

Supporting Materials for
**Two One-dimensional Copper-Oxalate-Framework with Jahn-Teller
Effect: $[(\text{CH}_3)_3\text{NH}]_2[[\text{Cu}(\mu-\text{C}_2\text{O}_4)(\text{C}_2\text{O}_4)] \cdot 2.5\text{H}_2\text{O}$ (I) and
 $[(\text{C}_2\text{H}_5)_3\text{NH}]_2[\text{Cu}(\mu-\text{C}_2\text{O}_4)(\text{C}_2\text{O}_4)] \cdot \text{H}_2\text{O}$ (II)**

Bin Zhang,^{*,a} Yan Zhang,^b Zheming Wang,^{*,c} Yang Sun,^d Tongling Liang,^d Mei Liu,^d and Daoben
Zhu^{*,a}

^a Organic Solid State Laboratory, Beijing National Laboratory of Molecular Sciences Institute of
Chemistry, Chinese Academy of Sciences, Beijing, 100190, P. R. China.

^b Institute of Condensed Matter and Material Physics, Department of Physics, Peking University,
Beijing, 100871, P. R. China.

^c State Key Laboratory of Rare Earth Materials and Chemistry and Applications, Beijing National
Laboratory of Molecular Sciences, Peking University, Beijing, 100871, P. R. China. Email: ^d CAS
Research/Education Center for Excellence in Molecular Science, CMS *BNLMS, Institute of
Chemistry, Chinese Academy of Science, Beijing, 100190, P. R. China.

* To whom correspondence should be addressed. E-mail: zhangbin@iccas.ac.cn,
zmw@pku.edu.cn, zhudb@iccas.ac.cn

Contents

Table S1. Crystallographic data of I and II	S3
Figure S1. IR spectra on crystalline I (top) and II (bottom).	S4
Figure S2. Experimental X-ray powder diffraction pattern of crystalline sample and simulated one based on single crystal structure of I . I shows preferred orientation.	S5
Figure S3. Experimental X-ray powder diffraction pattern of crystalline sample and simulated one based on single crystal structure of II .	S6
Figure S4. ZFCM/FCM of polycrystal of I under 100 G.	S7
Figure S5. ZFCM/FCM of polycrystal of II under 100 G.	S8

Table S1. Crystallographic data of **I** and **II**

Compound	I	II
formula	C10H25CuN2O10.5	C16H34CuN2O9
Fw	404.86	461.99
F(000)	424	980
T, K	293	293
crystal system	Triclinic	Monoclinic
space group	P $\bar{1}$	P 2 ₁ /c
a, Å	9.1043(3)	16.9291(3)
b, Å	9.4286(3)	9.6931(1)
c, Å	11.6225(4)	19.2582(3)
α , °	94.154(1)	90
β , °	112.273(1)	136.812(1)
γ , °	95.734(1)	90
V, Å ³	912.01(5)	2162.812(1)
Z	2	4
D_c , g/cm ³	1.474	1.419
μ (Mo K_{α}), mm ⁻¹	1.248	1.057
crystal size, mm ³	0.36 × 0.25 × 0.15	0.40 × 0.33 × 0.18
T_{\min} and T_{\max}	0.662, 0.835	0.744, 0.831
$\theta_{\min}, \theta_{\max.}$, °	3.496, 27.487	3.517, 27.498
no. total reflns.	14735	33283
no. uniq. reflns (R_{int})	4144(0.0361)	4944(0.0440)
no. obs. [$I \geq 2\sigma(I_0)$]	2963	3359
no. params	229	260
$R1, wR2$ [$I \geq 2\sigma(I_0)$]	0.0366, 0.0852	0.0394, 0.1036
$R1, wR2$ (all data)	0.0595, 0.0913	0.0652, 0.1139
GOF	0.980	1.032
^a $\Delta\rho$, e/Å ³	0.457, -0.350	0.773, -0.759
^b Max. and mean Δ/σ	0.001, 0.000	0.001, 0.000
CCDC	881974	843074

