

**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  $4000 - 400\text{ cm}^{-1}$  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**.

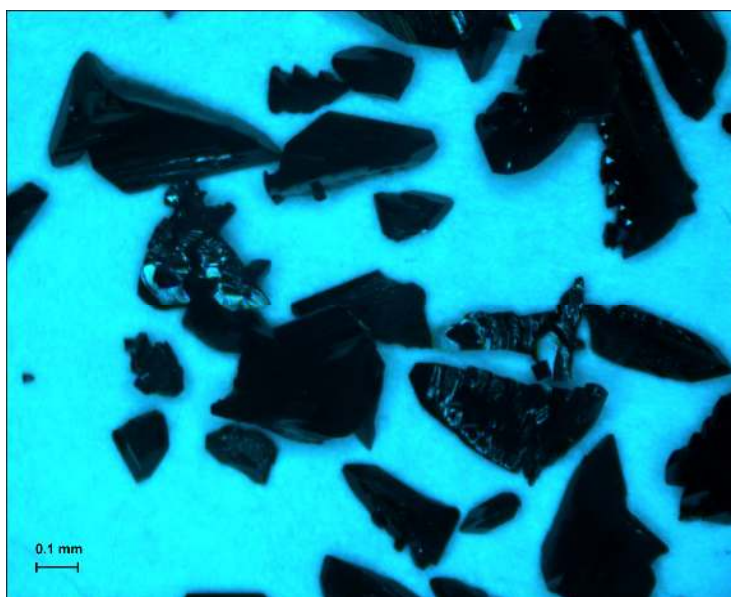
**Magnetic measurement.** Magnetic susceptibility measurements were carried out on a Quantum Design MPMS-5S SQUID system. Data were collected at 0.50 Tesla in the temperature range between 2 and 300 K. The experimental susceptibilities were corrected for the diamagnetism of the background of the sample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

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

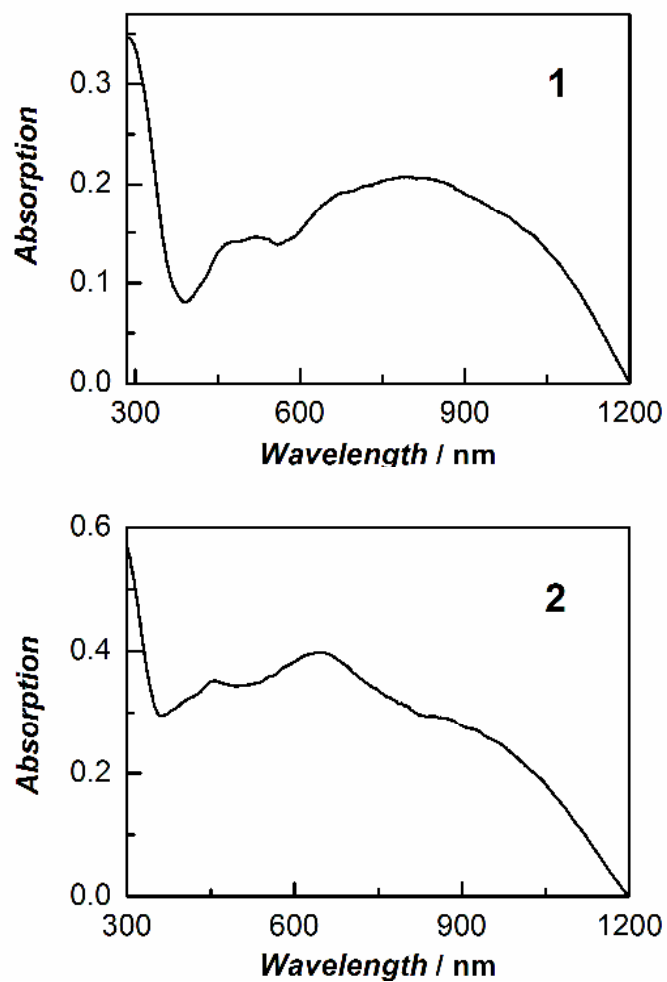
using a Rigaku CCD diffractometer with Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 123 K. Data collection, cell refinement and data reduction: CrystalClear 1.3.5 (Rigaku). The structures were solved by direct methods and refined by the full-matrix method based on  $F^2$  using the 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](http://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

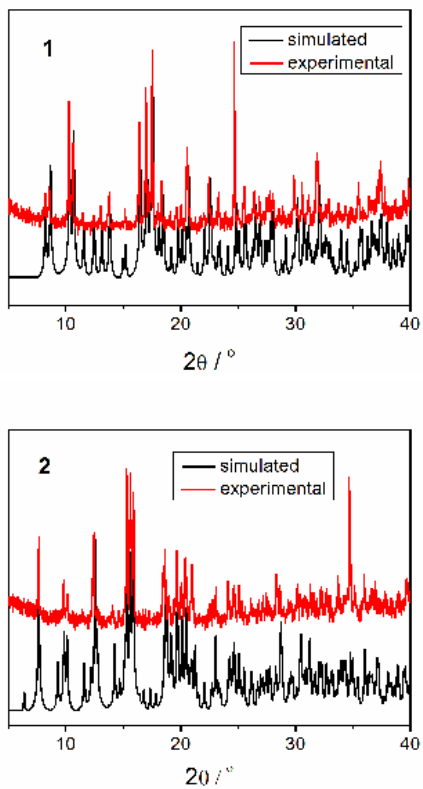
the samples.



