Supporting information for

A Nonlinear Optical Cadmium(II)-Based Metal–Organic Framework with Chiral Helical Chains Derived from an Achiral Bent Dicarboxylate Ligand

Kai Ting Hsu,[a,b,c] Pounraj Thanasekaran,[a] Ting-Wei Hsu,[b] Cing-Huei Su,[a] Bor-Chen Chang,[c] Yen-Hsiang Liu,[a,*] Chen-Hsiung Hung,[b,*] and Kuang-Lieh Lu[a,b,*]

[a]*Department of Chemistry, Fu Jen Catholic University, New Taipei City 242, Taiwan*
[b]*Institute of Chemistry, Academia Sinica, Taipei 115, Taiwan*
[c]*Department of Chemistry, National Central University, Taoyuan 320, Taiwan*

*E-Mail: 056461@gapp.fju.edu.tw (Y.-H. Liu)
*E-Mail: chhung@gate.sinica.edu.tw (C.-H. Hung)
*E-Mail: kllu@gate.sinica.edu.tw (K.-L. Lu)

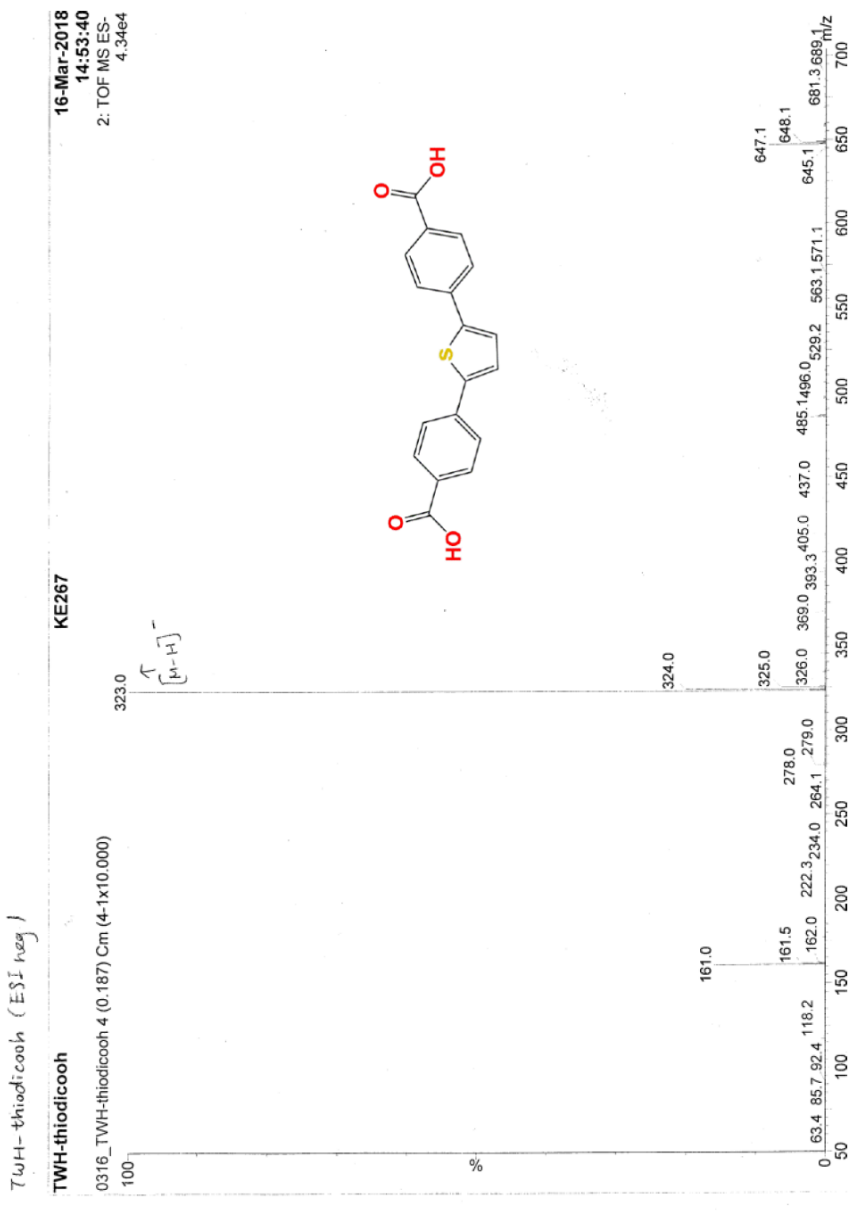

Fig. S1. ESI-MS spectrum of H_2TDB ligand.

