Electronic Supplementary Information (ESI)

Chiral uranyl-organic compounds assembled with achiral furandicarboxylic acid by spontaneous resolution

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Materials, Methods, Syntheses and Characterizations

All the reagents including 2,5-furandicarboxylic acid (H_2FDA) for synthesis were obtained commercially and used as received.

Elemental analyses (C, H and N) were performed on a Perkin-Elmer 240C analyzer. IR spectra were measured on a Tensor 27 OPUS (Bruker) FT-IR spectrometer with KBr pellets. The X-ray powder diffraction (XRPD) was recorded on a Rigaku D/Max-2500 diffractometer at 40 kV, 100 mA for a Cu-target tube and a graphite monochromator. Simulation of the XRPD pattern was carried out by the single-crystal data and diffraction-crystal module of the Mercury (Hg) program version 1.4.2.13. Thermogravimetric (TG) analyses were carried out on a Rigaku standard TG-DTA analyzer with a heating rate of 10 °C min^{-1} from ambient temperature to 700 °C, an empty Al_2O_3 crucible was used as reference. The solid-state circular dichroism (CD) spectra were recorded on a Jasco J-715 spectropolarimeter with KCl pellets.

Single-crystal X-ray diffraction measurements for **UOC-NH_4**, **UOC-Ca**, **UOC-Na-a** and **UOC-Na-b** were carried out on a Rigaku SCX-mini diffractometer equipped with a graphite crystal monochromator situated in the incident beam for data collection at 293(2) K. Data collections and cell refinement were performed with RAPID-AUTO (Rigaku, *RAPID-AUTO*. Rigaku Corporation, Japan, 2004). Data reduction was carried out using CrystalStructure

(Rigaku/MSC. CrystalStructure. Rigaku/MSC Inc. The Woodlands, USA, 2004). The structure was solved by direct methods using the SHELXS program of the SHELXTL package and refined with SHELXL (Sheldrick, G. M., *SHELXTL Version 6.1. Program for Solution and Refinement of Crystal Structures*, University of Göttingen, Germany, 1998). The final refinement was performed by full matrix least-squares methods with anisotropic thermal parameters for non-hydrogen atoms on F^2.

Photocatalytic experiments: at room temperature, 0.11 g **UOC-Na** was suspended in 200 mL MO aqueous solution (6.54 mg/L). The solution was stirred in the dark for about 60 min to ensure the establishment of adsorption equilibrium of MO onto the surface of samples. After that, the mixture was stirred and continuously exposed to UV irradiation from a 500 W high pressure mercury vapour lamp. A sample was taken every 15 min from the vessel, and subsequently analysed by UV−visible spectroscopy. For comparison, the photodegradation process of MO without any photocatalyst has also been studied under the same conditions.