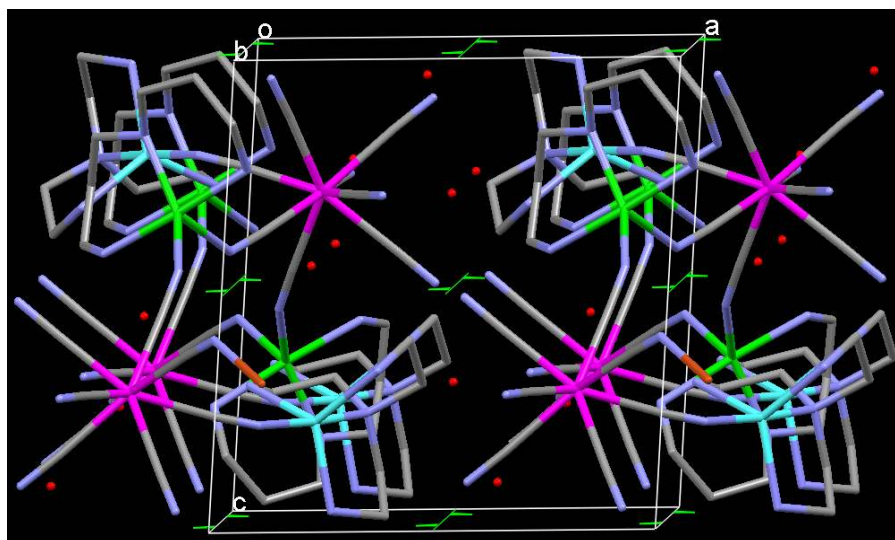
*Figure S1.* Crystal morphology of **1**.



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

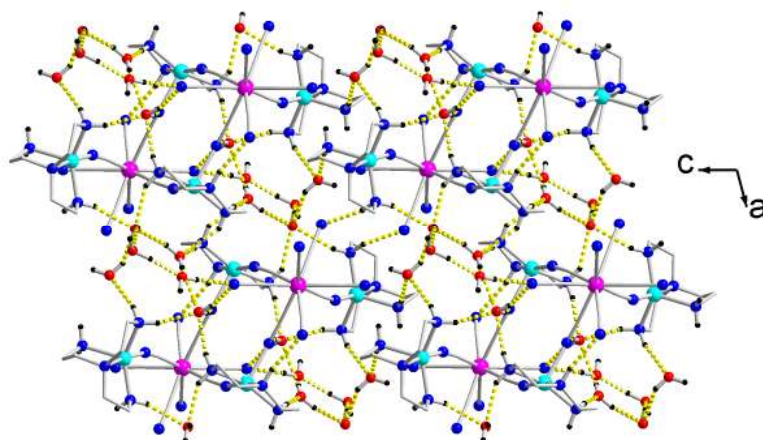


**Figure S3.** The powder X-ray diffraction patterns of bulky crystals of **1** and **2** with the simulated ones from single crystal X-ray diffraction data.

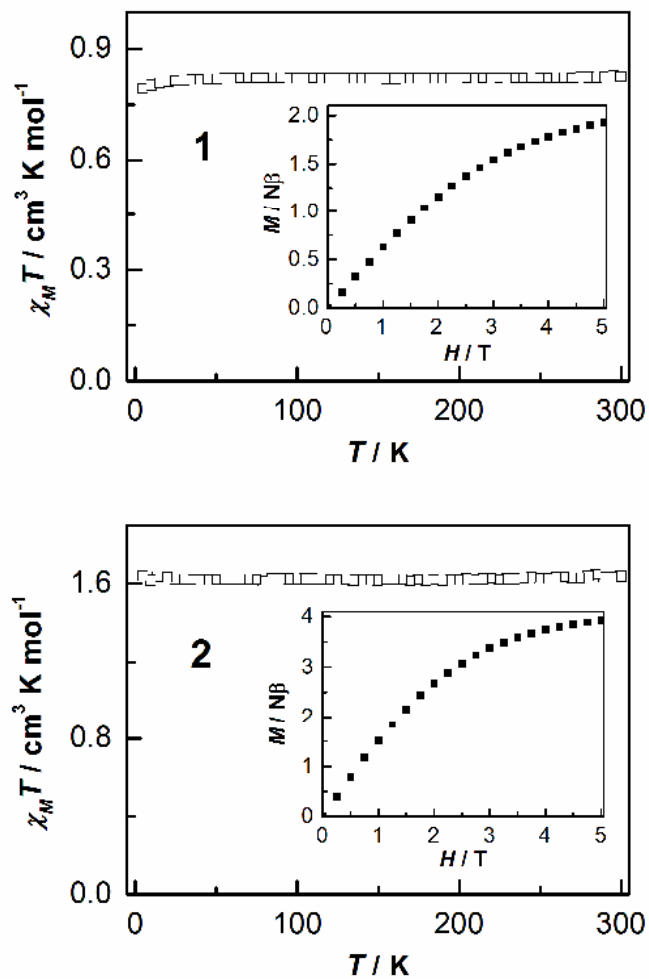


**Figure S4.** Packing diagram of **1** showing the relationship between the helical chain and the symmetric  $2_1$  screw axis (thin green lines).

