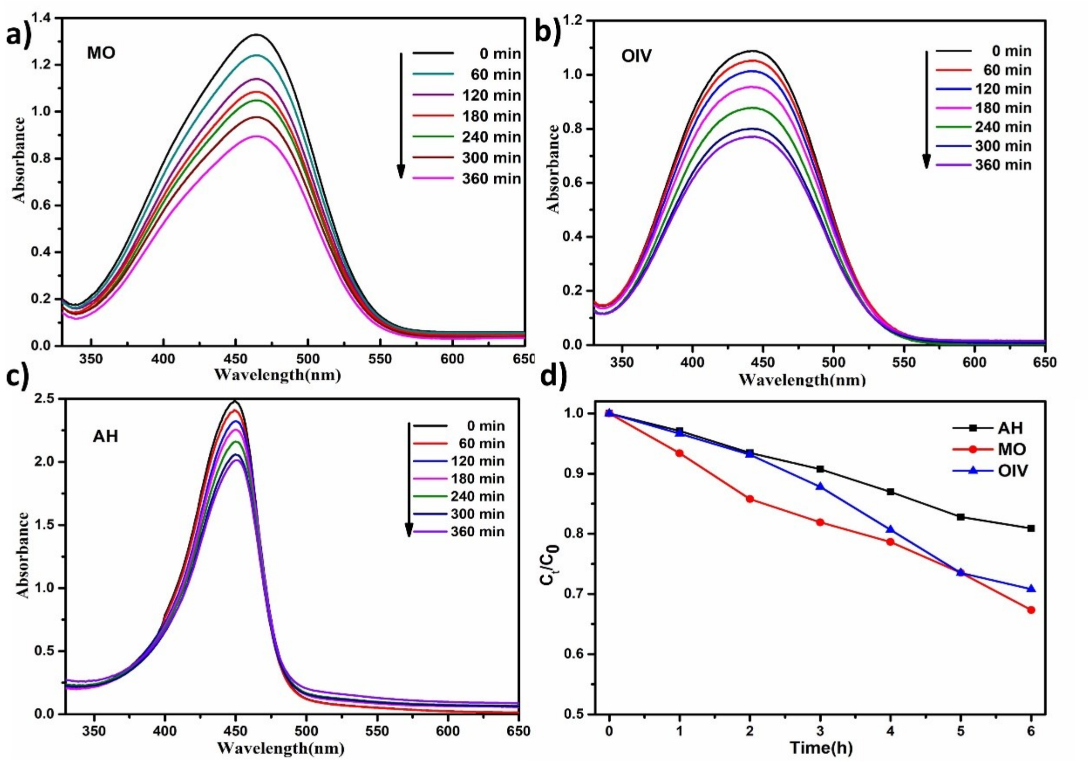


Figure. S3 (a)-(c) UV/Vis spectra of aqueous solution of MO/OIV/AH in the presence of freshly prepared complex **1** monitored with time. (d) Percentage of three dyes remaining in the solution monitored with time.

