Supporting Information

Energy-Dependent Photochromism at Room Temperature for Visually Detecting and Distinguishing X-Rays

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1. EXPERIMENTAL SECTION

Materials. All chemical reagents in AR grade were purchased from commercial companies and used without further purification.

Measurements. Elemental analyses of C, H, and N were measured on an Elementar Vario EL III microanalyzer. IR spectra were measured on a PerkinElmer Spectrum One FT-IR spectrometer using KBr pellets. UV–vis absorption spectra were measured in the diffuse reflectance mode on a PerkinElmer Lambda 950 UV/vis/near-IR spectrophotometer equipped with an integrating sphere, and a $BaSO_4$ plate was used as the reference. PXRD patterns were recorded using Cu-K_α radiation on a Rigaku Desktop MiniFlexII diffractometer powered at 30 kV and 15 mA. The simulated PXRD pattern was derived from the X-ray single crystal diffraction data using the Mercury software, which can be downloaded free from the Cambridge Crystallographic Data Centre (CCDC; https://www.ccdc.cam.ac.uk/support-and-resources/downloads/). The thermogravimetric analysis was conducted on a Mettler TOLECO simultaneous TGA/DSC apparatus in N2. EPR spectra were recorded on a Bruker ER-420 spectrometer with a 100 kHz magnetic field in the X band at room temperature. XPS studies were performed in a ThermoFisher ESCALAB 250Xi X-ray photoelectron spectrometer (powered at 150 W) using Al-K_α radiation. Solid-state NMR data were recorded in a Bruker-BioSpin AVANCE Ⅲ HD Solid-state NMR Spectrometer.

Al-K_α, Cu-K_α, and Mo-K_α X-rays used for coloration were generated, respectively, from the above-mentioned ThermoFisher ESCALAB250 X-ray photoelectron spectrometer (spot size of irradiation: 900 μm), the above-mentioned Rigaku Desktop MiniFlexII powder X-ray diffractometer (spot size of irradiation: 10 mm in width) and a Rigaku Pilatus 200K single-crystal X-ray diffractometer (powered at 50 kV and 80 mA; spot size of irradiation: 1 × 2 mm^2).

Synthesis of $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]\cdot 2H_2O$ (XP-3; Dg = diglycolate). The crystal structure of **XP-3** (CCDC No. 178915) has been reported by Tao et al (*Main Group Met. Chem.*, 2002, **25**, 321). In this work, it was synthesized with a minor modification of the reported method on temperature and time. A mixture of 4,4'-bipy (158 mg, 1.0 mmol), $Zn(NO_3)_2\cdot 6H_2O$ (297 mg, 1.0 mmol), diglycolic acid (134 mg, 1.0 mmol), NaOH (80 mg, 2.0 mmol) and H_2O (6 mL) was loaded into a 25 mL sealed Teflon−lined autoclave, and heated at 120 °C for 2 d before cooling down to room temperature. Pale yellow block crystals of **XP-3** were obtained by filtration of the solution and washed by ethanol and then dried in dark in air. The phase purity of the crystalline sample was checked by PXRD (Fig. S4), NMR (Fig. S16), and elemental analyses. Calcd. (%) for **XP-3**: C, 32.80; H, 4.28; N, 4.25. Found (%): C, 33.01; H, 4.35; N, 4.33. ^{13}C NMR (solid state, 101 MHz): δ 173.38 (COO in Dg); 148.02, 144.18, 122.17 (pyridyl); 65.82 (–CH_2– in Dg).

Theoretical Calculations. All calculations were performed at the B3LYP/6-31g* level using the Gaussian 09 suite.[1] The exchange correlation functional B3LYP[2] was chosen in view of its good compromise between accuracy and computational cost. It has been reported that electron-transfer photochromic compounds show only minor structural variation after photoinduced coloration.[3] So, the structural geometry of $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]$ was not optimized for the calculation of the Mülliken charges of **XP-3** under the closed-shell singlet and triplet states. However, to compare energy levels of the free water molecule and the $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]$ complex in **XP-3**, both structures were optimized before frequency analysis. Likewise, to study the population of spin density, the open-shell singlet ground state of the $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]$ complex was also optimized using the "guess mix" keyword in the Gaussian software.

2. ADDITIONAL FIGURES.

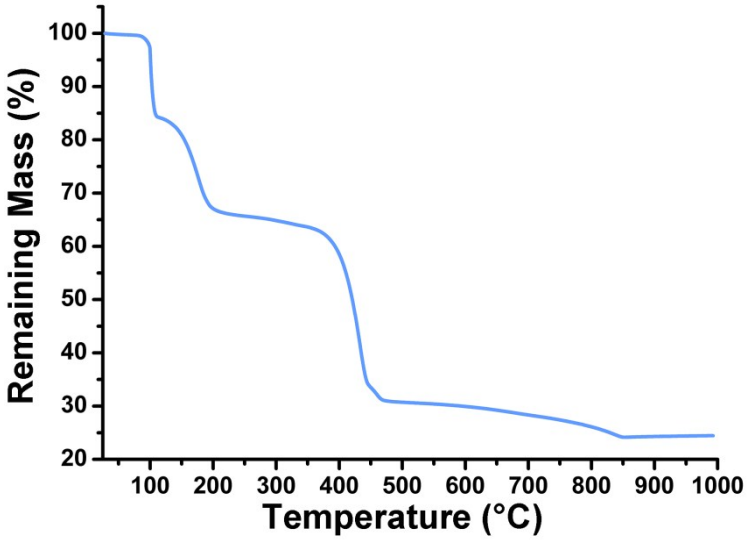

Fig. S1 Thermogravimetric curve of **XP-3** recorded in N_2 with a ramping temperature of 10 °C min^{-1}.

