Supplementary Material (ESI) for CrystEngComm

A one-dimensional homochiral Mo(IV)-Cu(II) coordination polymer: spontaneous resolution and photoresponsive properties

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Experimental section

General Procedures. All reagents and solvents in the syntheses were of reagent grade and used without further purification. (***Caution****! $Cu(ClO_4)_2 \cdot 6H_2O$ is potentially explosive and should be handled with much care.*) Elemental analyses of carbon, hydrogen, and nitrogen were carried out at the Center of Elemental Analysis, College of Science, Kyushu University. Infrared spectroscopy studies were performed on a JASCO FT/IR-600 Plus spectrometer in the 4000 – 400 cm^{-1} region. UV-Vis spectra were recorded on a Shimadzu UV-3100PC spectrometer with MPC 3100 unit. Powder X-ray diffraction was measured on a Rigaku D/MAX 2000 PC X-Ray Diffraction instrument. ESR spectra were recorded on a JOEL JES-FA200 spectrometer at X-band frequency with 100 kHz field modulation. Supportive CD spectra could not be obtained because of the tiny crystal size of the compound **1**.

Magnetic measurement. Magnetic susceptibility measurements were carried out on a Quantum Design MPMS-5S SQUID system. Data were collected at 0.50 Tesla in the temperature range between 2 and 300 K. The experimental susceptibilities were corrected for the diamagnetism of the background of the sample holder and the constituent atoms.

X-ray crystallography. X-ray diffraction experiments were carried out on **1** and **2**

using a Rigaku CCD diffractometer with Mo-Kα radiation (λ = 0.71073 Å) at 123 K. Data collection, cell refinement and data reduction: CrystalClear 1.3.5 (Rigaku). The structures were solved by direct methods and refined by the full-matrix method based on F^2 using the SHELXL97 software package (Sheldrick, 1997). All non-hydrogen atoms were refined anisotropically and the positions of all hydrogen atoms were generated geometrically. CCDC-671018 contains the supplementary crystallographic data of **2**, which can be obtained free of charge from *The Cambridge Crystallographic Data Centre* via www.ccdc.cam.ac.uk/data_request/cif.

Illumination experiments. The illumination measurements were carried out by using a transparent tape loaded with a thin layer of the powder sample (less than 1.0 mg) and a UV light source. The light source for the irradiation was a Hayashi LA-310UV instrument with a multi-line spectrum (300 ~ 450 nm). In the photomagnetic experiment, the tape was placed on the edge of an optical fiber. The sample was irradiated continuously at 5 K on a Quantum Design MPMS-5S SQUID system. The diamagnetic contribution and the exact weight were estimated by comparing the magnetic curves before irradiation with those recorded in a routine mode (about 20 mg of sample in gel capsule). The relatively large noise on the experimental data above 200 K came from the use of very small quantities of

the samples.

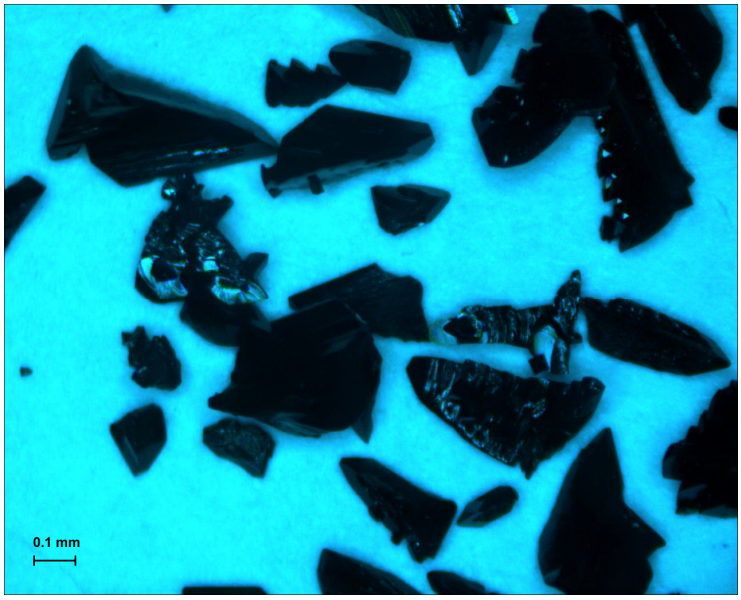

Figure S1. Crystal morphology of **1**.