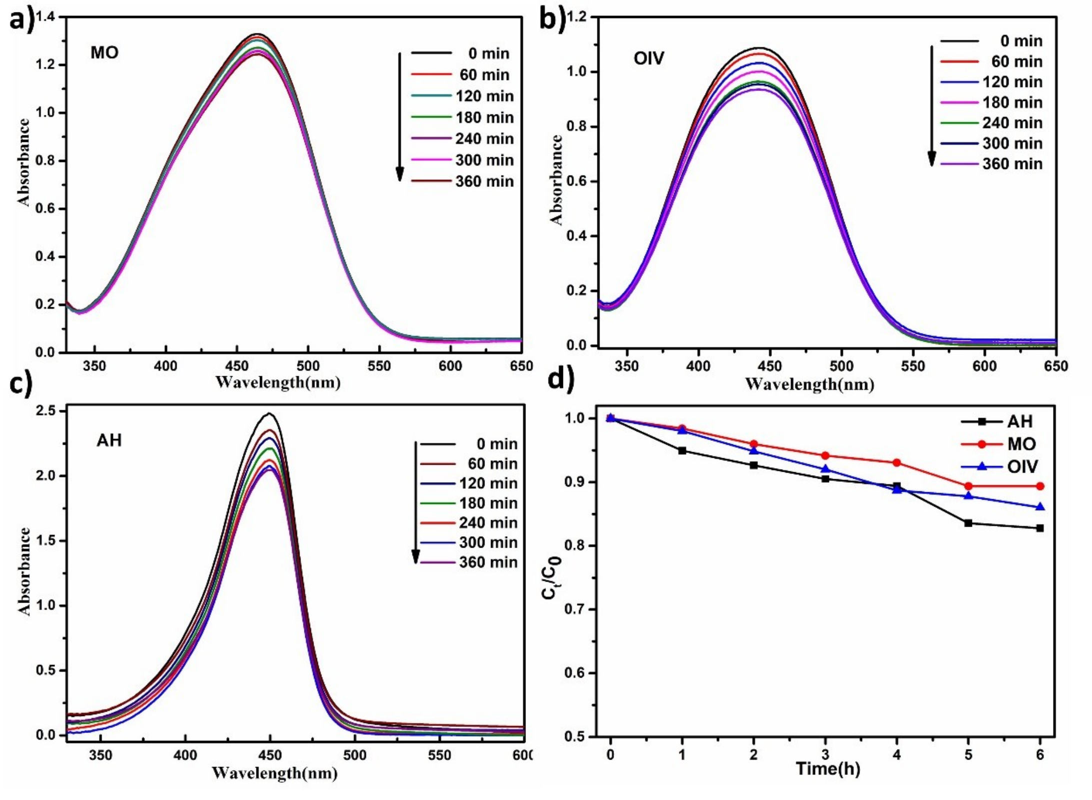


Figure. S4 (a)-(c) UV/Vis spectra of aqueous solution of MO/OIV/AH in the presence of freshly prepared complex **2** monitored with time. (d) Percentage of three dyes remaining in the solution monitored with time.

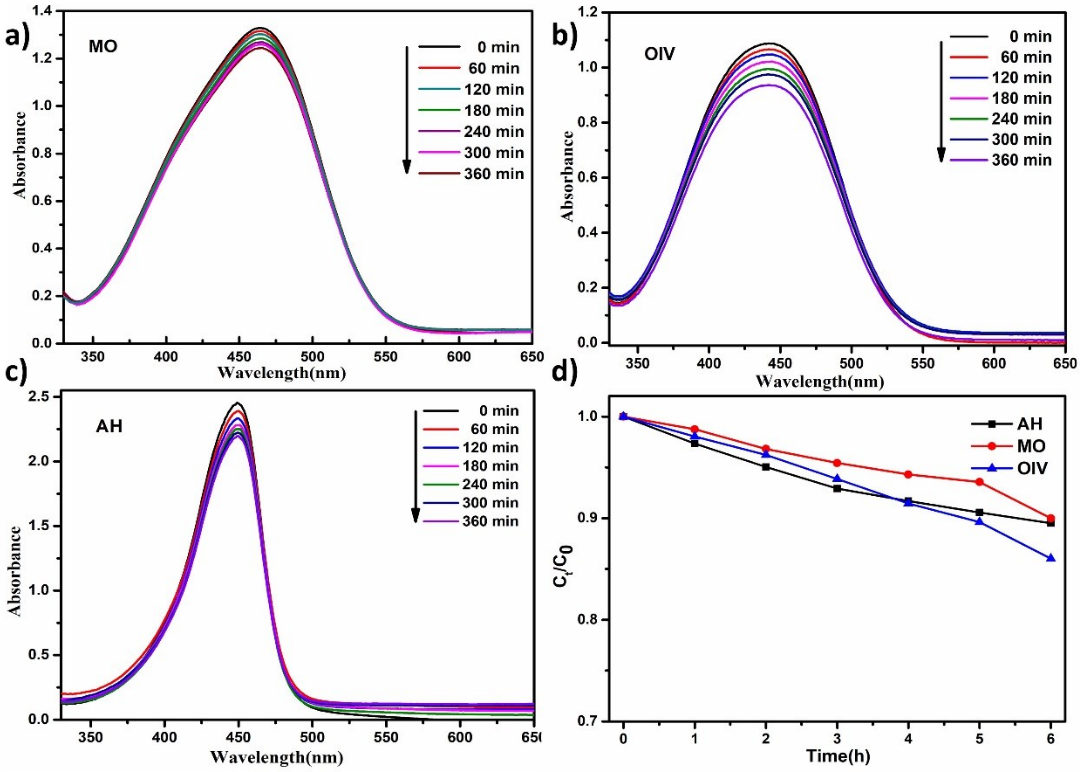


Figure. S5 (a)-(c) UV/Vis spectra of aqueous solution of MO/OIV/AH in the presence of freshly prepared complex **3** monitored with time. (d) Percentage of three dyes remaining in the solution monitored with time.