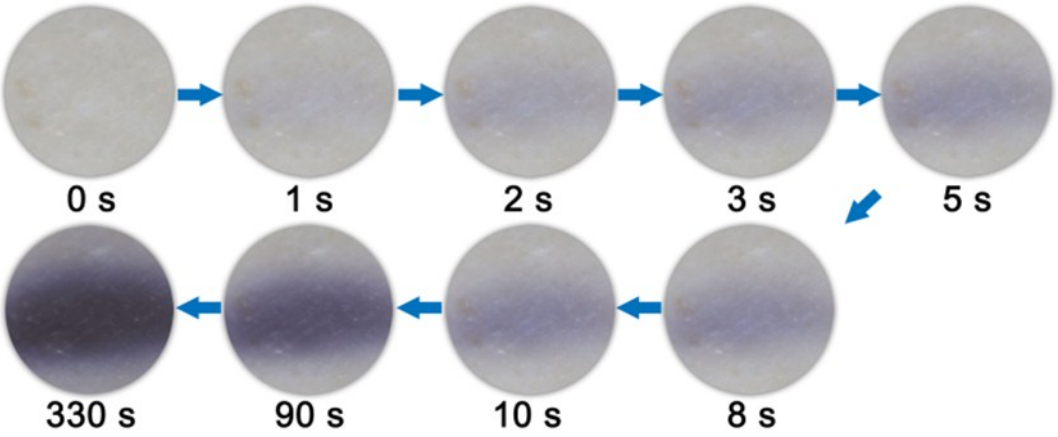

Fig. S2 Time-dependent color change of a tableted sample of **XP-3** under successive irradiation of Al-K_α X-ray (λ = 8.357 Å; spot size, 900 µm; power, 150 W) from the ThermoFisher ESCALAB250 X-ray photoelectron spectrometer at room temperature.

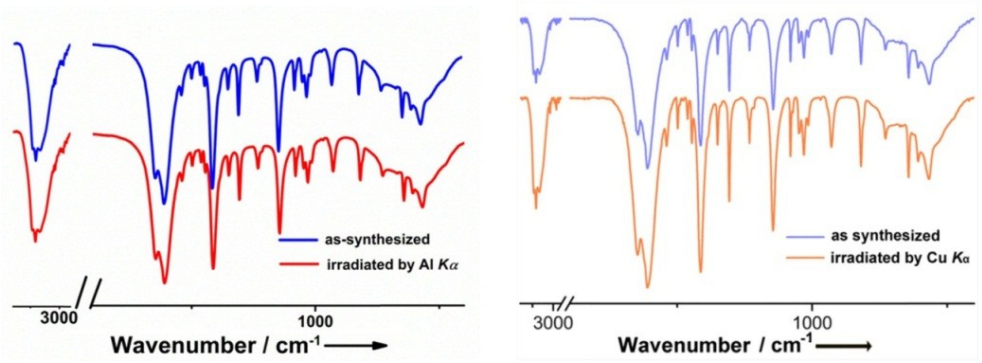

Fig. S3 IR spectra of **XP-3** before and after irradiation by Al-K_α (left) and Cu-K_α (right) X-rays.

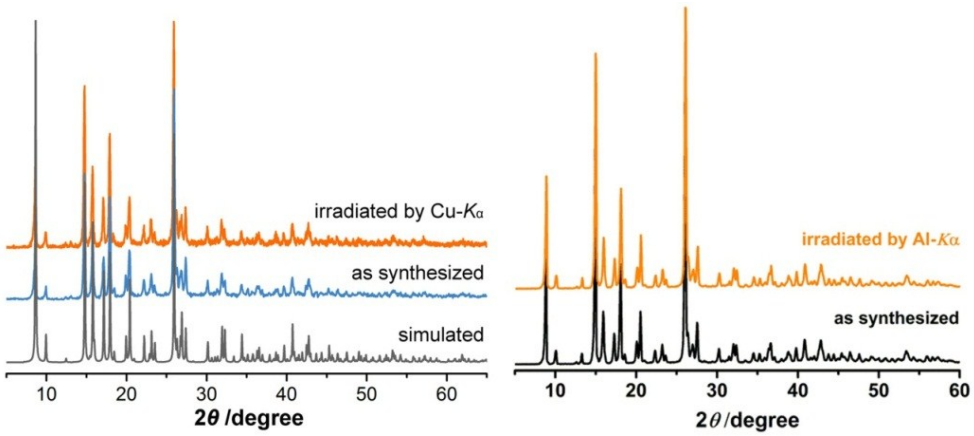

Fig. S4 PXRD patterns of **XP-3** before and after irradiation by Cu-K_α (left) and Al-K_α (right) X-rays. The simulated data was derived from the single crystal X-ray diffration data.

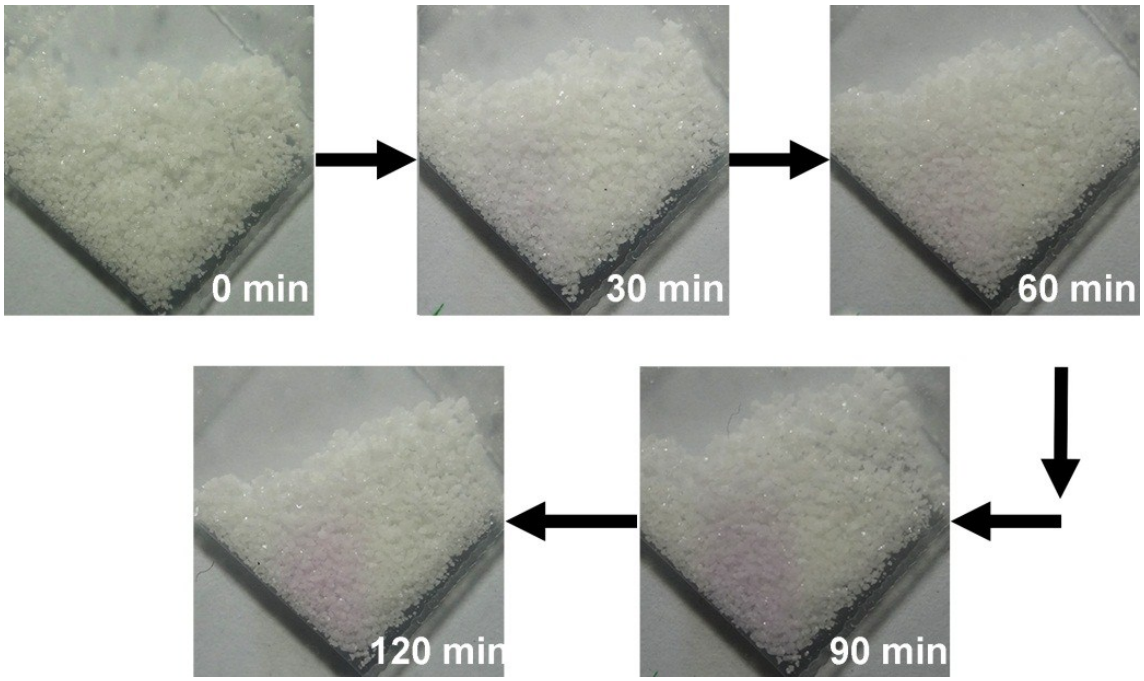

Fig. S5 Color evolution of a single-crystal sample of **XP-3** upon irradiation of Cu-K_α X-ray (λ = 1.54056 Å, 8.0478 keV) from the Rigaku Desktop MiniFlexII powder X-ray diffractometer (powered at 450 W).