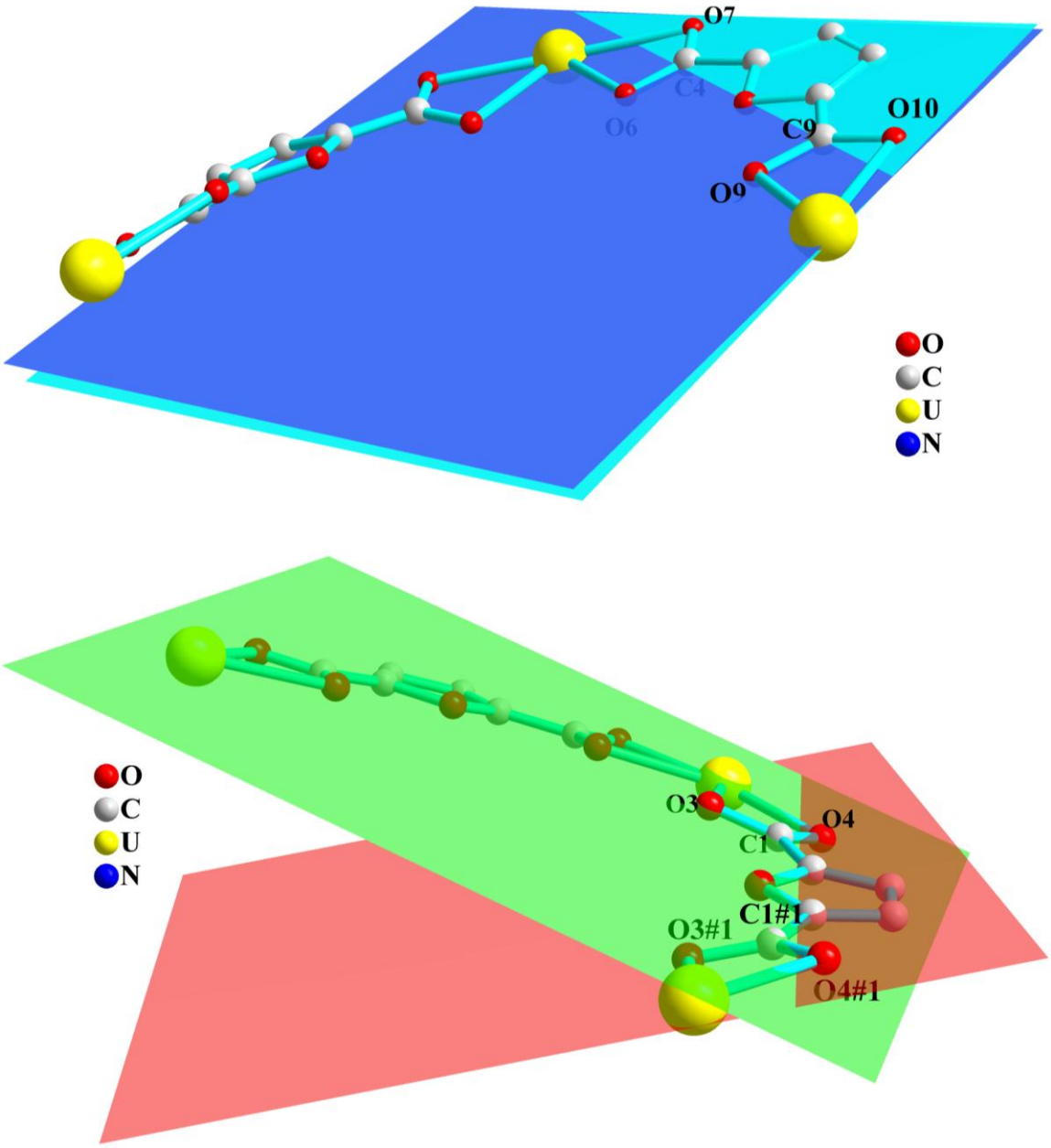

Fig. S1 The dihedral angle between the two carboxyl group (-COO) in each ligand in **UOC-NH$_4$** (top, 2.3° and down, 30.0°. Symmetry code #1: 1-x, y, 0.5-z).