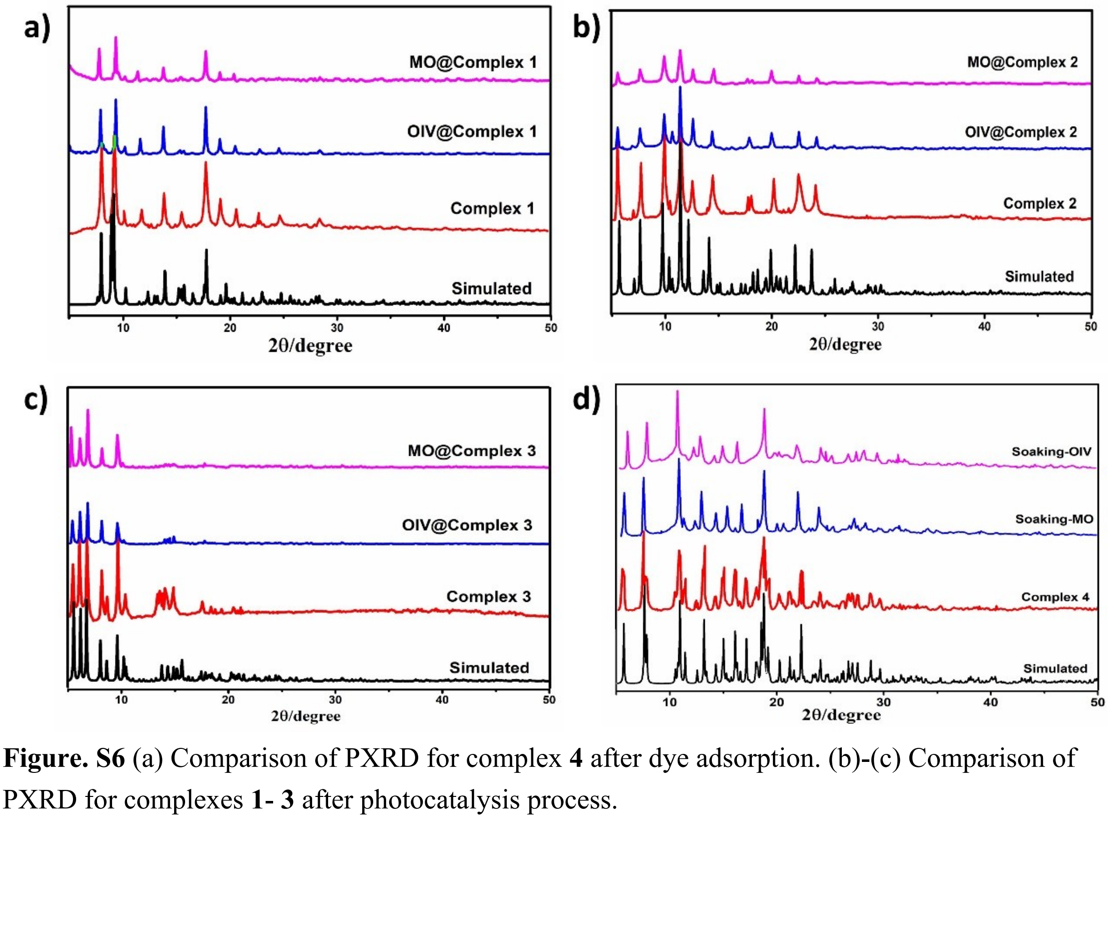


Figure. S6 (a) Comparison of PXRD for complex **4** after dye adsorption. (b)-(c) Comparison of PXRD for complexes **1- 3** after photocatalysis process.

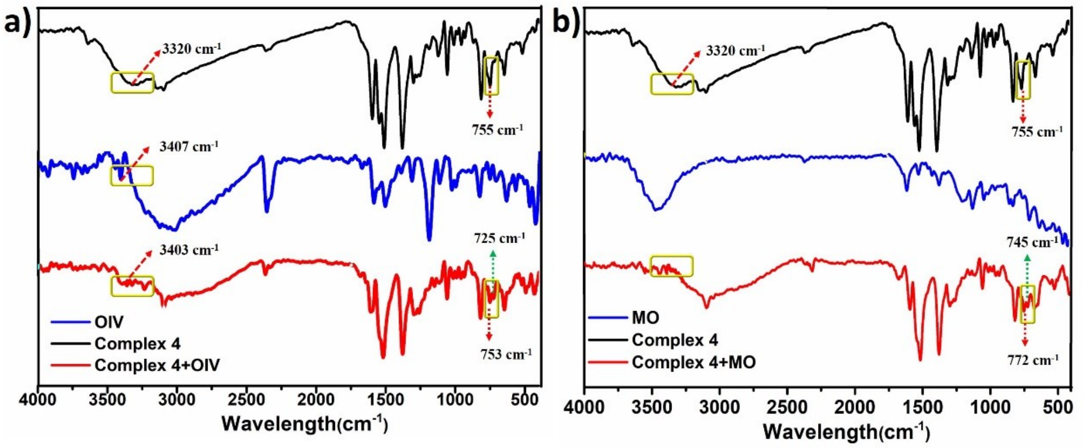
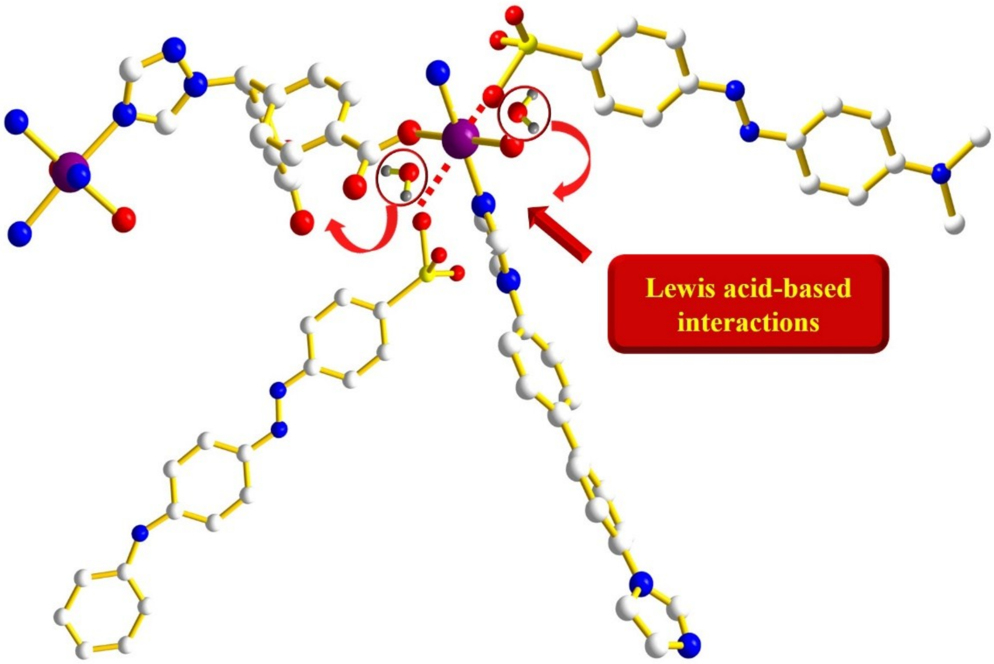