Fig. S6 A single-crystal sample of **XP-3** after irradiation by the Cu-K_α X-ray (λ = 1.54056 Å, 8.0478 keV) for 10 h.

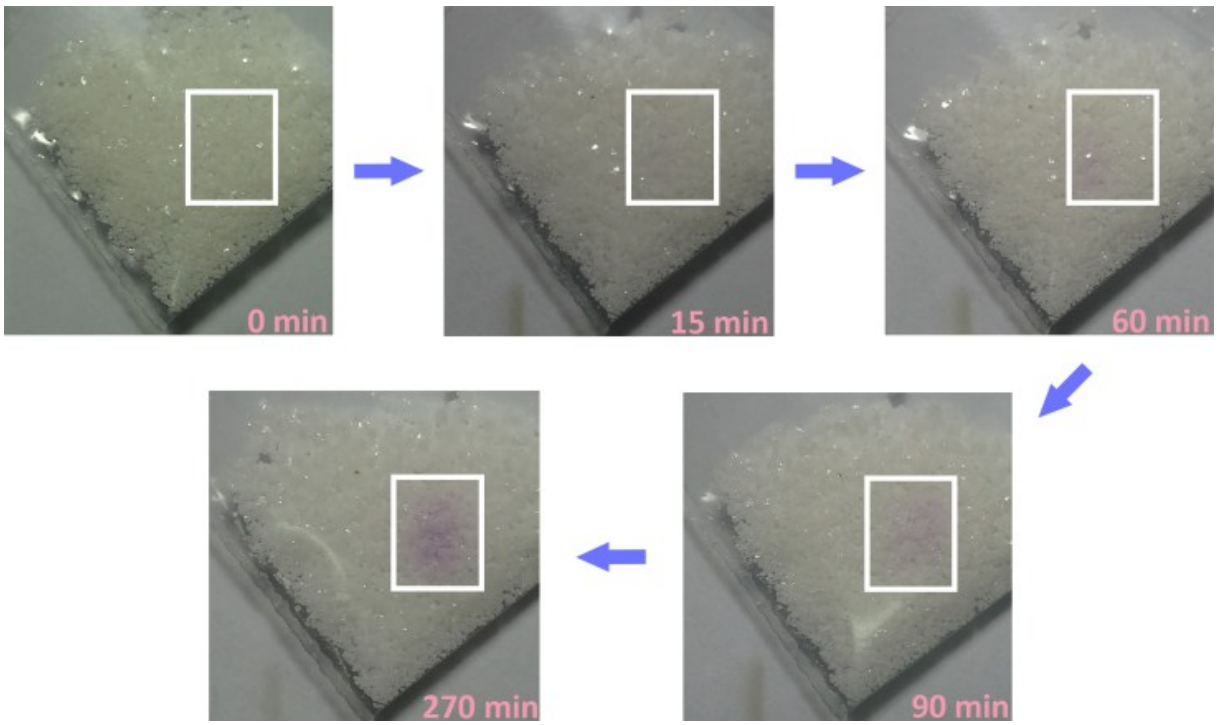

Fig. S7 Color evolution of a single-crystal sample of **XP-3** upon irradiation of Mo-K_α X-ray (λ = 0.7107 Å, 17.4793 keV) from the Rigaku Pilatus 200K single-crystal X-ray diffractometer powered at 4 kW.

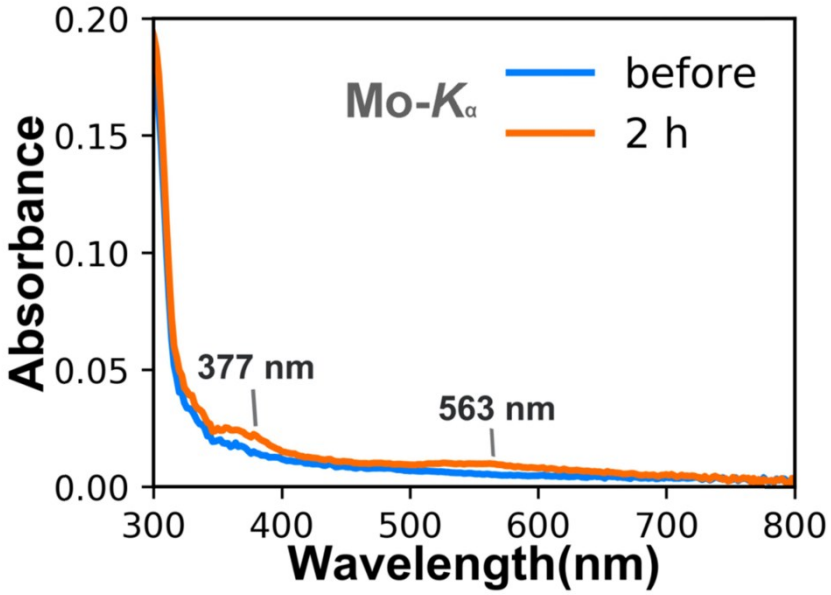

Fig. S8 UV–vis absorption spectra of **XP-3** before and after irradiation by Mo-K_α X-ray (λ = 0.7107 Å) from the Rigaku Pilatus 200K single-crystal X-ray diffractometer for 2 h.