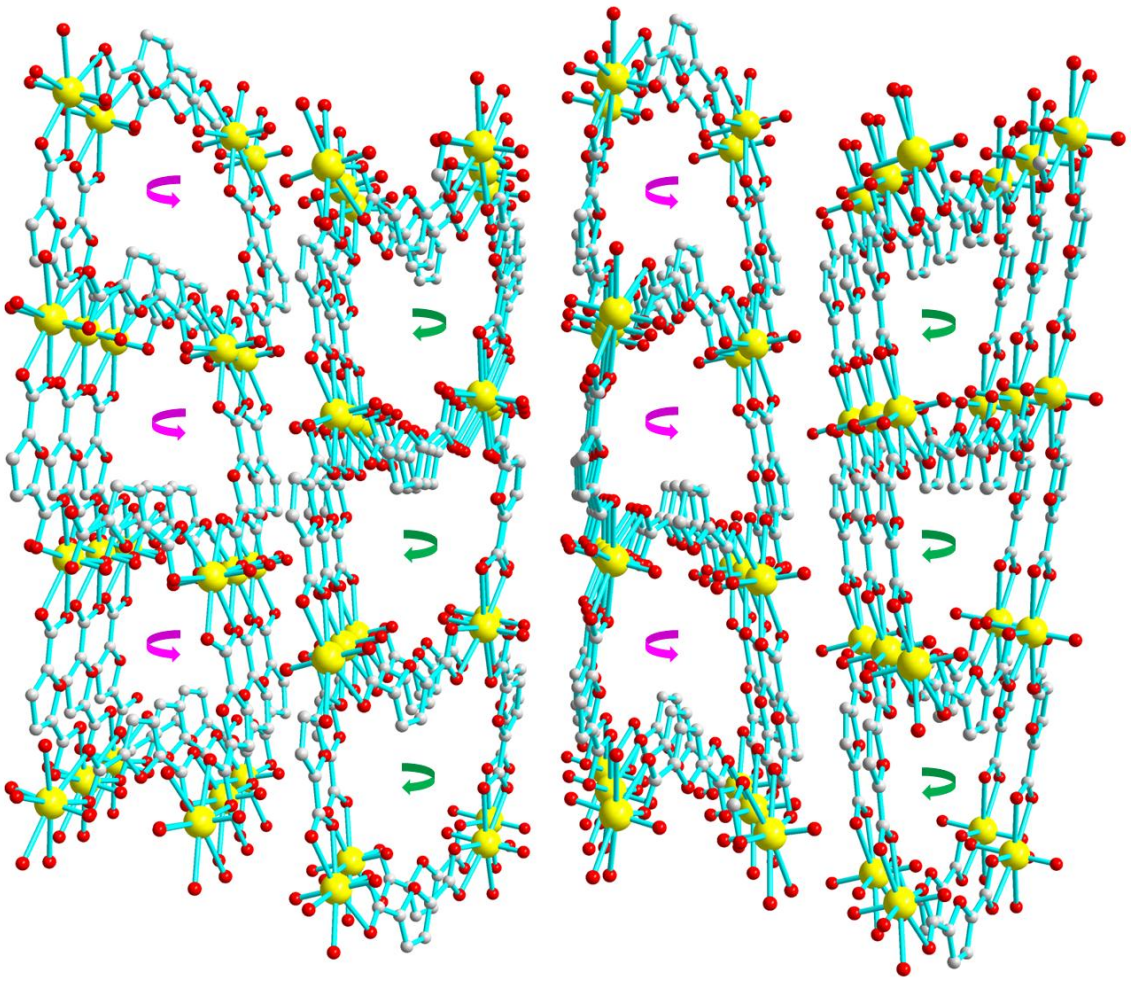

Fig. S2 Neighboring layers with opposite chirality in **UOC-Ca** (The calcium ions were omitted for clarity).

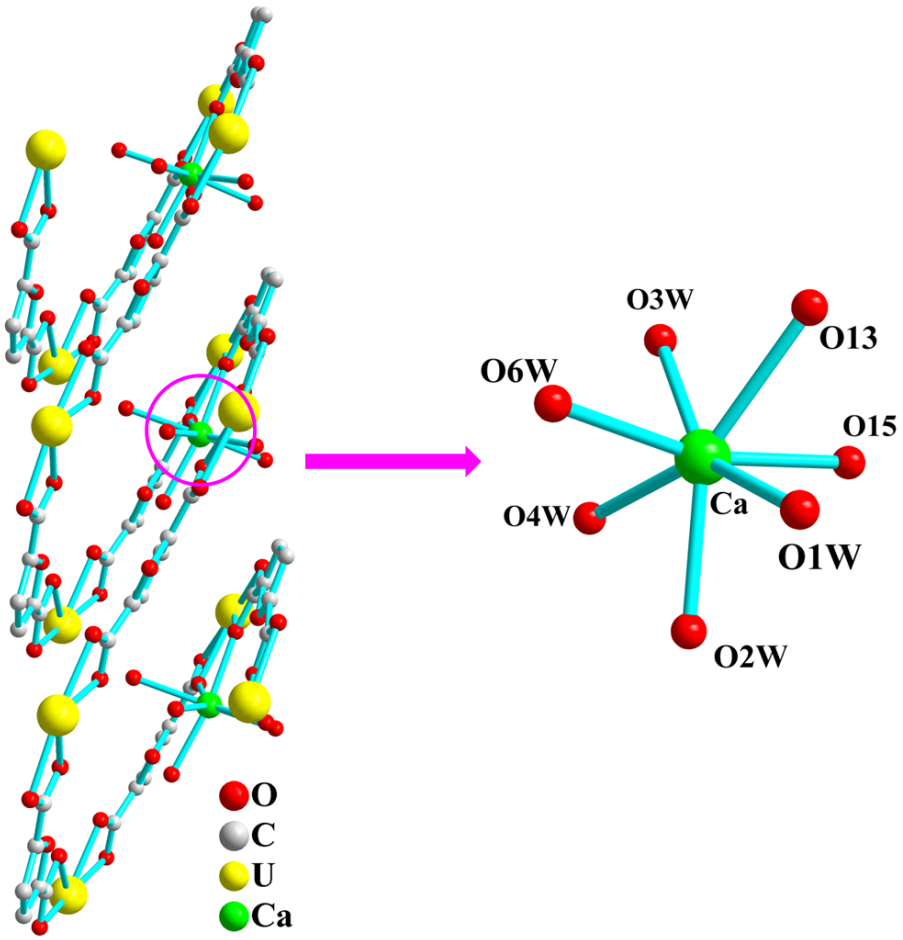

Fig. S3 Coordination environment of the calcium ions located inside the helical chain in **UOC-Ca**.