Figure. S7 IR spectra of complex **4** before and after the absorption of dyes.



Scheme S1. The possible mechanism of OIV/MO adsorbed into complex **4**.

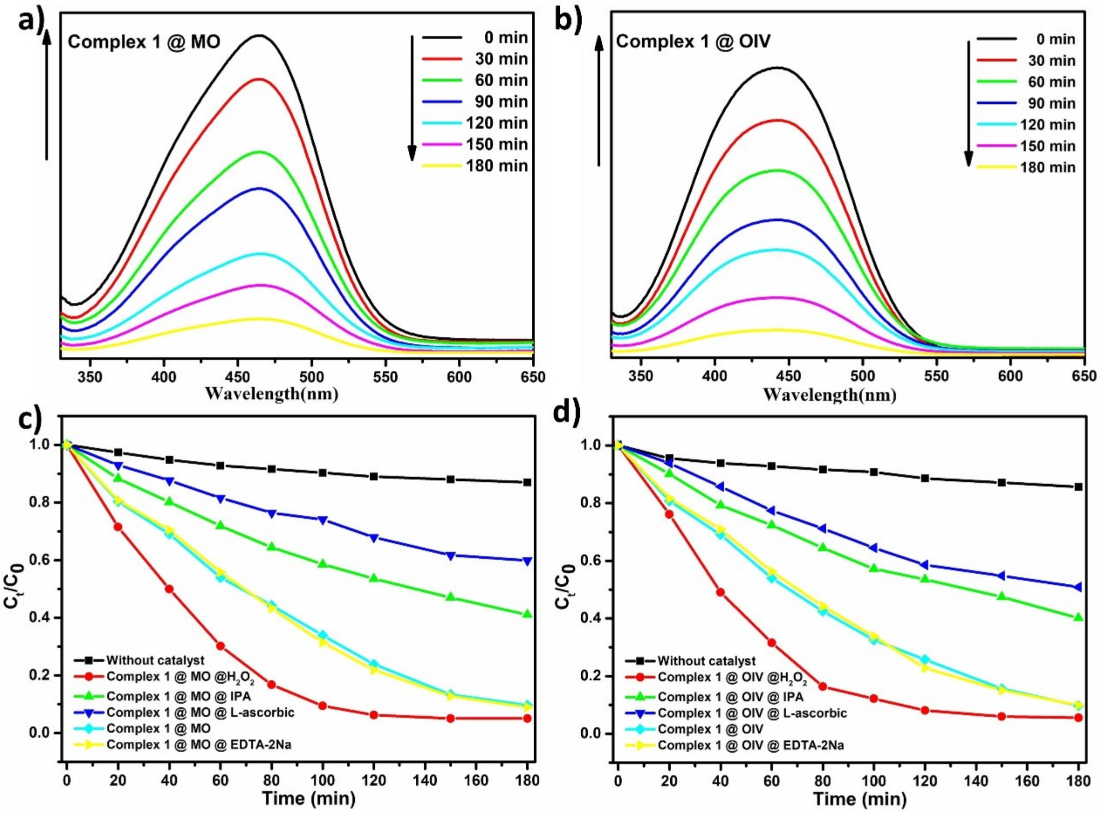


Figure. S8 (a) and (b) UV-vis spectra of MO/OIV solutions in the presence of **1** under UV irradiation at different time intervals. (c) and (d) Plots of concentration ratios of MO/OIV against irradiation time (min) in the presence of complex **1**, radical scavenger (IPA, EDTA-2Na, L-ascorbic) and H_2O_2 during the decomposition reaction under UV irradiation.