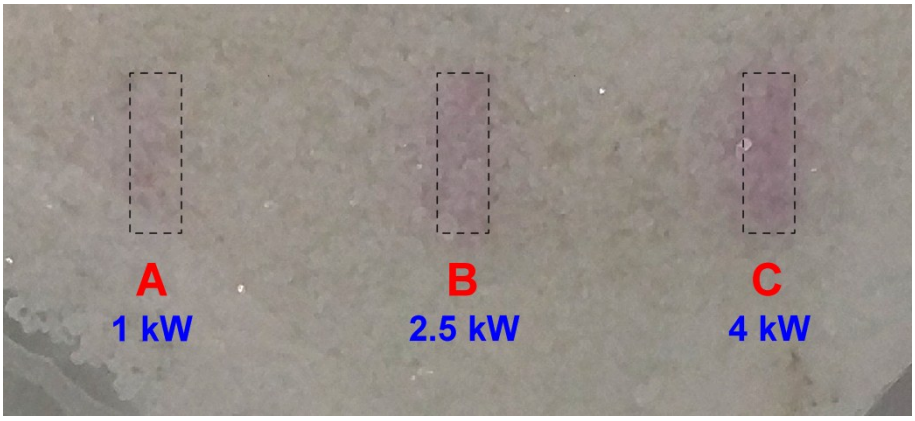

Fig. S9 Irradiation intensity-dependent coloration behavior for a single-crystal sample of **XP-3**, evaluated in a single-crystal X-ray diffractometer (Mo-K_α X-ray; 5-h irradiation each spot). Powers of the diffractometer: A, 1 kW, 533018 mR/h; B, 2.5 kW, 1578808 mR/h; C, 4 kW, 226941 mR/h.

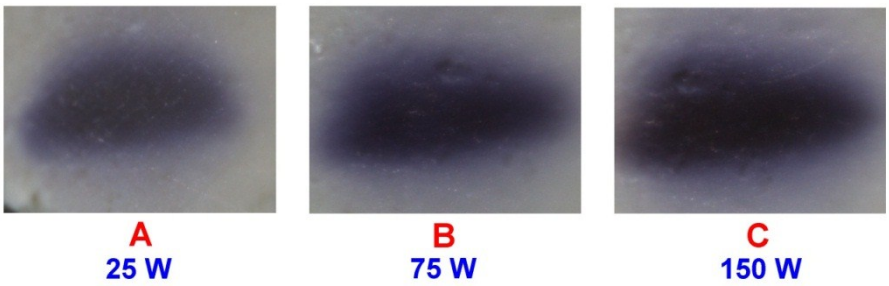

Fig. S10 Irradiation intensity-dependent coloration behavior for tableted samples of **XP-3**, evaluated in a photoelectron spectrometer (Al-K_α X-ray, 2-min irradiation each spot). Powers of the diffractometer are labeled.

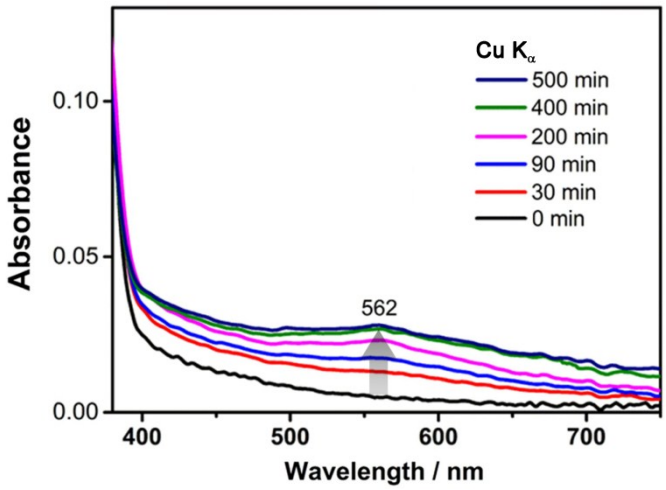

Fig. S11 Time-dependent absorption spectra of **XP-3** irradiated by Cu-K_α X-ray. The power of the PXRD instrument is 450 W.

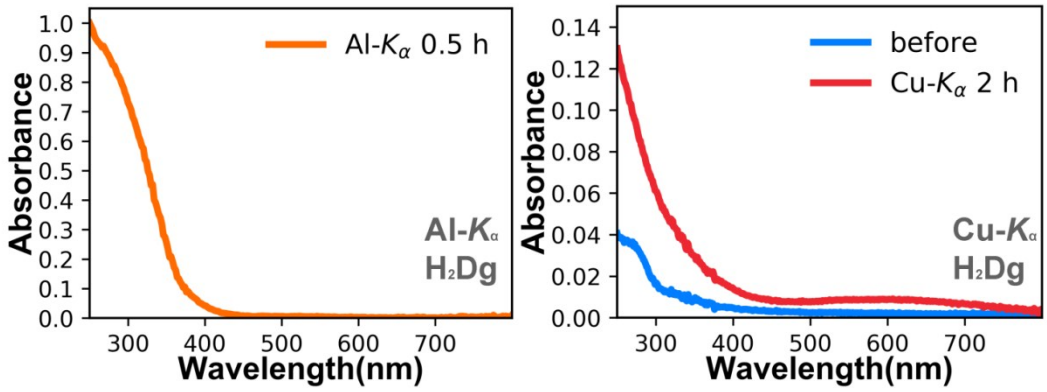

Fig. S12 UV–vis absorption spectra of diglycolic acid (H_2Dg) after irradiation by Al-K_α X-ray (λ = 8.357 Å) for 30 min (left) and Cu-K_α X-ray (λ = 1.54056 Å) for 2 h (right). The data in the right graph were measued using the same sample, and thus the intensities are comparable.

