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Electronic Supplementary Information (ESI) for

Homochiral 3D Coordination Polymer with Unprecedented Three-Directional Helical Topology from Achiral Precursor: Synthesis, Crystal Structure, and Luminescence Properties of Uranyl Succinate Metal-Organic Framework

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I. Experimental section

Materials and methods

All materials were of analytical grade and were used without further purification. Deionized water was used throughout. Elemental analysis (Cand H) was performed on a Vario Micro Cube element analyzer. The infrared spectrum was recorded as a KBr pellet on a Spectrum One fourier transform infra-red spectrometer in the range 4000–450 cm^{-1}.The electronic absorption spectra were taken on a Shimadzu UV-240 spectrophotometer. X-ray powder diffractometry study of the complex was performed on a Bruker SMART APEX CCD sealed tube diffractometer with Cu K_α radiation. The XPS spectrum wascarried out on XSAM800 spectrometer. Fluorescence data were collected on anEdinburgh FL-FS920 TCSPC system. The solid-sate circular dichroism(CD) spectra were recorded with KCl pellets on a JASCO J-810 spectropolarimeter.

Synthesis of Complex I

UO_2 (142.5 mg, 0.53 mmol) was dissolved in concentrated nitric acid (20 mL) and the pH was adjusted to ~3 with concentrated ammonia water.Then succinic acid(59.0 mg, 0.50 mmol) was added to the resultant yellow solution. The whole was stirred with a magnetic bar until the acid was dissolved, followed by addition of ammonia aqueous solution until the pH reached 2~2.5. Next, the mixture was transferred to a Teflon-lined stainless steel autoclave(25mL), and the temperature was heated to 170℃and maintained at this temperature for four days. The autoclave was allowed to cool down to room temperature, and the mixture was filtered to remove excess black powders. Slow evaporation of the resulting yellow clear solutionfor four weeks gave yellow crystals of complex **I** in 20.0% yield. Elemental analysis: calculated for $C_{24}H_{28}O_{32}U_4 \cdot 2H_2O$ (%): C 15.87, H 1.78; found: C 15.73, H 1.50.

II. Physical measurements

X-ray Crystallography

A single-crystal with dimensions 0.22 × 0.24 × 0.28 mm^3 for compound **I** was selected for X-ray crystallographic analyses, which was performed at 291(2) K on a Bruker SMART APEX CCD sealed tube diffractometer with graphite monochromated Mo–Kα(0.71073 Å) radiation. Data collection, indexing, andinitial cell refinements were carried out using SMART software. Frame integration and final cell refinements were carried out usingSAINT software.[1] Absorption corrections for each data set were applied using SADABSprogram.[2] The structure was solved by direct methods with SHELXS-2000 program and refined using full-matrix least-squares techniques on F^2 with SHELXL-2000.[3] All non-hydrogen atoms were refined anisotropically. Crystal data and details of data collection as well as the structure refinement are given Table **1**, and selected of the bond lengths and bond angles are listed in Table **2.**

Table 1. Crystal data and structure refinement for complex **1**

Empirical formula	$C_{24}H_{28}O_{32}U_4 \cdot 2H_2O$	
Formula weight	1816.62	
Temperature	291 K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	*P32 (No.145)*	
Unit cell dimensions	a = 19.0913(3) Å ,	α=90.00°
	b= 19.0913(3) Å,	β= 90.00°
	c= 11.7929(5) Å,	γ= 120.00°
Volume	3722.4(2)$Å^3$	
Z	3	
Density (calculated)	2.431 g · cm^{-3}	
Absorption coefficient	13.105 mm^{-1}	
F(000)	2448	
Crystal Size	0.22 × 0.24 × 0.28 mm^3	
Theta range for data collection	2.1 to 26.0°	
Index ranges	$-23 \le h \le 23$; $-23 \le k \le 15$; $-14 \le l \le 14$	

Reflections collected	20888
Unique reflections	9586 (R_{int} = 0.036)
Obs. Reflections [$I>2\sigma(I)$]	8242
Goodness-of-fit on F^2	1.056
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0440 , wR_2 = 0.1154
Flack x	0.086(11)
Largest diffraction peak and hole	-1.741 and 1.46 e · Å^{-3}

a $R_1=\sum||F_o|-|F_c|| /\sum|F_o|$; b $wR_2=\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]^{1/2}$

c $w^{-1}=[\sigma^2(F_o)^2+(0.07P)^2+1.99P]$, $P=(F_o^2+2F_c^2)/3$

Table 2. Selected bond lengths (nm) and angles (°) for complex **1**

U1 -O6	2.367(8)	U3 -O15	2.543(9)
U1 -O24	2.480(10)	U3 -O18	2.326(9)
U1 -O25	1.771(10)	U3 -O29	1.773(10)
U1 -O26	1.773(11)	U3 -O30	1.789(10)
U2 -O9	2.495(9)	U4 -O19	2.399(11)
U2 -O10	2.340(11)	U4 -O4	2.578(11)
U2 -O27	1.821(8)	U4 -O31	1.686(11)
U2 -O28	1.780(8)	U4 -O32	1.824(10)
O1-U1-O2	49.54(3)	O25-U1 -O26	178.3(4)
O1-U1 -O5	74.4(3)	O8 -U2 -O10	177.5(4)
O1-U1 -O26	81.5(4)	O31 -U4 -O32	172.2(5)
O29 -U3 -O30	176.2(4)	U1 -O6-H6C	111.57

III. Characterization

CD spectrum

Three times CD measurements were performed using three different single crystals. The results of the three experiments are consistent. The splitting peak is observed in the spectra at 307 nm, again corroborating the homochirality of the single crystal. The first Cotton effect is positive, and the second is negative, proving that coordination polymer I is R- chiral.

Powder x-ray diffraction

The powder diffraction of complex 1 was done twice using ground up powder composed of many crystals from the bulk product. Every time XRD powder diffraction pattern is basically the same as that of the single crystal structure data. It can be explained that the solid powder is consistent with the single crystal in the microstructure.

IR spectrum

The IR spectrum of complex **I** exhibits a strong absorption at 3606cm^{-1} and 3455cm^{-1}due to the stretching vibration of the O-H moiety, indicating that the coordination polymer contains water molecules. The peaks at 955, 926, 868 and808 cm^{-1} can be assigned to the stretching vibration of the UO_2^{2+}, while the two sets of absorption bands at 1697 and 1416cm^{-1}, and 1298and 1284 cm^{-1} belong to the asymmetric and symmetric vibration of the dicarboxylate groups. Therefore, IR spectrum is also in line with the structure of **I**.

XPS spectrum

The binding energies(E_b) for UO_3 in the $U_{4f7/2}$ peak are between 382.1 and 382.5 eV with an average value of 382.3 eV. The E_b for UO_2 in the $U_{4f7/2}$ peak are between 381.1 and 381.5 eV with an average value of 381.3 eV.[4] The $U_{4f7/2}$binding energy value in **I** was found to be 382.8 eV, which could be assigned to U(□), demonstrating that the U of complex is in the oxidation state of +□.

Supplementary material

Crystallographic data for the structure reported in this paper have been deposited with Cambridge Crystallographic Data Center as supplementary publication No.899501. Copiesof the data can be obtained free from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ (fax: +44 1223 336 033; e-mail: deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

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