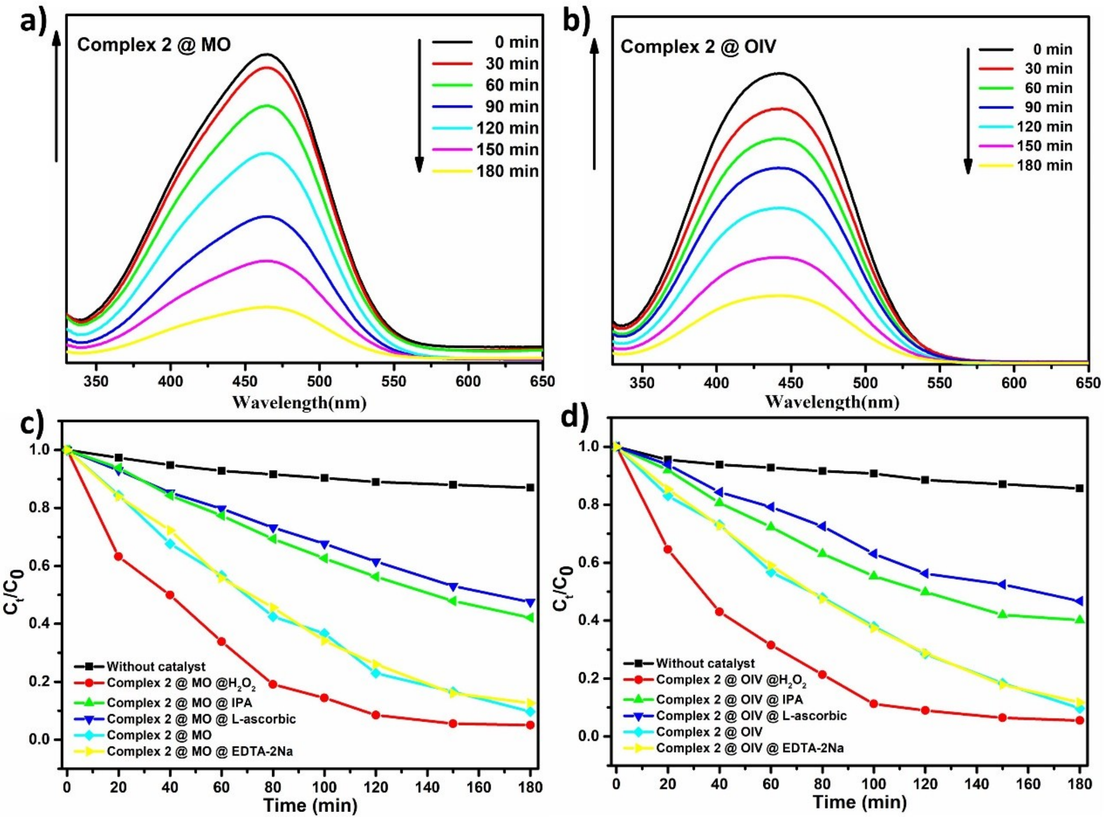


Figure. S9 (a) and (b) UV-vis spectra of MO/OIV solutions in the presence of **2** under UV irradiation at different time intervals. (c) and (d) Plots of concentration ratios of MO/OIV against irradiation time (min) in the presence of complex **2**, radical scavenger (IPA, EDTA-2Na, L-ascorbic) and H_2O_2 during the decomposition reaction under UV irradiation.