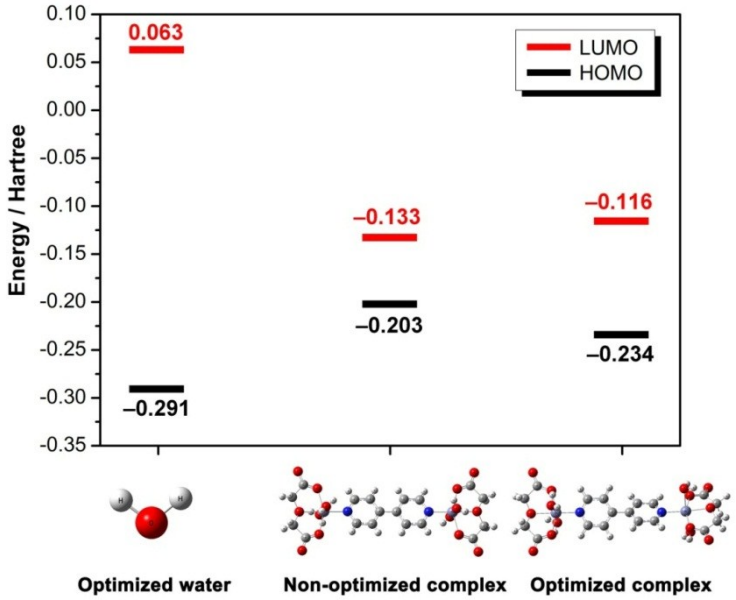

Fig. S13 HOMO and LUMO energy levels and molecule structures for a free water molecule and the coordinated complex in **XP-3** under the closed-shell singlet states.

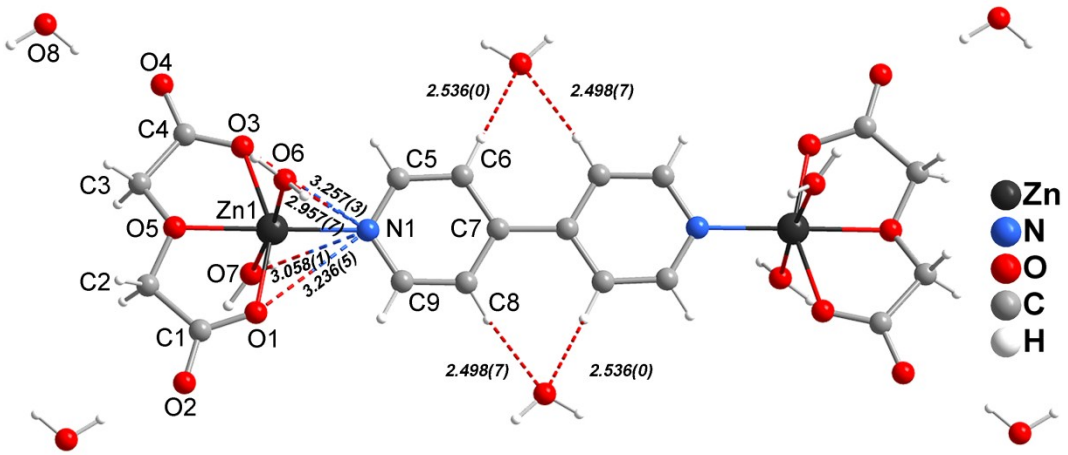

Fig. S14 A molecular structural diagram of **XP-3** showing partial intramolecular and intermolecular O···O separations in angstrom.

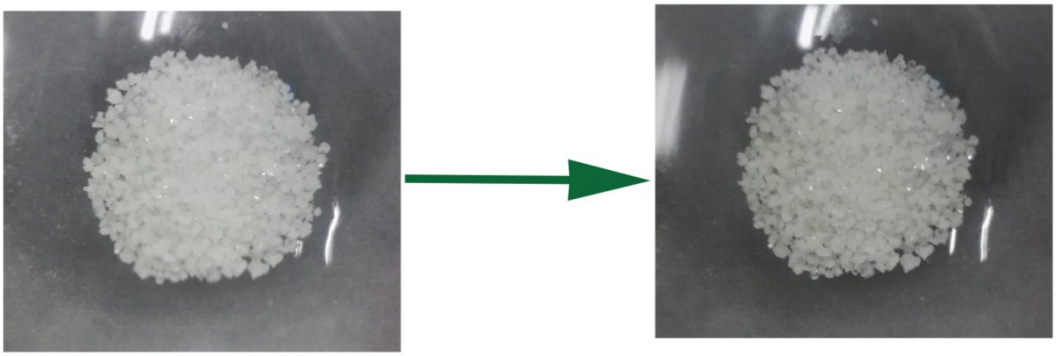

Fig. S15 Color comparison of a single-crystal sample of **XP-3** before and after irradiation in vacuum using a 300 W xenon lamp system (155 mW/cm^2; 4 h).

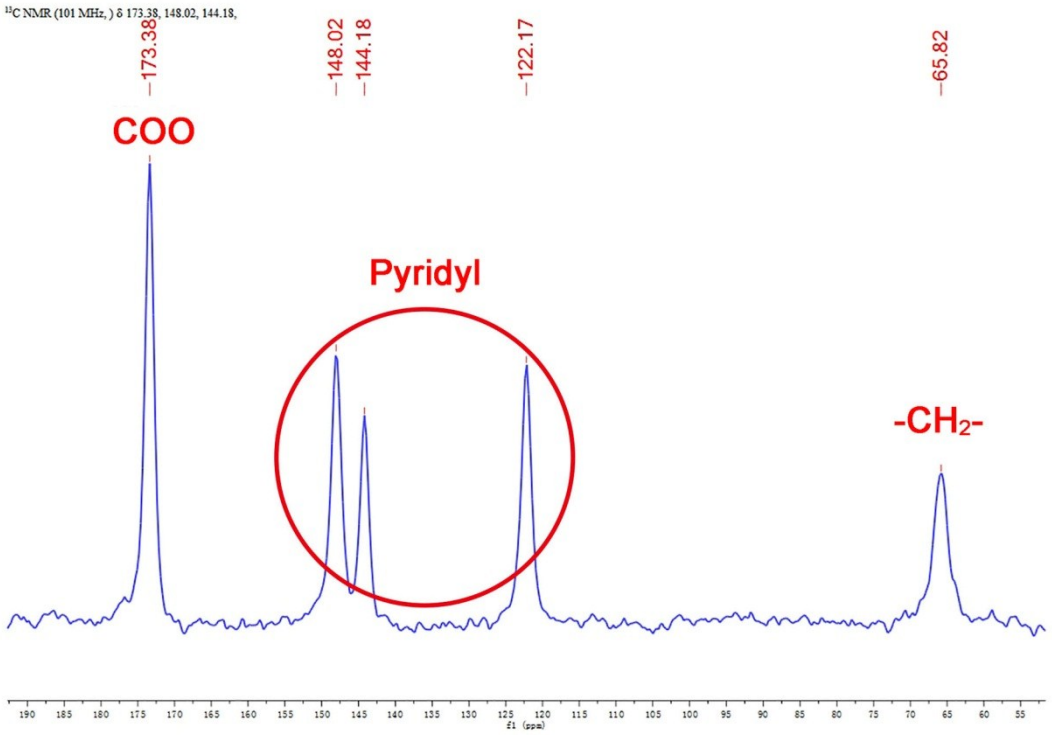

Fig. S16 Solid-state ^{13}C NMR spectrum of **XP-3**.