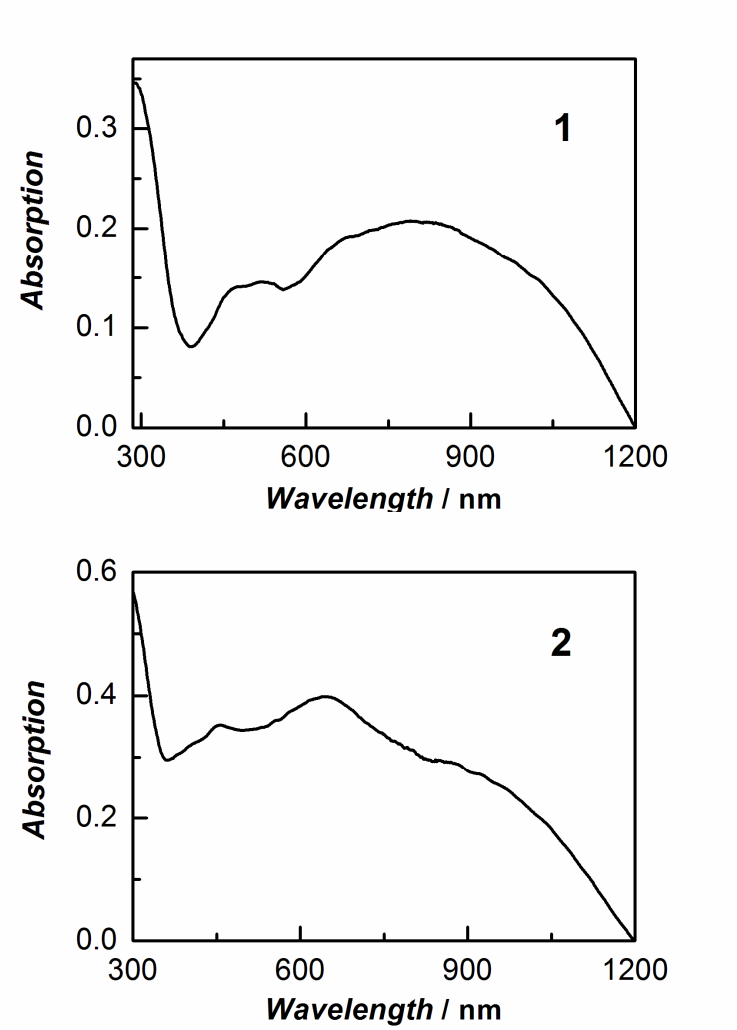

Figure S2. Solid-state UV-Vis spectra of **1** and **2**.