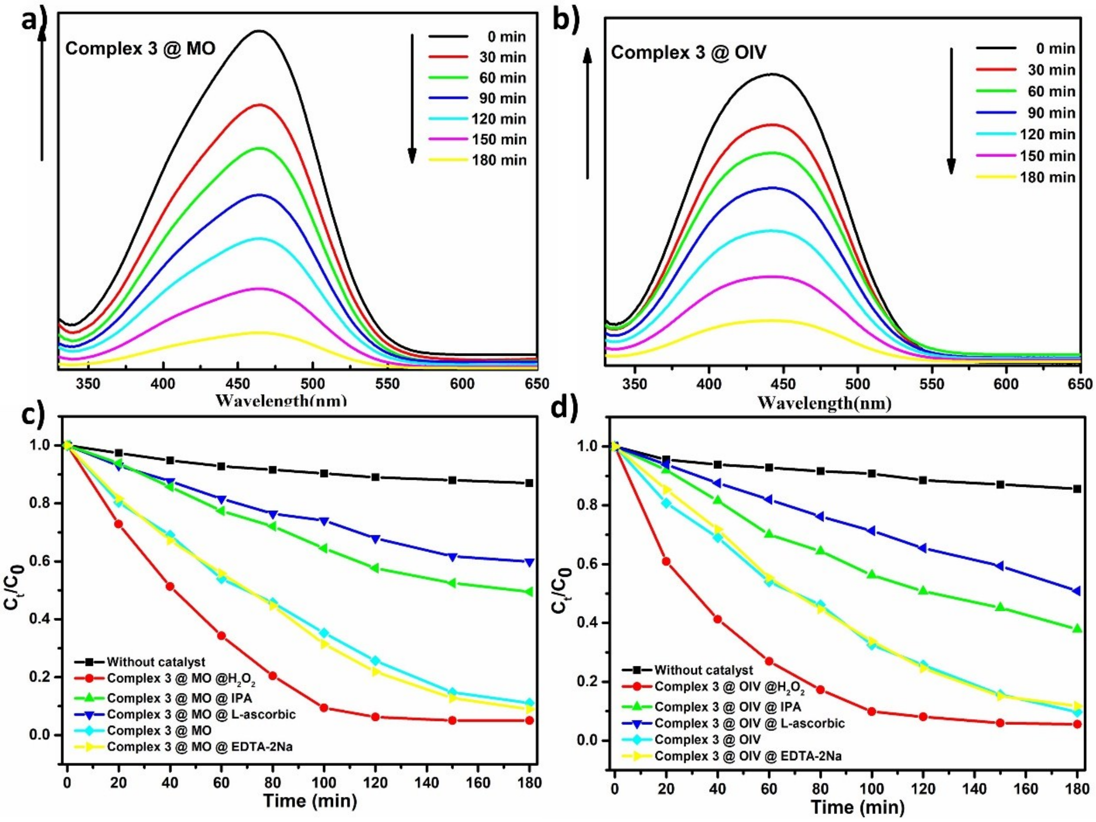


Figure. S10 (a) and (b) UV-vis spectra of MO/OIV solutions in the presence of **2** under UV irradiation at different time intervals. (c) and (d) Plots of concentration ratios of MO/OIV against irradiation time (min) in the presence of complex **3**, radical scavenger (IPA, EDTA-2Na, L-ascorbic) and H_2O_2 during the decomposition reaction under UV irradiation.

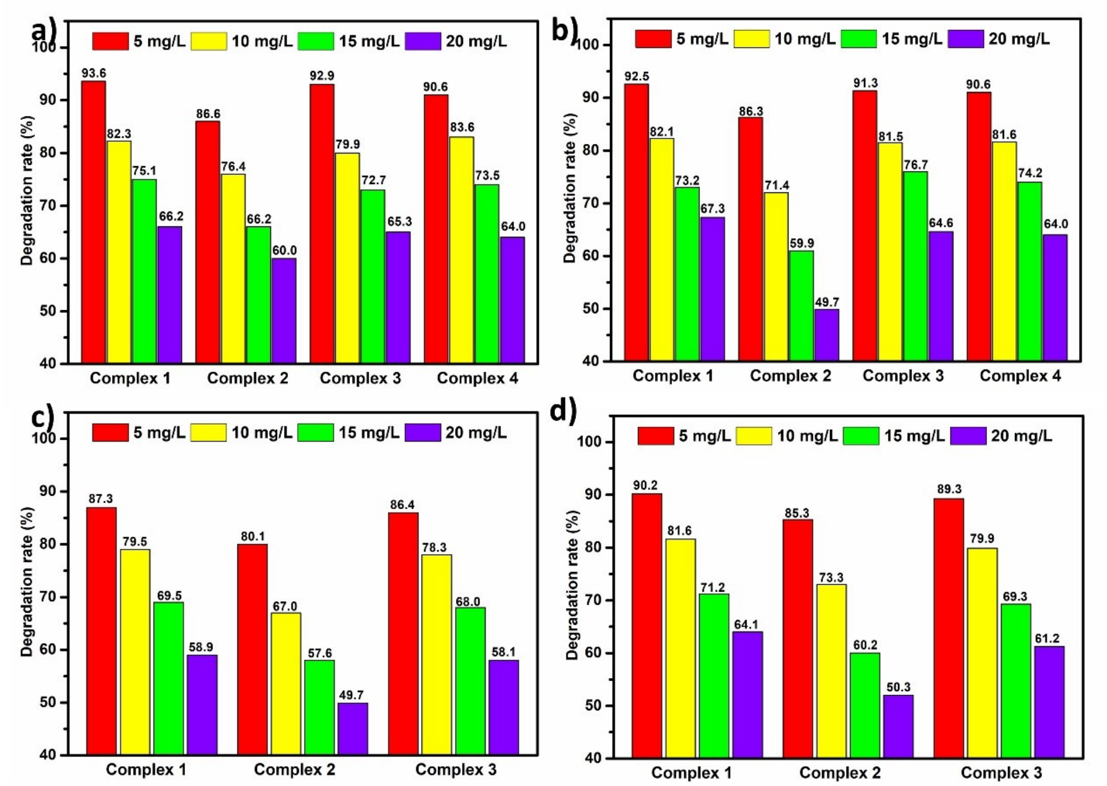


Figure. S11 Effect of initial concentration of different dyes ((a)for MB, (b) for MV, (c) for OIV and (d) for MO) aqueous solution on degradation process in 3 hours.