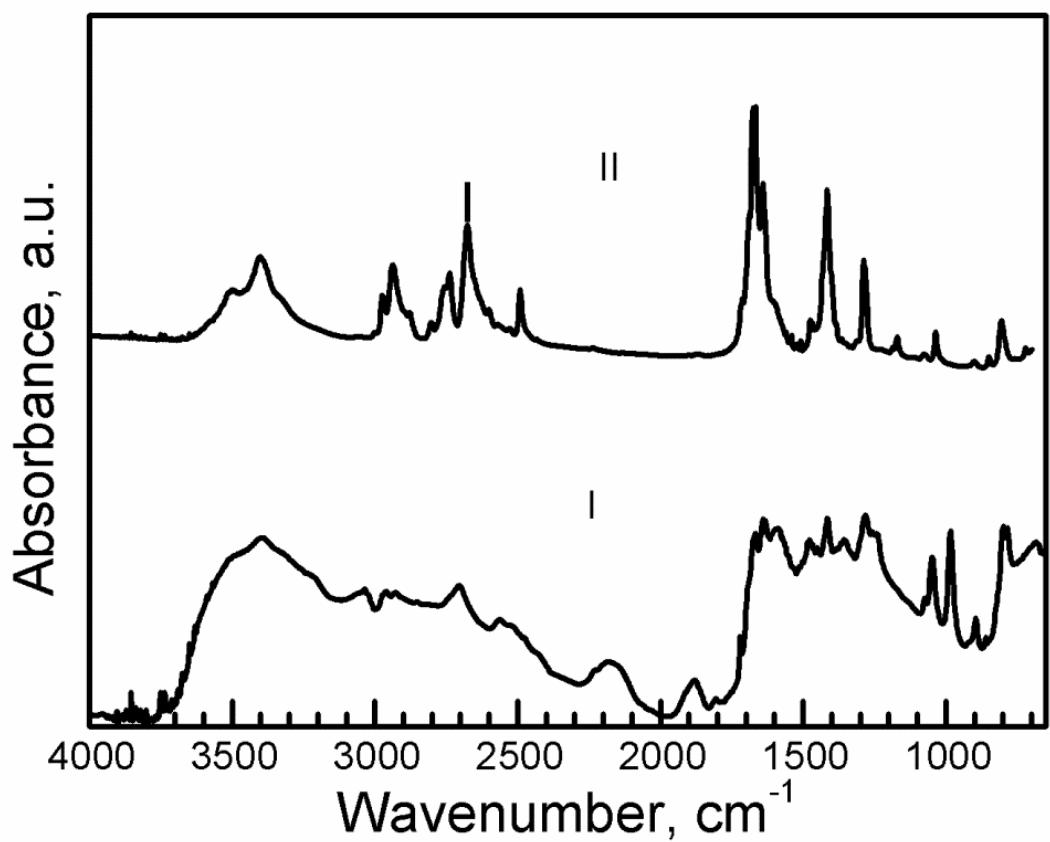


Figure S1. IR spectra of **I** and **II**.