3. ADDITIONAL TABLES.

Table S1. Geometry for the optimized $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]$ complex under the closed-shell and open-shell singlet ground states.

Closed-shell singlet ground state							
Zn							
N	1	B1					
O	1	B2	2	A1			
O	3	B3	1	A2	2	D1	0
O	1	B4	3	A3	4	D2	0
O	5	B5	1	A4	3	D3	0
O	1	B6	5	A5	6	D4	0
O	1	B7	5	A6	6	D5	0
O	1	B8	5	A7	6	D6	0
C	4	B9	3	A8	1	D7	0
C	7	B10	1	A9	5	D8	0
C	7	B11	1	A10	5	D9	0
C	6	B12	5	A11	1	D10	0
C	2	B13	1	A12	5	D11	0
C	14	B14	2	A13	1	D12	0
C	15	B15	14	A14	2	D13	0
C	16	B16	15	A15	14	D14	0
C	2	B17	1	A16	5	D15	0
H	8	B18	1	A17	5	D16	0
H	8	B19	1	A18	5	D17	0
H	9	B20	1	A19	5	D18	0
H	9	B21	1	A20	5	D19	0
H	11	B22	7	A21	1	D20	0
H	11	B23	7	A22	1	D21	0
H	12	B24	7	A23	1	D22	0
H	12	B25	7	A24	1	D23	0

H	14	B26	2	A25	1	D24	0
H	15	B27	14	A26	2	D25	0
H	17	B28	16	A27	15	D26	0
H	18	B29	2	A28	1	D27	0
Zn	16	B30	15	A29	14	D28	0
N	31	B31	16	A30	15	D29	0
O	31	B32	16	A31	15	D30	0
O	33	B33	31	A32	16	D31	0
O	31	B34	16	A33	15	D32	0
O	35	B35	31	A34	16	D33	0
O	31	B36	16	A35	15	D34	0
O	31	B37	16	A36	15	D35	0
O	31	B38	16	A37	15	D36	0
C	34	B39	33	A38	31	D37	0
C	37	B40	31	A39	16	D38	0
C	37	B41	31	A40	16	D39	0
C	36	B42	35	A41	31	D40	0
C	32	B43	31	A42	16	D41	0
C	44	B44	32	A43	31	D42	0
C	45	B45	44	A44	32	D43	0
C	46	B46	45	A45	44	D44	0
C	32	B47	31	A46	16	D45	0
H	38	B48	31	A47	16	D46	0
H	38	B49	31	A48	16	D47	0
H	39	B50	31	A49	16	D48	0
H	39	B51	31	A50	16	D49	0
H	41	B52	37	A51	31	D50	0
H	41	B53	37	A52	31	D51	0
H	42	B54	37	A53	31	D52	0
H	42	B55	37	A54	31	D53	0

H	44	B56	32	A55	31	D54	0
H	45	B57	44	A56	32	D55	0
H	47	B58	46	A57	45	D56	0
H	48	B59	32	A58	31	D57	0

B1	2.07376354
B2	1.96893584
B3	2.25888114
B4	1.95867976
B5	2.25687781
B6	2.17692130
B7	2.27676660
B8	2.31544909
B9	1.21854754
B10	1.43567742
B11	1.43295710
B12	1.21924074
B13	1.34401411
B14	1.38951463
B15	1.40287132
B16	1.40299181
B17	1.34381938
B18	0.97094197
B19	0.98027591
B20	0.97449434
B21	0.96927883
B22	1.09753802
B23	1.09460947
B24	1.09426483
B25	1.09780682

B26	1.08641106
B27	1.08484949
B28	1.08482005
B29	1.08653140
B30	6.35214950
B31	2.07357547
B32	1.96916992
B33	2.25878294
B34	1.95664415
B35	2.25685583
B36	2.17982344
B37	2.27673682
B38	2.31632841
B39	1.21862279
B40	1.43540978
B41	1.43294757
B42	1.21919145
B43	1.34387273
B44	1.38966010
B45	1.40288118
B46	1.40291857
B47	1.34389351
B48	0.97097210
B49	0.98007473
B50	0.97458964
B51	0.96929034
B52	1.09758701
B53	1.09462092
B54	1.09425726
B55	1.09775399

B56	1.08644485
B57	1.08479016
B58	1.08479184
B59	1.08655914
A1	102.41295672
A2	142.50629596
A3	157.13674243
A4	145.51851379
A5	80.16477777
A6	108.59423073
A7	76.49737908
A8	27.74223742
A9	107.20079642
A10	109.96241731
A11	27.83270365
A12	120.01666152
A13	122.20009975
A14	119.53031267
A15	117.54721721
A16	120.84170587
A17	106.77793283
A18	83.00649700
A19	90.41669446
A20	130.51716264
A21	109.78702079
A22	110.56359726
A23	110.41329715
A24	109.92844198
A25	115.61227754
A26	119.43993893

A27	121.01411856
A28	115.75225402
A29	122.06748400
A30	2.82804284
A31	101.45054510
A32	142.67006322
A33	100.87756313
A34	145.50875514
A35	169.58884401
A36	85.96481476
A37	101.31544793
A38	27.74303955
A39	107.16093779
A40	109.76729685
A41	27.84261015
A42	120.41170918
A43	122.22500271
A44	119.51084551
A45	117.53686073
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A48	83.20934912
A49	90.30134295
A50	130.60923140
A51	109.78322101
A52	110.57660216
A53	110.42663093
A54	109.89643778
A55	115.67548179
A56	119.46122212