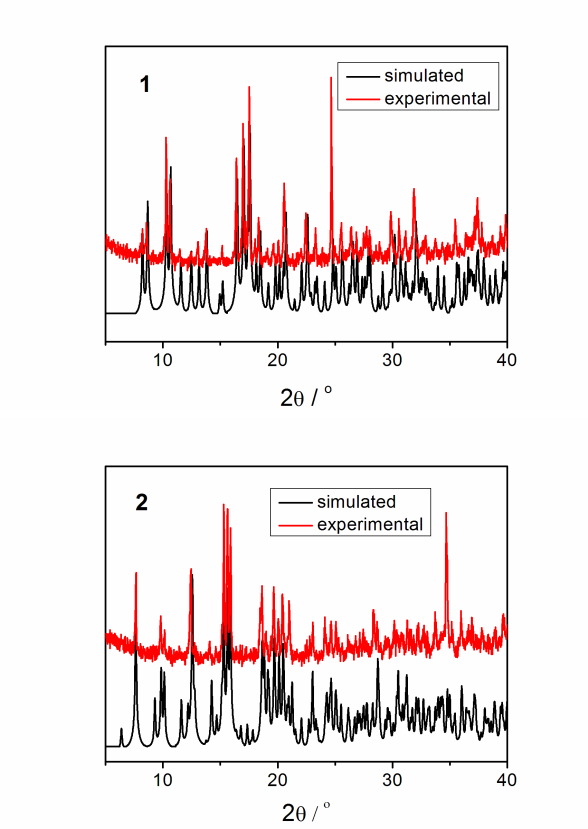

Figure S3. The powder X-ray diffraction patterns of bulky crystals of **1** and **2** with the simulated ones from single crystal X-ray diffraction data.

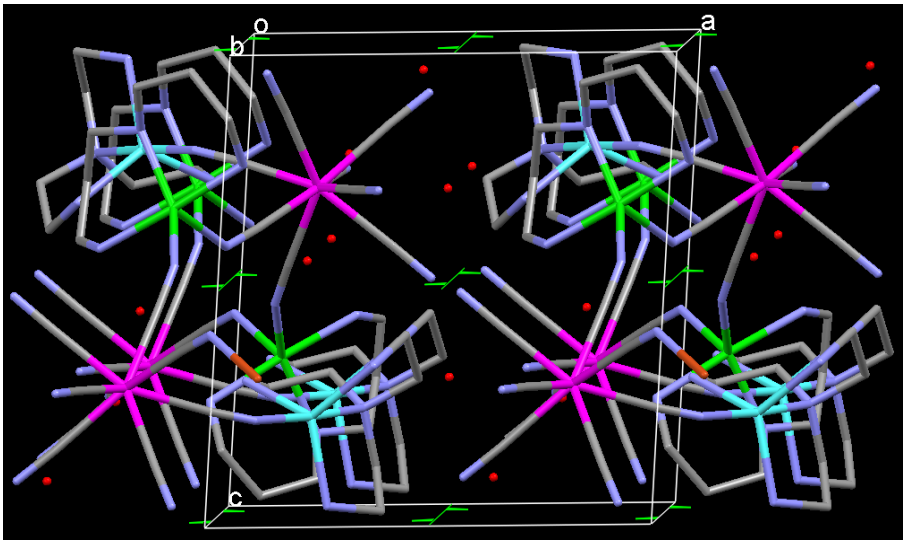

Figure S4. Packing diagram of **1** showing the relationship between the helical chain and the symmetric 2_1 screw axis (thin green lines).

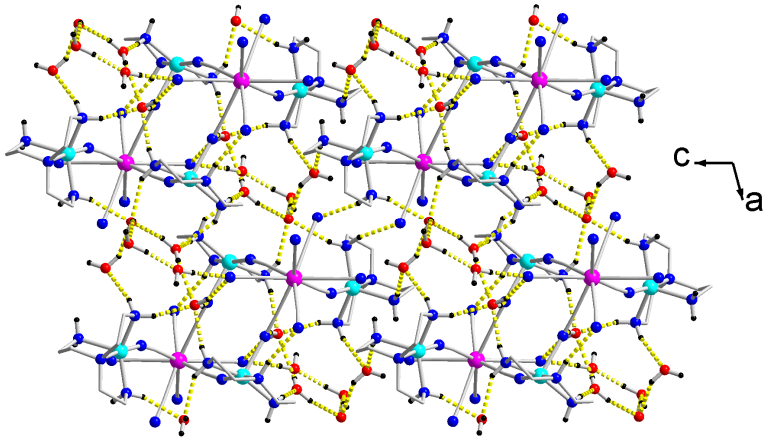

Figure S5. Hydrogen bonds in **2** shown as yellow dashed lines. Sphere colors: purple, Mo; cyan, Cu1; green, Cu2; blue, N; gray, C; O, red; black, H.