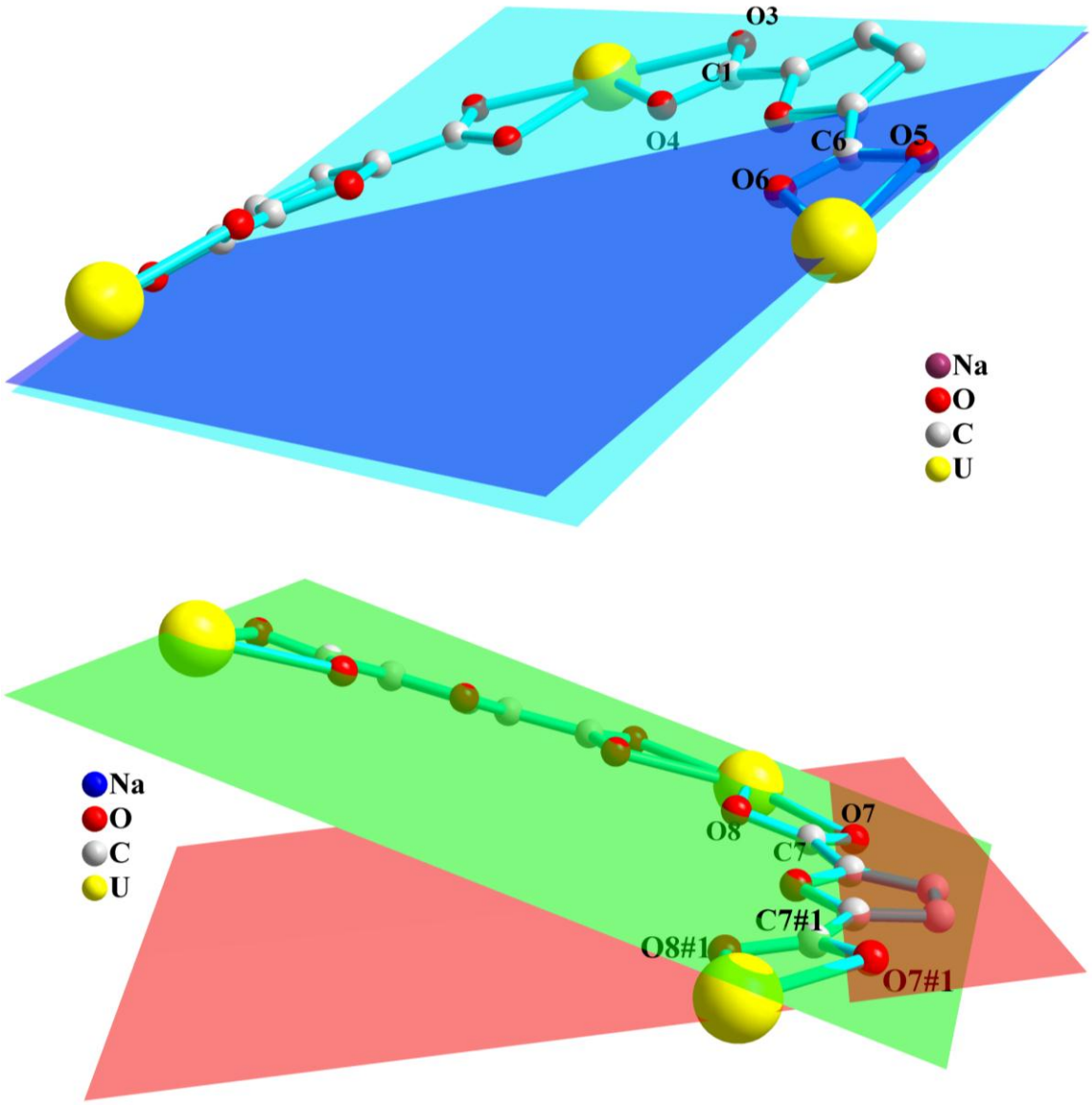

Fig. S4 The dihedral angle between the two carboxyl group (-COO) in each ligand in **UOC-Na** (top, 3.3° and down, 25.3°. Symmetry code #1: 2-x, y, 0.5-z).