A57	121.01765464
A58	115.72259456
D1	-155.92740439
D2	8.17259261
D3	23.83321003
D4	0.41204265
D5	-79.72762070
D6	91.64765306
D7	-18.60665089
D8	142.45620593
D9	12.32471615
D10	-5.92291938
D11	11.66267660
D12	175.71646567
D13	-0.26754498
D14	0.13426914
D15	-172.92132718
D16	52.50070585
D17	155.70156711
D18	15.63514365
D19	129.45592995
D20	-89.83639666
D21	150.23064776
D22	-139.75299936
D23	100.86245759
D24	-3.96482990
D25	-178.57306969
D26	178.55565860
D27	4.39677306
D28	178.73623616

D29	54.15987743
D30	-40.07021588
D31	159.09914878
D32	135.02666736
D33	169.45521042
D34	-129.87139320
D35	-117.12291829
D36	56.84238606
D37	18.35417308
D38	120.50011892
D39	-109.57831176
D40	5.63457789
D41	87.68690475
D42	-175.16163812
D43	-0.07227843
D44	-0.03478789
D45	-87.41655704
D46	-152.50021793
D47	104.23857536
D48	82.81298027
D49	-30.88609062
D50	89.55454536
D51	-150.51354143
D52	139.98663008
D53	-100.61946678
D54	4.91926383
D55	-178.68187822
D56	178.42735710
D57	-4.00025468

Open-shell singlet ground state

Zn							
N	1	B1					
O	1	B2	2	A1			
O	3	B3	1	A2	2	D1	0
O	1	B4	3	A3	4	D2	0
O	5	B5	1	A4	3	D3	0
O	1	B6	5	A5	6	D4	0
O	1	B7	5	A6	6	D5	0
O	1	B8	5	A7	6	D6	0
C	4	B9	3	A8	1	D7	0
C	7	B10	1	A9	5	D8	0
C	7	B11	1	A10	5	D9	0
C	6	B12	5	A11	1	D10	0
C	2	B13	1	A12	5	D11	0
C	14	B14	2	A13	1	D12	0
C	15	B15	14	A14	2	D13	0
C	16	B16	15	A15	14	D14	0
C	2	B17	1	A16	5	D15	0
H	8	B18	1	A17	5	D16	0
H	8	B19	1	A18	5	D17	0
H	9	B20	1	A19	5	D18	0
H	9	B21	1	A20	5	D19	0
H	11	B22	7	A21	1	D20	0
H	11	B23	7	A22	1	D21	0
H	12	B24	7	A23	1	D22	0
H	12	B25	7	A24	1	D23	0
H	14	B26	2	A25	1	D24	0
H	15	B27	14	A26	2	D25	0
H	17	B28	16	A27	15	D26	0
H	18	B29	2	A28	1	D27	0

Zn	16	B30	15	A29	14	D28	0
N	31	B31	16	A30	15	D29	0
O	31	B32	16	A31	15	D30	0
O	33	B33	31	A32	16	D31	0
O	31	B34	16	A33	15	D32	0
O	35	B35	31	A34	16	D33	0
O	31	B36	16	A35	15	D34	0
O	31	B37	16	A36	15	D35	0
O	31	B38	16	A37	15	D36	0
C	34	B39	33	A38	31	D37	0
C	37	B40	31	A39	16	D38	0
C	37	B41	31	A40	16	D39	0
C	36	B42	35	A41	31	D40	0
C	32	B43	31	A42	16	D41	0
C	44	B44	32	A43	31	D42	0
C	45	B45	44	A44	32	D43	0
C	46	B46	45	A45	44	D44	0
C	32	B47	31	A46	16	D45	0
H	38	B48	31	A47	16	D46	0
H	38	B49	31	A48	16	D47	0
H	39	B50	31	A49	16	D48	0
H	39	B51	31	A50	16	D49	0
H	41	B52	37	A51	31	D50	0
H	41	B53	37	A52	31	D51	0
H	42	B54	37	A53	31	D52	0
H	42	B55	37	A54	31	D53	0
H	44	B56	32	A55	31	D54	0
H	45	B57	44	A56	32	D55	0
H	47	B58	46	A57	45	D56	0
H	48	B59	32	A58	31	D57	0

B1	2.07375802
B2	1.96893626
B3	2.25888171
B4	1.95869747
B5	2.25687813
B6	2.17690708
B7	2.27676569
B8	2.31545473
B9	1.21854681
B10	1.43567547
B11	1.43295381
B12	1.21924101
B13	1.34401522
B14	1.38951470
B15	1.40287133
B16	1.40299075
B17	1.34381941
B18	0.97094191
B19	0.98027343
B20	0.97449664
B21	0.96928052
B22	1.09753893
B23	1.09461084
B24	1.09426576
B25	1.09780830
B26	1.08641009
B27	1.08484885
B28	1.08481896
B29	1.08653070

B30	6.35215052
B31	2.07357944
B32	1.96917265
B33	2.25878299
B34	1.95664444
B35	2.25685623
B36	2.17981431
B37	2.27672712
B38	2.31634641
B39	1.21862210
B40	1.43540673
B41	1.43294588
B42	1.21919127
B43	1.34387293
B44	1.38966108
B45	1.40287979
B46	1.40291903
B47	1.34389295
B48	0.97097323
B49	0.98007262
B50	0.97458954
B51	0.96929185
B52	1.09758846
B53	1.09462280
B54	1.09425779
B55	1.09775411
B56	1.08644380
B57	1.08479021
B58	1.08479108
B59	1.08655818

A1	102.41248685
A2	142.50602703
A3	157.13684988
A4	145.51830783
A5	80.16432078
A6	108.59440235
A7	76.49638351
A8	27.74220494
A9	107.20124148
A10	109.96336047
A11	27.83258708
A12	120.01557973
A13	122.20003462
A14	119.53028935
A15	117.54733965
A16	120.84281131
A17	106.77743241
A18	83.00620335
A19	90.41657956
A20	130.51491716
A21	109.78710646
A22	110.56362639
A23	110.41350874
A24	109.92847728
A25	115.61232600
A26	119.44009509
A27	121.01409096
A28	115.75224433
A29	122.06770089
A30	2.82801203