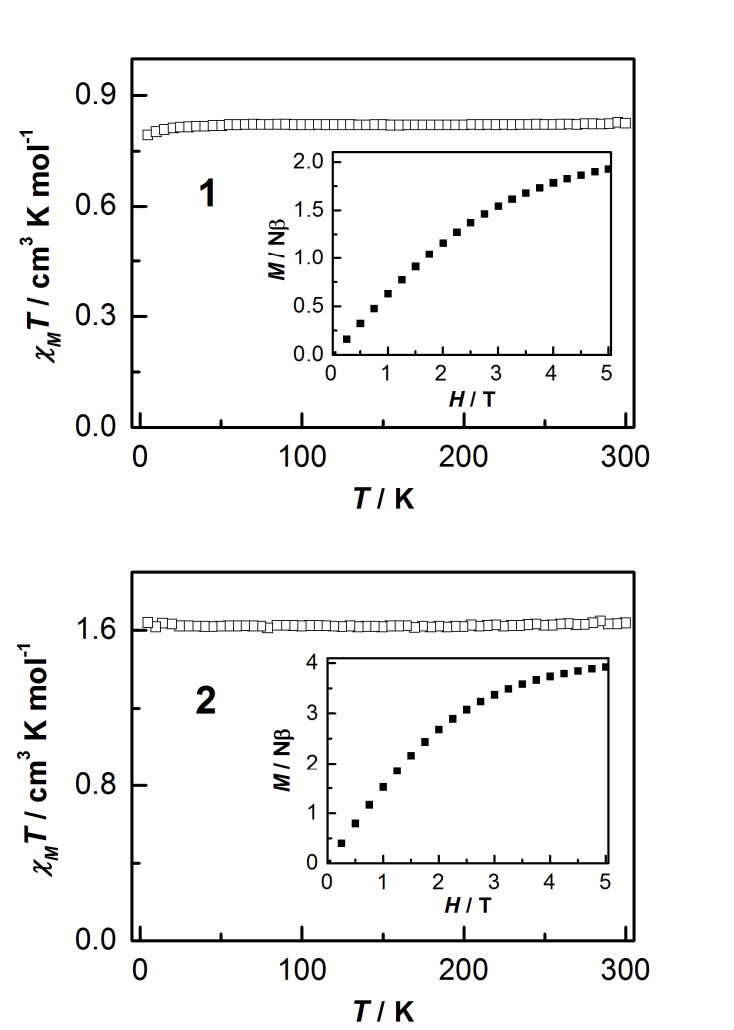

Figure S6. $\chi_M T$ vs T plots of **1** and **2**. Inset: Plot of magnetization vs H at 2 K.