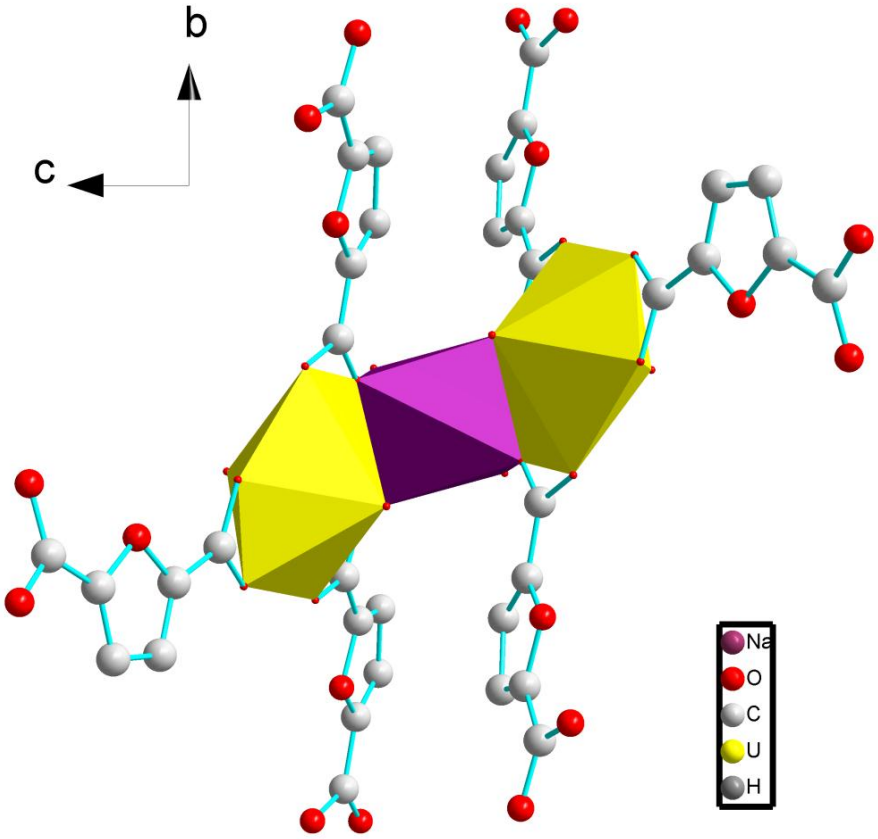

Fig. S5 Trinuclear heterometal cluster (U_2Na) as a SBU in **UOC-Na**.

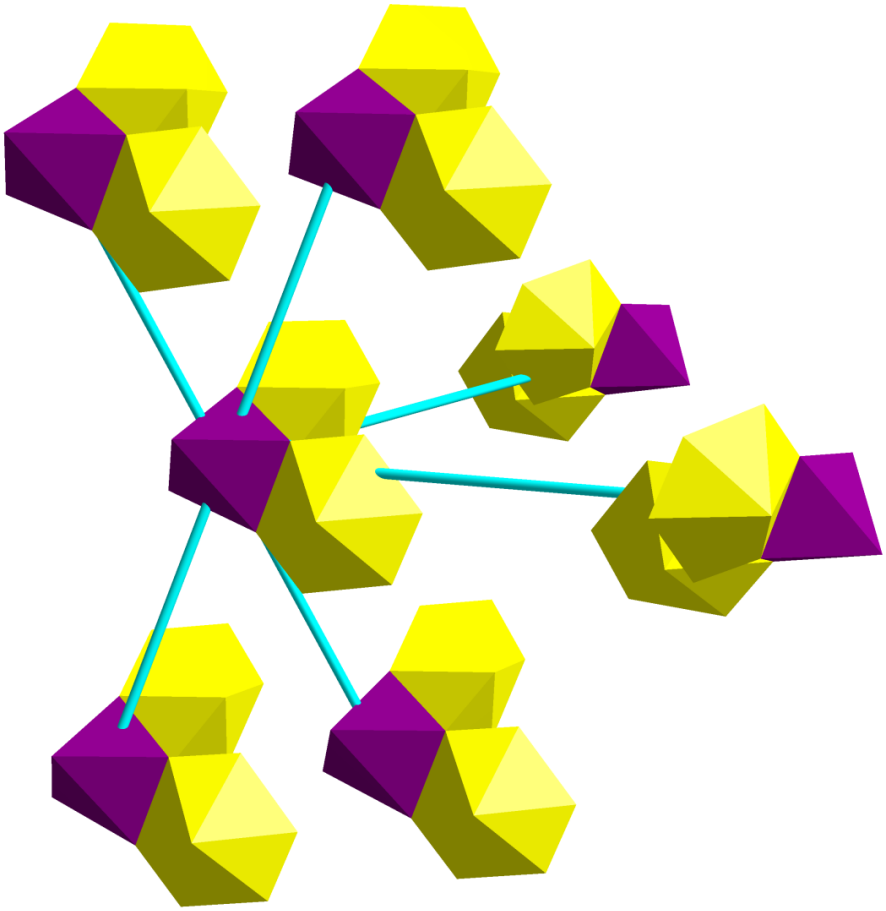

Fig. S6 View of the six-connected node of the (U_2Na) SBU in **UOC-Na**.