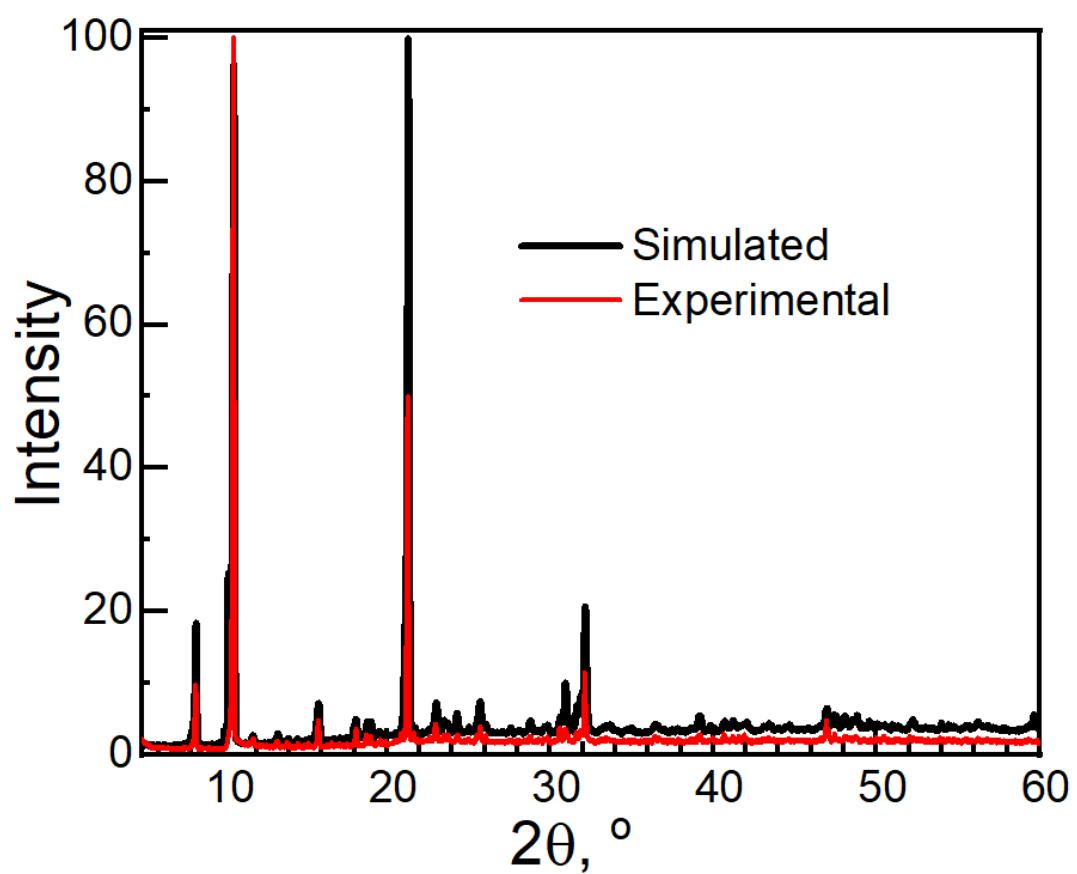


Figure S2. Experimental X-ray powder diffraction pattern of crystalline sample and simulated one based on single crystal structure of **I**. **I** shows preferred orientation.

