Reversible photoswitchable ferromagnetic thin film based on a cyanido-bridged RbCuMo complex

Shin-ichi Ohkoshi*[,a], Koki Shiraishi[a], Kosuke Nakagawa[a], Yusuke Ikeda[a], Olaf Stefanczyk[a], Hiroko Tokoro[a,b], and Asuka Namai[a]

[a]*Department of Chemistry, School of Science, The University of Tokyo*
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
[b]*Department of Materials Science, Faculty of Pure and Applied Sciences, University of Tsukuba*
1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan

*To whom correspondence should be addressed
E-mail: ohkoshi@chem.s.u-tokyo.ac.jp

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§ 1. Structural details of RbCuMo

Table S1-1. Structural parameters of **RbCuMo** obtained from the Rietveld analysis.

Formula	$C_{31}H_{24}O_{12}N_{31}Rb_{1.5}Cu_7Mo_{3.875}$
Formula weight	1967.5
Crystal System	Tetragonal
Space group	*I*4/*mmm*
a / Å	7.2066(1)
c / Å	28.4148(4)
V / Å^3	1475.71(4)
d_{cal} / g cm^{-3}	2.1873
Z	4
Temperature / K	293
R_{wp} / R_p	3.095 / 2.365

Table S1-2. Atomic position of **RbCuMo** obtained from the Rietveld analysis.

Atom	*x*	*y*	*z*	Occ.
Rb	0	0.5	0.25	0.375
Mo	0	0	0.36814	0.96875
Cu1	0	0	0.17406	1
Cu2	0.42909	0	0	0.375
C1	0.28861	−0.28861	0.15584	0.96875
C2	0.05053	0.23662	0.42851	0.364
C3	0	0	0.2854	0.96875
N1	0.19173	−0.19173	0.17003	0.96875
N2	0.17578	0.42917	0.05326	0.364
N3	0	0	0.25387	0.96875
O1	0	0	0.06797	1
O2	0.07689	0.07689	0	0.25
O3	0.19173	−0.19173	0.17003	0.03
O4	0.17578	0.42917	0.05326	0.011
O5	0	0	0.25387	0.03
O6	0	0.5	0.19574	0.57
O7	0.325	0.325	0.215	0.03

Table S1-3. List of bond lengths (Mo–C and Cu–N) and bond angles (∠C–Mo–C, ∠N–Cu–N, ∠Mo–C–N, ∠Cu–N–C) of **RbCuMo** at 293 K.

	RbCuMo@293 K
Mo1–C1	2.2596(1)
Mo1–C2	2.446(1)
Mo1–C3	2.351(1)
Cu1-N1/O3	1.9575(1)
Cu1-N3/O5	2.2676(1)
Cu2-N2/O4	1.9736(1)
C1–Mo1–C1	84.7805(2)
C1–Mo1–C1	144.8908(7)
C1–Mo1–C2	68.9717(8)
C1–Mo1–C2	80.9045(6)
C1–Mo1–C2	125.5307(1)
C1–Mo1–C2	141.4337(1)
C1–Mo1–C3	72.4454(3)
C2–Mo1–C2	60.5376(7)
C2–Mo1–C2	73.4847(9)
C2–Mo1–C2	88.393(1)
C2–Mo1–C2	90.934(1)
C2–Mo1–C3	134.5332(6)
Mo1–C1–N1	175.3534(1)
Mo1–C2–N2	174.0506
Mo1–C3–N3	180
Cu1–N1–C1	161.1584(3)
Cu1–N3–C3	180
Cu2–N2–C2	165.2954(1)
N1–Cu1–N1	89.8032
N1–Cu1–N1	173.2809(1)
N1–Cu1–N3	93.3596(1)
N2–Cu2–N2	79.860(1)
N2–Cu2–N2	100.140(1)
N2–Cu2–N2	179.9674