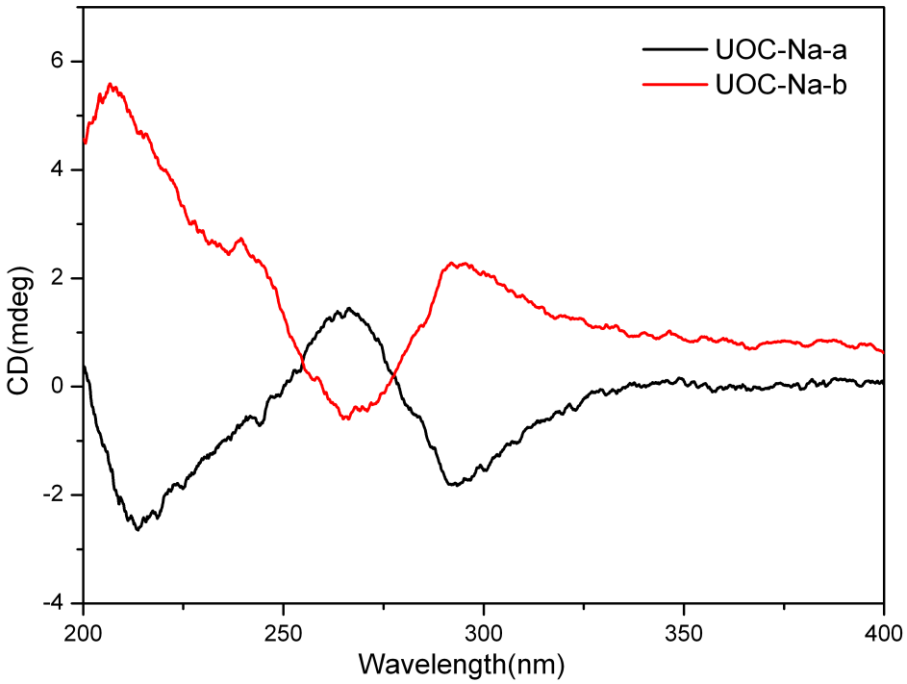

Fig. S7 Solid-state CD spectra of compounds **UOC-Na-a** (black) and **UOC-Na-b** (red).

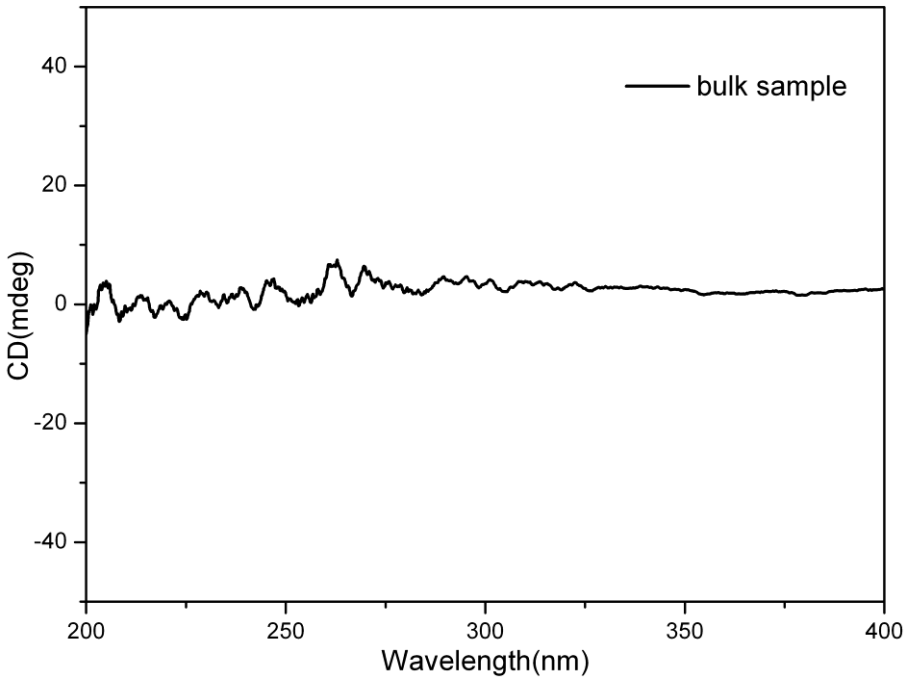

Fig. S8 Solid-state CD spectra of compound **UOC-Na** (bulk sample).