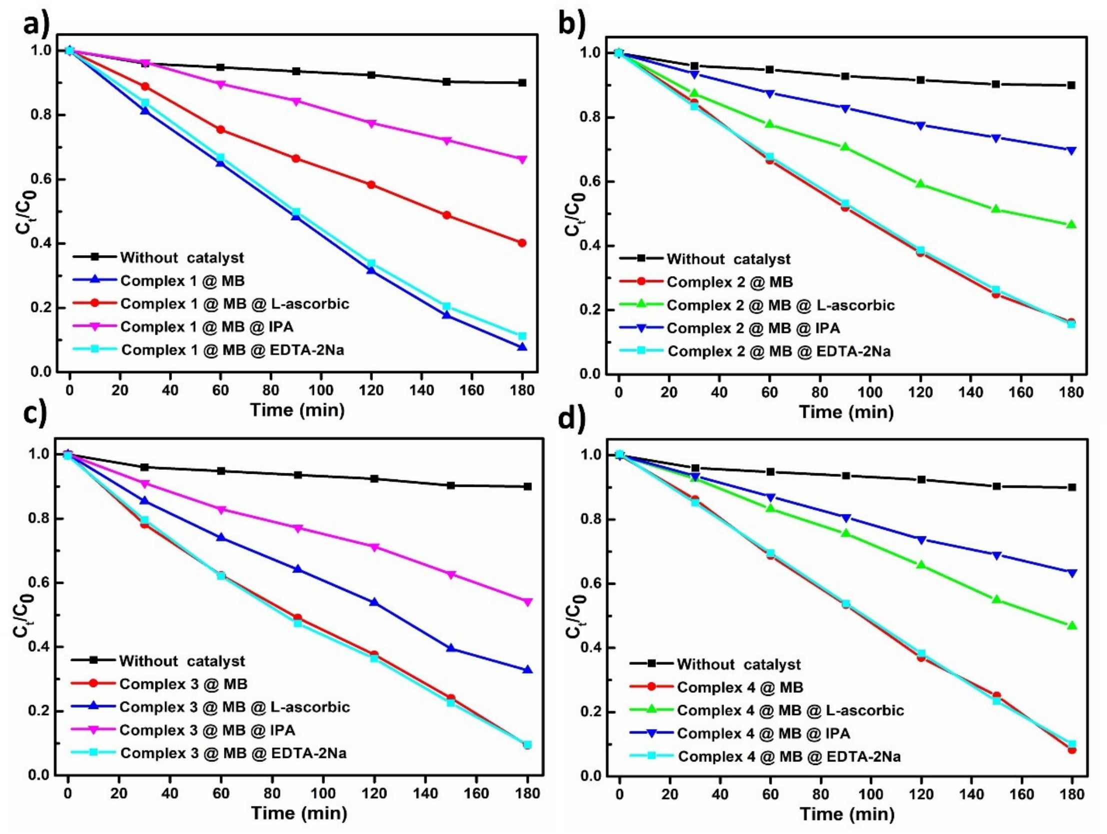


Figure. S12 Plots of concentration ratios of MB against irradiation time (min) in the presence of complexes **1-4** and radical scavenger (IPA, EDTA-2Na, L-ascorbic) during the decomposition reaction under UV irradiation.

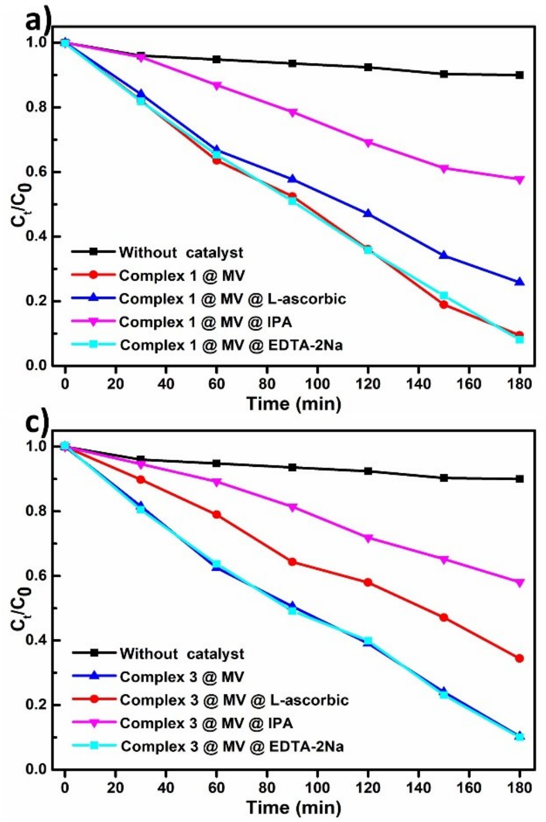


Figure. S13 Plots of concentration ratios of MV against irradiation time (min) in the presence of complexes **1-4** and radical scavenger (IPA, EDTA-2Na, L-ascorbic) during the decomposition reaction under UV irradiation.