A31	101.44946877
A32	142.66974465
A33	100.87799462
A34	145.50882514
A35	169.59090095
A36	85.96577342
A37	101.31444936
A38	27.74300194
A39	107.16083901
A40	109.76765768
A41	27.84250720
A42	120.41184082
A43	122.22496504
A44	119.51076606
A45	117.53703561
A46	120.43321648
A47	106.74993039
A48	83.20940759
A49	90.30084946
A50	130.60907179
A51	109.78334585
A52	110.57674863
A53	110.42661723
A54	109.89653119
A55	115.67553281
A56	119.46138015
A57	121.01764472
A58	115.72263145
D1	-155.92977125
D2	8.16986415

D3	23.83595354
D4	0.41407139
D5	-79.72563578
D6	91.65080803
D7	-18.60505867
D8	142.45765845
D9	12.32479556
D10	-5.92508702
D11	11.66333688
D12	175.71736259
D13	-0.26771446
D14	0.13425246
D15	-172.91982759
D16	52.50055649
D17	155.70146907
D18	15.63373967
D19	129.45359237
D20	-89.83844802
D21	150.22870775
D22	-139.75399933
D23	100.86120513
D24	-3.96439852
D25	-178.57299674
D26	178.55574614
D27	4.39570820
D28	178.73677432
D29	54.15821845
D30	-40.07258905
D31	159.09811653
D32	135.02395752

D33	169.45949771
D34	-129.87017823
D35	-117.12542813
D36	56.83970579
D37	18.35312256
D38	120.49611718
D39	-109.58176663
D40	5.63191847
D41	87.68833528
D42	-175.16148320
D43	-0.07287437
D44	-0.03407599
D45	-87.41511389
D46	-152.50203409
D47	104.23706673
D48	82.81304599
D49	-30.88493535
D50	89.55383705
D51	-150.51417341
D52	139.98565774
D53	-100.62032994
D54	4.91884215
D55	-178.68240027
D56	178.42678305
D57	-4.00040596

Table S2. Population of spin density for the non-optimized or optimized $[Zn_2(Dg)_2(4,4'\text{-bipy})(H_2O)_4]$ complex under the open-shell singlet ground states.

Non-optimized

1	Zn	0.000000
2	N	-0.000003
3	O	0.000000
4	O	0.000000
5	O	0.000000
6	O	0.000000
7	O	0.000000
8	O	0.000000
9	O	0.000000
10	C	0.000000
11	C	0.000000
12	C	0.000000
13	C	0.000000
14	C	0.000004
15	C	-0.000004
16	C	0.000003
17	C	-0.000004
18	C	0.000004
19	H	0.000000
20	H	0.000000
21	H	0.000000
22	H	0.000000
23	H	0.000000
24	H	0.000000
25	H	0.000000
26	H	0.000000
27	H	0.000000
28	H	0.000000
29	H	0.000000
30	H	0.000000

31	Zn	0.000000
32	N	-0.000003
33	O	0.000000
34	O	0.000000
35	O	0.000000
36	O	0.000000
37	O	0.000000
38	O	0.000000
39	O	0.000000
40	C	0.000000
41	C	0.000000
42	C	0.000000
43	C	0.000000
44	C	0.000004
45	C	-0.000004
46	C	0.000003
47	C	-0.000004
48	C	0.000004
49	H	0.000000
50	H	0.000000
51	H	0.000000
52	H	0.000000
53	H	0.000000
54	H	0.000000
55	H	0.000000
56	H	0.000000
57	H	0.000000
58	H	0.000000
59	H	0.000000
60	H	0.000000

Optimized		
1	Zn	0.000000
2	N	-0.000003
3	O	0.000000
4	O	0.000000
5	O	0.000000
6	O	0.000000
7	O	0.000000
8	O	0.000000
9	O	0.000000
10	C	0.000000
11	C	0.000000
12	C	0.000000
13	C	0.000000
14	C	0.000004
15	C	-0.000004
16	C	0.000003
17	C	-0.000004
18	C	0.000004
19	H	0.000000
20	H	0.000000
21	H	0.000000
22	H	0.000000
23	H	0.000000
24	H	0.000000
25	H	0.000000
26	H	0.000000
27	H	0.000000
28	H	0.000000
29	H	0.000000

30	H	0.000000
31	Zn	0.000000
32	N	-0.000003
33	O	0.000000
34	O	0.000000
35	O	0.000000
36	O	0.000000
37	O	0.000000
38	O	0.000000
39	O	0.000000
40	C	0.000000
41	C	0.000000
42	C	0.000000
43	C	0.000000
44	C	0.000004
45	C	-0.000004
46	C	0.000003
47	C	-0.000004
48	C	0.000004
49	H	0.000000
50	H	0.000000
51	H	0.000000
52	H	0.000000
53	H	0.000000
54	H	0.000000
55	H	0.000000
56	H	0.000000
57	H	0.000000
58	H	0.000000
59	H	0.000000

60 H 0.000000

Table S3. Mülliken charges of **XP-3** in the singlet closed shell and triplet ground states. The atom symbols agree with those shown in **Fig. S14**.

Atoms	Mülliken charges		
	Singlet closed shell	**Triplet**	**Change**
Zn1	0.905388	0.925241	↑
N1	–0.57377	–0.61375	↓
O1 (COO)	–0.606907	–0.57553	↑
O2 (COO)	–0.513928	–0.44599	↑
O3 (COO)	–0.607578	–0.5813	↑
O4 (COO)	–0.514933	–0.46547	↑
O5 (COC)	–0.560454	–0.55653	–
O6 (water)	–0.745128	–0.74708	–
O7 (water)	–0.740757	–0.73731	–
O8 (water)	-0.813881	-0.806385	–
C1	0.559944	0.577882	↑
C2	–0.107732	–0.10727	–
C3	–0.101463	–0.09841	–
C4	0.559638	0.583753	↑
C5	0.139914	0.100807	↓
C6	–0.170302	–0.18165	–
C7	0.135375	0.112743	↓
C8	–0.170208	–0.18106	–
C9	0.131608	0.092727	↓

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