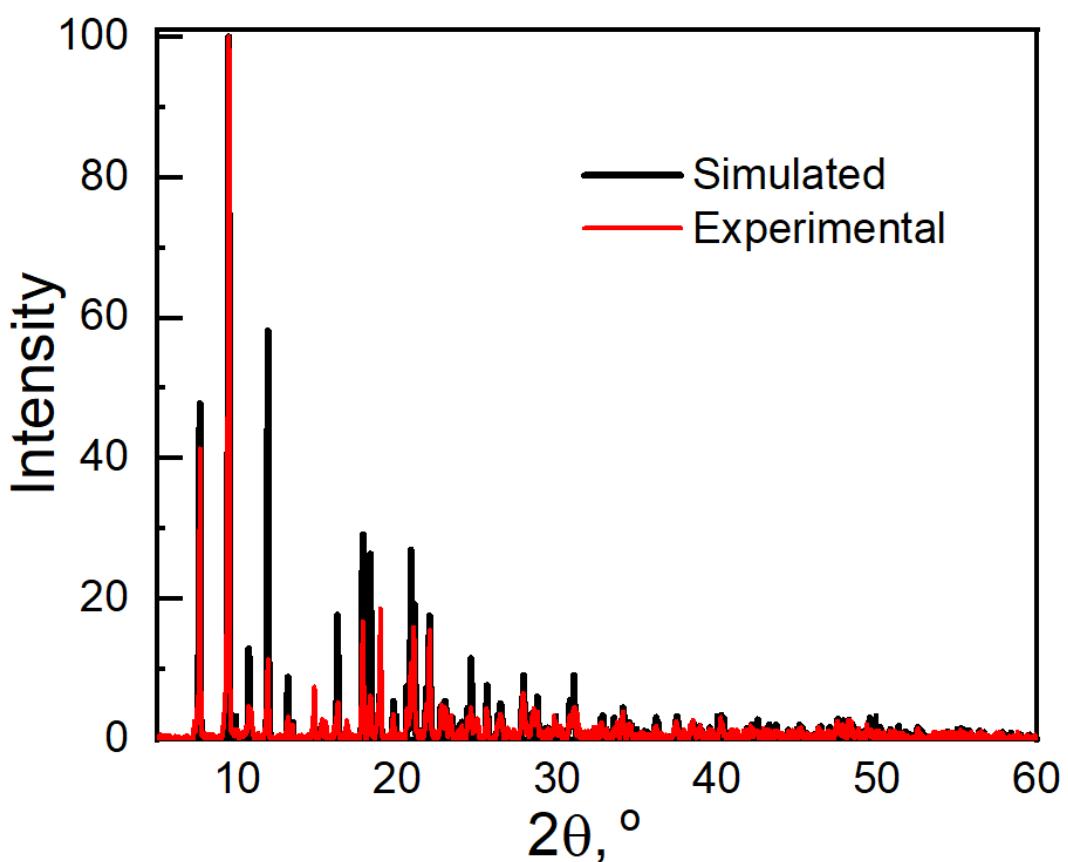


Figure S3. Experimental X-ray powder diffraction pattern of crystalline sample and simulated one based on single crystal structure of **II**.