§ 2. Change in the XRD patterns upon light irradiation

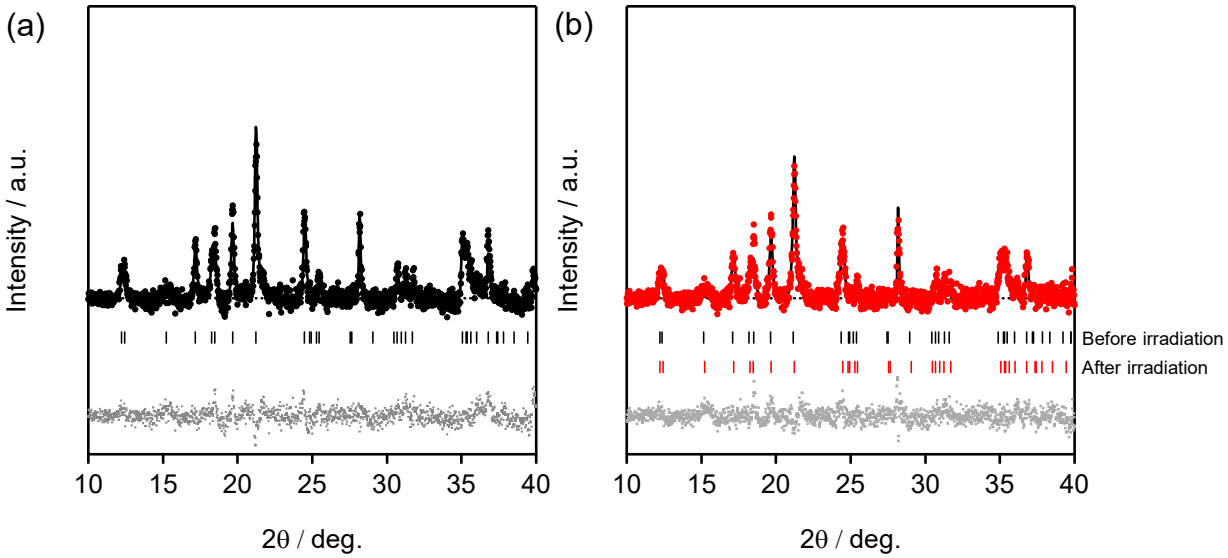

Figure S1. (a) XRD pattern with Rietveld analysis of **RbCuMo** before light irradiation. Red dots, black lines, and blue lines are the observed patterns, calculated patterns, and their differences, respectively. Green bars represent the calculated positions of the Bragg reflections. (b) XRD pattern with Rietveld analysis of **RbCuMo** after 473-nm-light irradiation. Red dots, black lines, and blue lines are the observed patterns, calculated patterns, and their differences, respectively. Black and red bars represent the calculated positions of the Bragg reflections of the initial and photoinduced states, respectively.

§ 3. Comparison of the structural parameter before and after light irradiation

Table S2-1. Structural parameters of the initial phase obtained from the Rietveld analysis of the XRD pattern before light irradiation.

Formula	$C_{31}H_{24}O_{12}N_{31}Rb_{1.5}Cu_7Mo_{3.875}$
Formula weight	1967.5
Crystal System	Tetragonal
Space group	*I*4/*mmm*
a / Å	7.1837(7)
c / Å	28.354(5)
V / Å^3	1463.2(3)
d_{cal} / g cm^{-3}	2.21
Z	4
Temperature / K	12
R_{wp} / R_p	0.47 / 0.36

Table S2-2. Structural parameters of the photoinduced phase obtained from the Rietveld analysis of the XRD pattern after 473-nm-light irradiation.

Formula	$C_{31}H_{24}O_{12}N_{31}Rb_{1.5}Cu_7Mo_{3.875}$
Formula weight	1967.5
Crystal System	Tetragonal
Space group	*I*4/*mmm*
a / Å	7.217(2)
c / Å	28.332(15)
V / Å^3	1475.7(11)
d_{cal} / g cm^{-3}	2.19
Z	4
Temperature / K	14
R_{wp} / R_p	0.44 / 0.36

Table S2-3. Change in the bond length of Cu1–N_{eq} and Cu1–N_{ax} upon light irradiation.

	Cu1–N_{eq} / Å	Cu1–N_{ax} / Å
Before the light irradiation	1.95119(19)	2.2629(4)
After the 473-nm light irradiation	1.9602(6)	2.2612(12)

§ 4. Preparation and characterization of powder-form sample

The powder form of cyanido-bridged rubidium-copper-molybdenum bimetallic assembly was synthesized by dissolving $Rb_3[Mo^V(CN)_8]\cdot 2H_2O$ (98.9 mg, 0.166 mmol), RbCl (112.3 mg, 0.929 mol), and $CuCl_2\cdot 2H_2O$ (61.3 mg, 0.359 mol) in a 100 dm^3 HCl acidic solution (pH~3). Then the solution was placed in an incubator at 35 ℃ for 10 days. The formula is almost the same as that of the film (*i.e.*, $Rb_{1.72}Cu_7[Mo^{IV}(CN)_8]_{3.93}\cdot 11H_2O$). Calculated: Rb, 7.4; Cu, 22.4; Mo, 19.0; C, 19.0; H, 1.1; N, 22.2%. Found: Rb, 7.5; Cu, 22.4; Mo, 18.9; C, 19.3; H, 1.2; N, 22.4%.