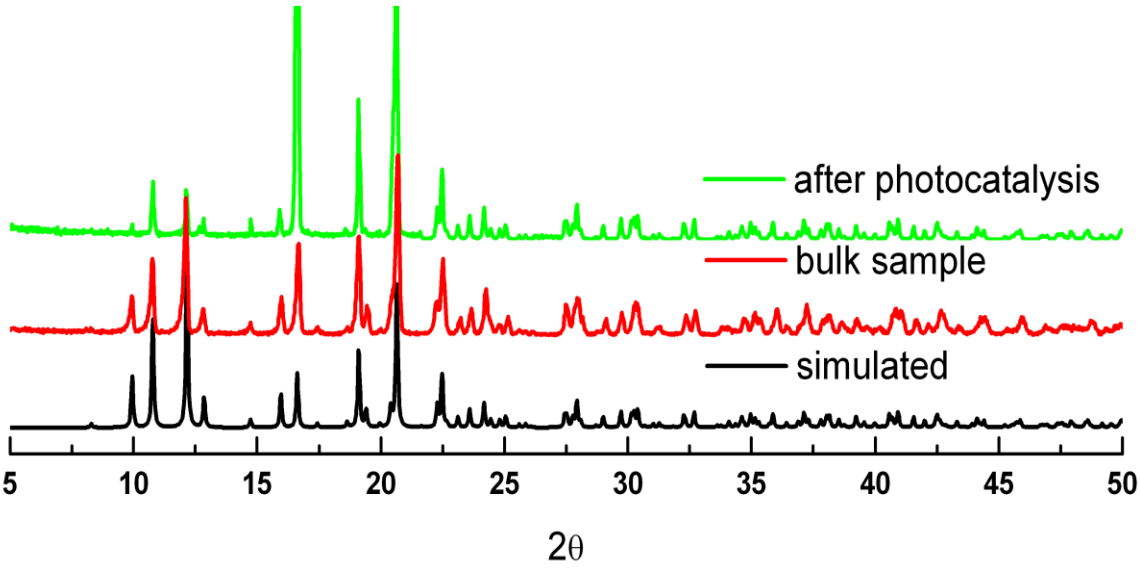

Fig. S9 XRPD patterns of **UOC-Na**.

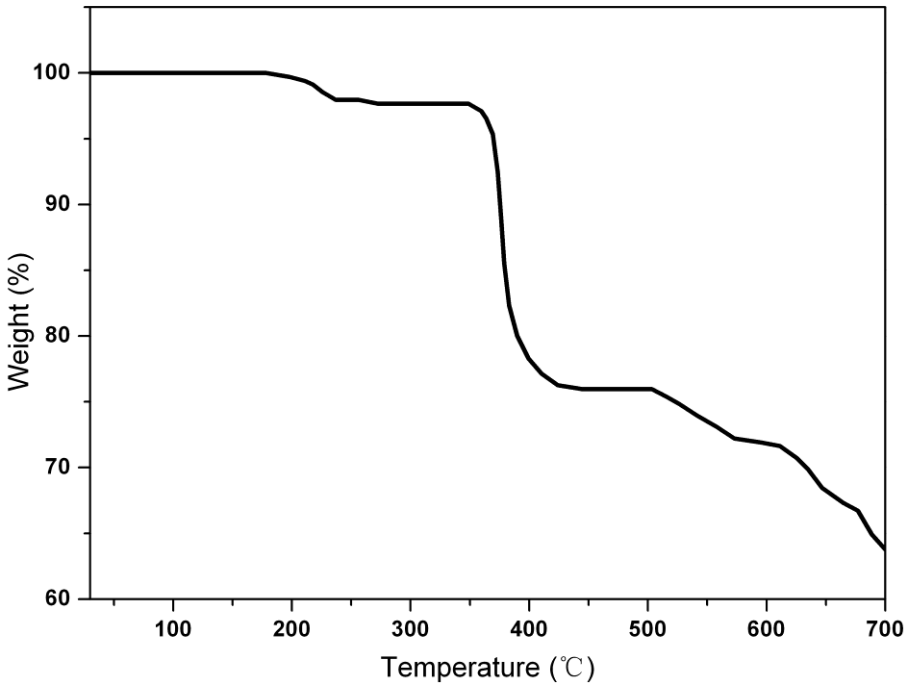

Fig. S10 TG curve of compound **UOC-Na**.