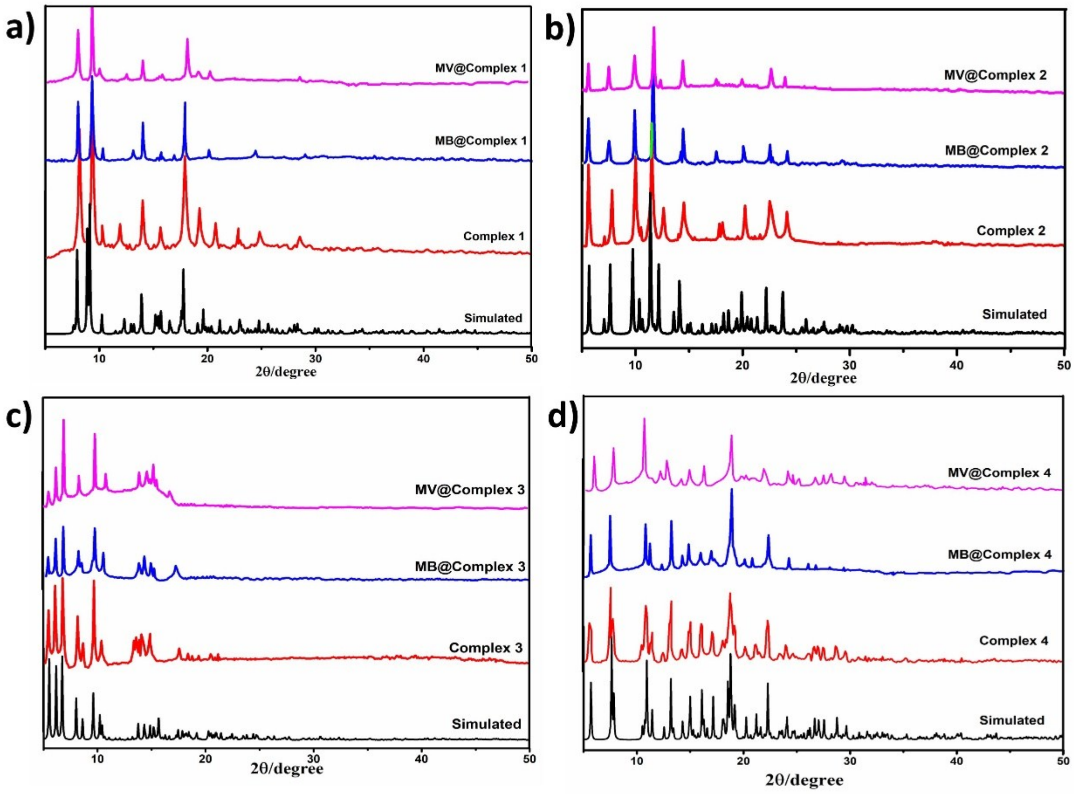


Figure. S14 Comparison of PXRD for complexes **1- 4** after photocatalysis process.

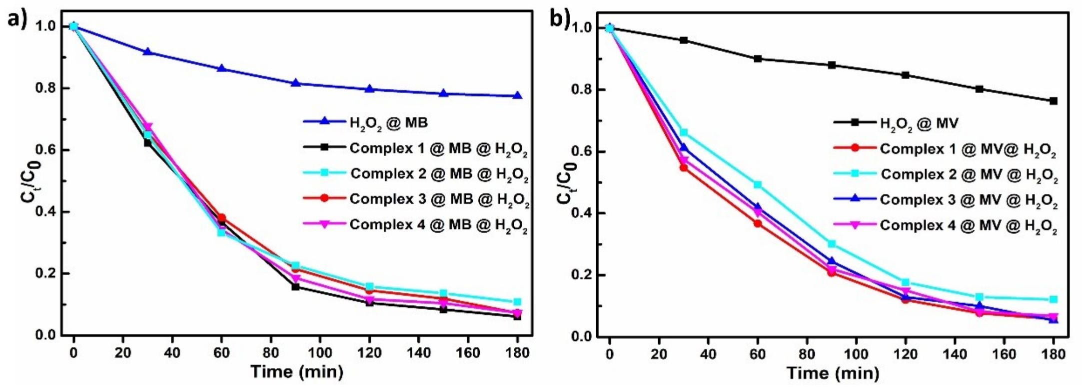


Figure. S15 (a) and (b) Plots of concentration ratios of MB/MV against irradiation time (min) in the presence of complexes **1-4** and H_2O_2 during the decomposition reaction under UV irradiation.