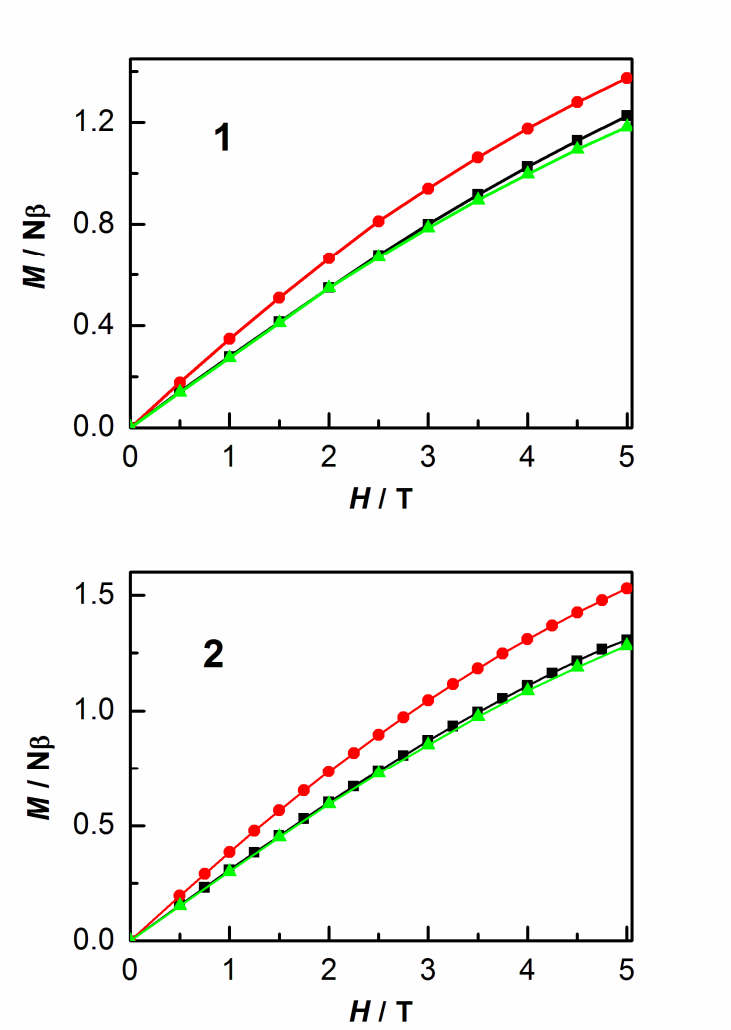

Figure S7. Plots of magnetization vs *H* of **1** and **2** at 5 K upon light irradiation: (■) before irradiation; (●) after irradiation; (▲) after thermal treatment at 300 K. Lines are guides for the eye.

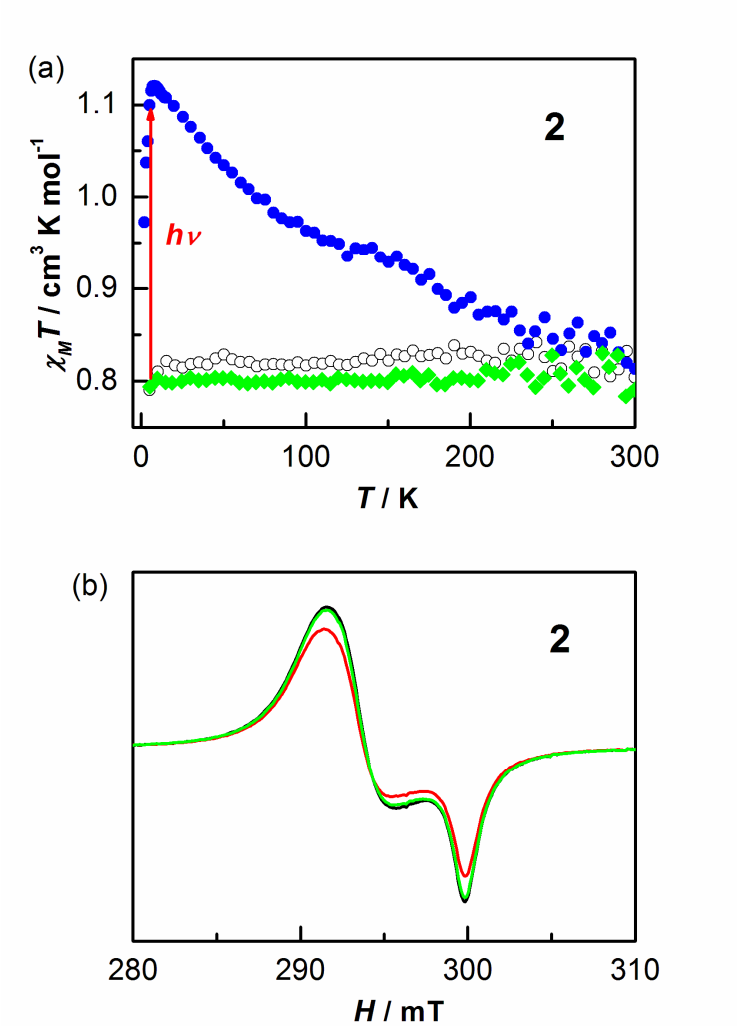

Figure S8. (a) $\chi_M T$ versus T plot of **2**: (○) before irradiation; (●) after irradiation; (♦) after thermal treatment at 300 K. (b) ESR spectra of **2** at 77 K upon light irradiation: (—) before irradiation; (—) after irradiation; (—) after thermal treatment at 300 K.

Table S1. Hydrongen bonds in **1** and **2**.