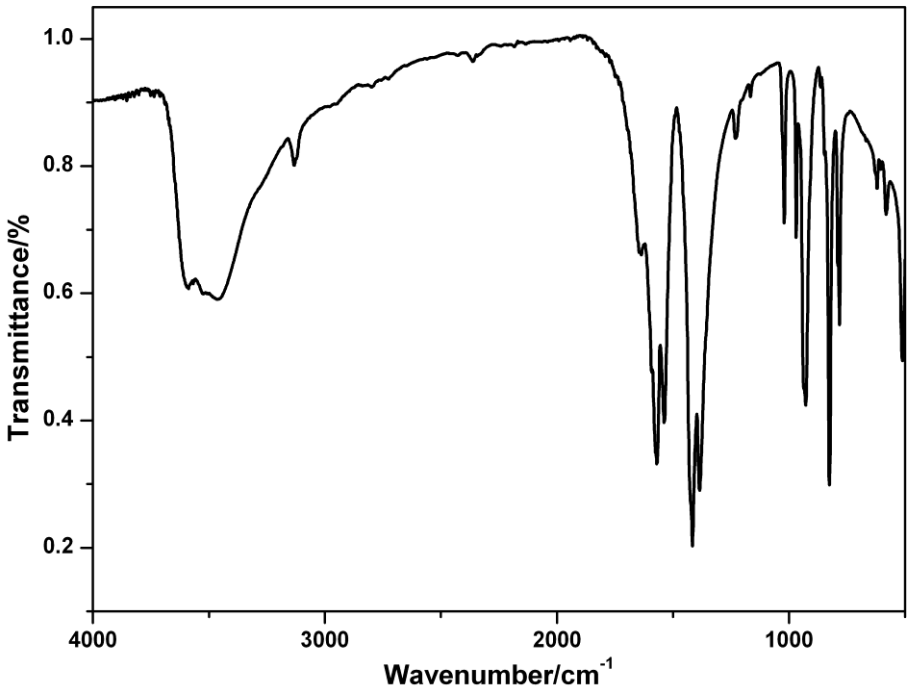

Fig. S11 IR curve of compound **UOC-Na**.

Table S1 A summary of structure determinations of 10 randomly selected crystals in the products of compound **UOC-Na** from the same crystallization: the *R* factors and Flack absolute structure parameters for each refinement with the same set of position coordinates.

	a	*b*	*c*	R_1	wR_2	Flack parameter	Goodness-of-fit on F^2
1	7.9757(16)	17.707(4)	21.218(4)	0.0312	0.0764	-0.001(13)	1.048
2	7.9714(16)	17.775(4)	21.312(4)	0.0429	0.0942	0.010(17)	1.083
3	7.9919(16)	17.682(4)	21.189(4)	0.0706	0.1245	0.00(2)	1.079
4	7.9577(16)	17.760(4)	21.311(4)	0.0610	0.1141	0.05(2)	1.095
5	8.0110(16)	17.769(4)	21.349(4)	0.0582	0.1332	0.04(2)	1.092
6	7.9674(16)	17.755(4)	21.296(4)	0.0502	0.1314	0.96(3)	1.039
7	7.9962(16)	17.743(4)	21.314(4)	0.0579	0.1337	0.99(3)	1.068
8	7.9541(16)	17.713(4)	21.235(4)	0.0589	0.1409	0.95(3)	1.074
9	8.0136(16)	17.765(4)	21.273(4)	0.0714	0.1634	0.99(3)	1.091
10	7.9416(16)	17.707(4)	21.177(4)	0.0519	0.1281	0.94(3)	1.040

Table S2 A summary of structure determinations of crystals 6-10 with inverted atomic coordinates

	a	b	c	R_1	wR_2	Flack parameter	Goodness-of-fit on F^2
6	7.9674(16)	17.755(4)	21.296(4)	0.0335	0.0827	0.045(15)	1.072
7	7.9962(16)	17.743(4)	21.314(4)	0.0430	0.0841	0.022(16)	1.091
8	7.9541(16)	17.713(4)	21.235(4)	0.0444	0.0952	0.060(18)	1.083
9	8.0136(16)	17.765(4)	21.273(4)	0.0590	0.1157	0.02(2)	1.087
10	7.9416(16)	17.707(4)	21.177(4)	0.0364	0.0790	0.066(15)	1.078