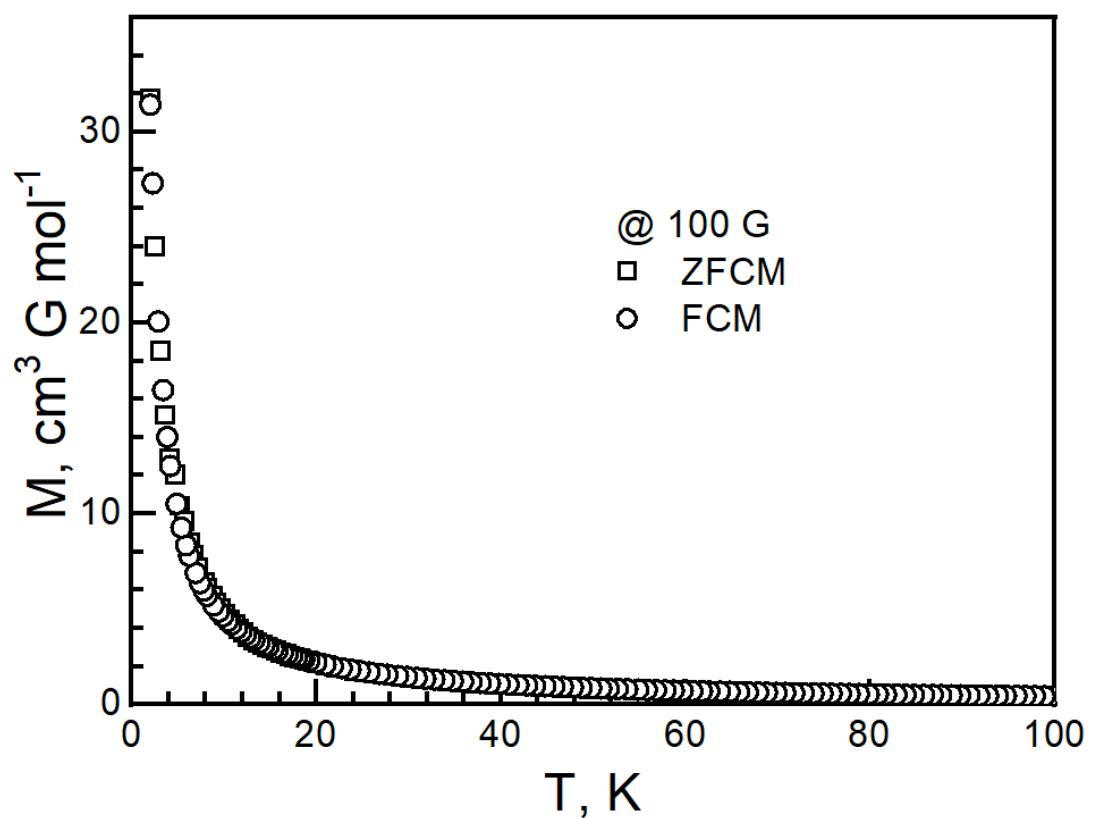


Figure S4. ZFCM/FCM of polycrystal of **I** under 100 G.

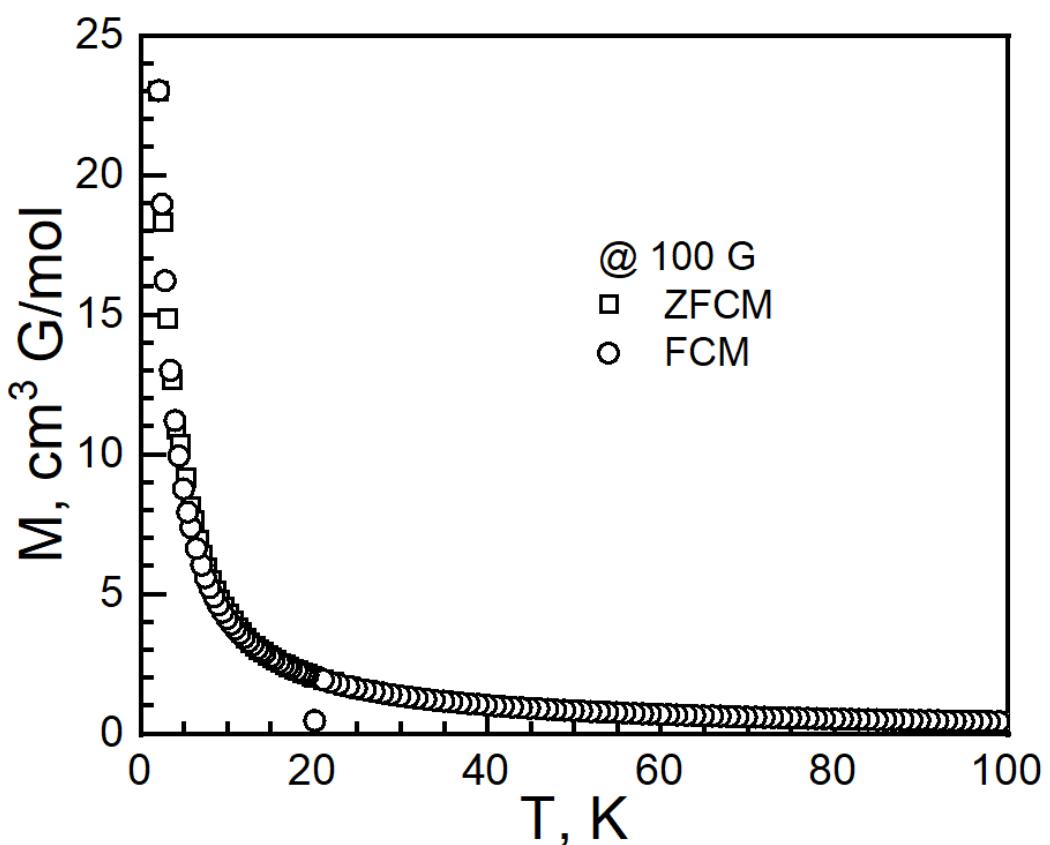


Figure S5. ZFCM/FCM of polycrystal of **II** under 100 G.