D−H	A [Symmetry code]	d (D−H) / Å	d (H···A) / Å	<DHA / °	d (D···A) / Å
1					
N1−H1A	O1 [x−1, y, z−1]	0.900	2.140	161.87	3.009
N1−H1B	N14 [−x, y−1/2, −z]	0.900	2.407	150.92	3.224
N2−H2A	O4 [x−1, y, z]	0.900	2.195	157.97	3.048
N3−H3A	N10	0.900	2.437	148.04	3.236
N3−H3B	N11 [−x, y−1/2, −z+1]	0.900	2.343	148.02	3.143
N6−H6A	N10	0.900	2.484	172.41	3.379
N6−H6B	O3 [−x+1, y−1/2, −z+1]	0.900	2.243	170.04	3.133
N7−H7	N14 [−x, y−1/2, −z+1]	0.910	2.560	164.16	3.444
N8−H8A	O4 [x−1, y, z]	0.900	2.229	163.28	3.101
N8−H8B	N14 [−x, y−1/2, −z+1]	0.900	2.619	153.62	3.448
O1−H1E	N13 [x, y, z+1]	0.884	2.007	171.94	2.886
O1−H1F	O3 [−x+1, y−1/2, −z+1]	0.856	1.928	169.99	2.774
O2−H2E	N10	0.933	2.020	165.09	2.931
O2−H2F	O1 [−x+1, y−1/2, −z+1]	0.968	1.942	177.36	2.909
O3−H3E	N12 [−x+1, y+1/2, −z+1]	0.895	1.943	168.35	2.826
O3−H3F	N15	0.878	1.977	159.70	2.818
O4−H4F	O2 [−x+1, y+1/2, −z+1]	0.920	1.889	161.38	2.776
O4−H4E	N9 [x+1, y, z]	0.874	2.360	147.44	3.132
2					
N1−H1B	O1 [−x+1, −y+1, −z+1]	0.900	2.366	145.64	3.150
N2−H2A	O2 [−x+1, −y+1, −z]	0.900	2.225	163.19	3.097
N2−H2B	N14 [−x+1, −y+1, −z]	0.900	2.655	140.82	3.401
N3−H3A	O5 [−x, −y+1, −z+1]	0.900	2.313	140.37	3.060
N3−H3B	N15 [−x, −y+1, −z]	0.900	2.265	164.50	3.141
N6−H6A	O6 [−x+2, −y+1, −z+1]	0.900	2.334	145.96	3.121
N6−H6B	O6	0.900	2.029	170.78	2.921
N7−H7	N10	0.910	2.419	163.09	3.301
N8−H8A	O1	0.900	2.128	164.45	3.004
N8−H8B	O5 [x+1, y, z]	0.900	2.220	147.10	3.016
O1−H1E	N11	0.793	2.176	153.06	2.905
O1−H1F	N12 [−x+1, −y+1, −z+1]	0.826	2.242	158.56	3.027
O2−H2E	N14 [−x+1, −y+1, −z]	0.85	2.61	96.8	2.839
O2−H2E	N15 [x+1, y, z]	0.85	2.54	100.3	2.815
O2−H2F	O5 [−x+1, −y+1, −z+1]	0.850	2.317	136.59	2.992
O3−H3E	O4	0.946	1.755	173.79	2.698
O3−H3F	N13 [x+1, y−1, z]	0.888	1.951	167.45	2.824
O4−H4F	N10 [x, y−1, z]	0.893	1.910	174.41	2.800
O4−H4E	N11 [−x+1, −y+1, −z+1]	0.861	1.982	169.04	2.833
O5−H5C	O3 [−x+1, −y+1, −z+1]	0.911	1.943	138.26	2.692
O5-H5F	O3 [−x+1, −y+1, −z+1]	0.850	1.973	141.69	2.692
O6−H6F	O1 [−x+1, −y+1, −z+1]	0.850	2.307	120.33	2.833
O6−H6E	O5 [−x+1, −y+1, −z+1]	0.850	2.016	156.44	2.816