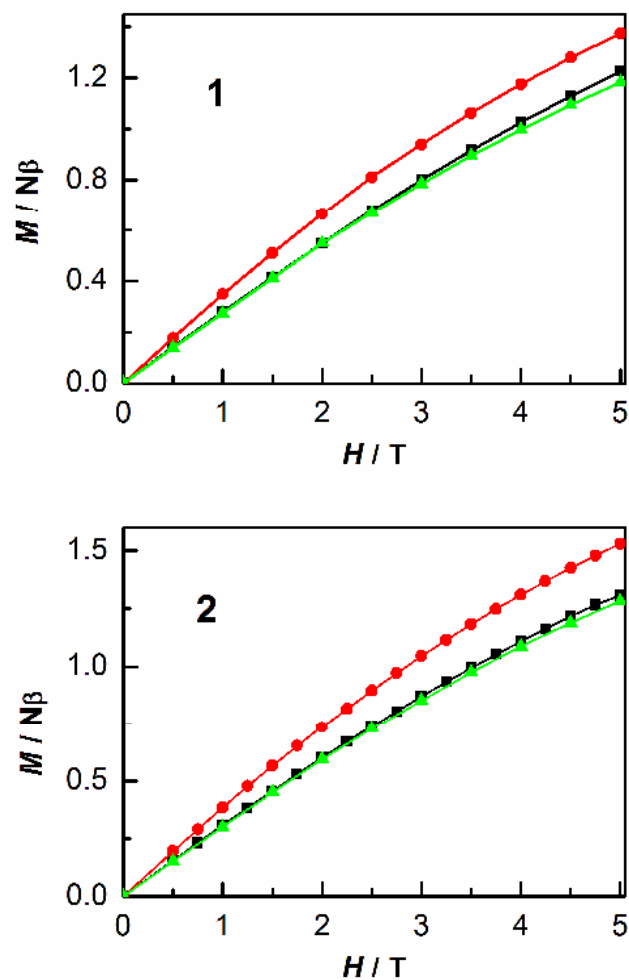




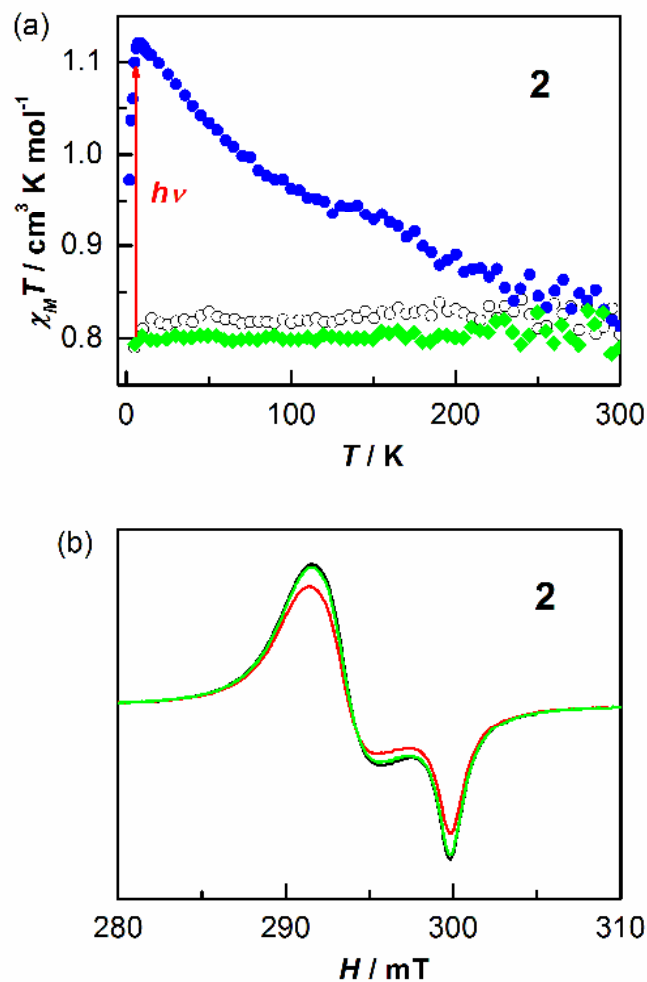
**Figure S5.** Hydrogen bonds in **2** shown as yellow dashed lines. Sphere colors: purple, Mo; cyan, Cu1; green, Cu2; blue, N; gray, C; O, red; black, H.



**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.** Hydrogen bonds in **1** and **2**.

D-H	A [Symmetry code]	d (D-H) / Å	d (H...A) / Å	<DHA / °	d (D...A) / Å
<b>1</b>					
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
<b>2</b>					
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