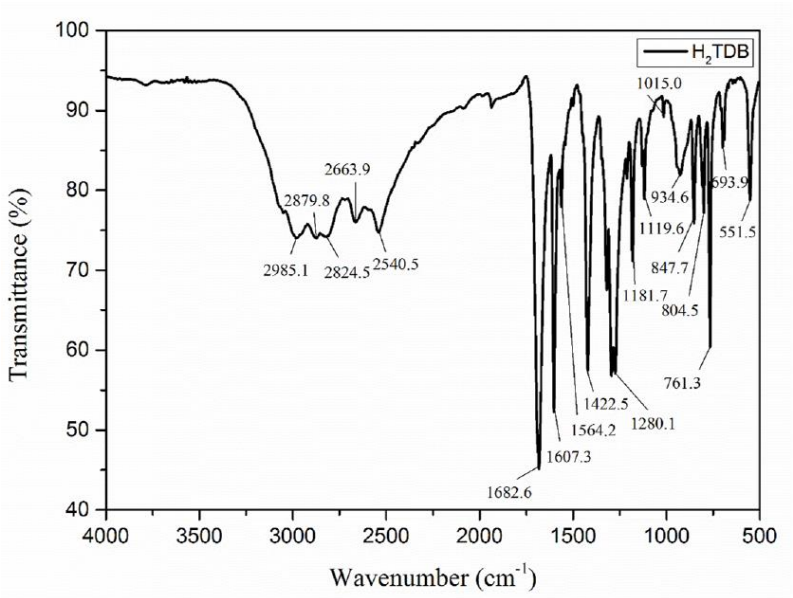

Fig. S2. FT-IR spectrum of H_2TDB ligand.

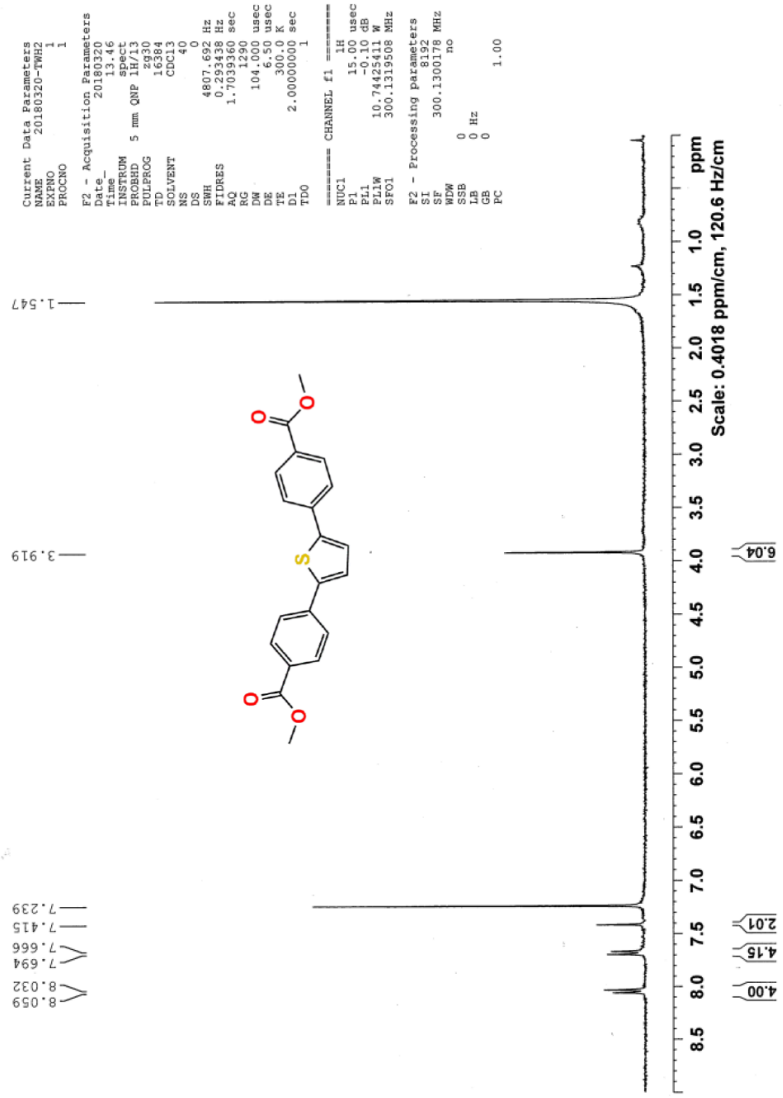

Fig. S3. ^{1}H NMR spectrum of 2,5-TDBMe ligand in $CDCl_3$.

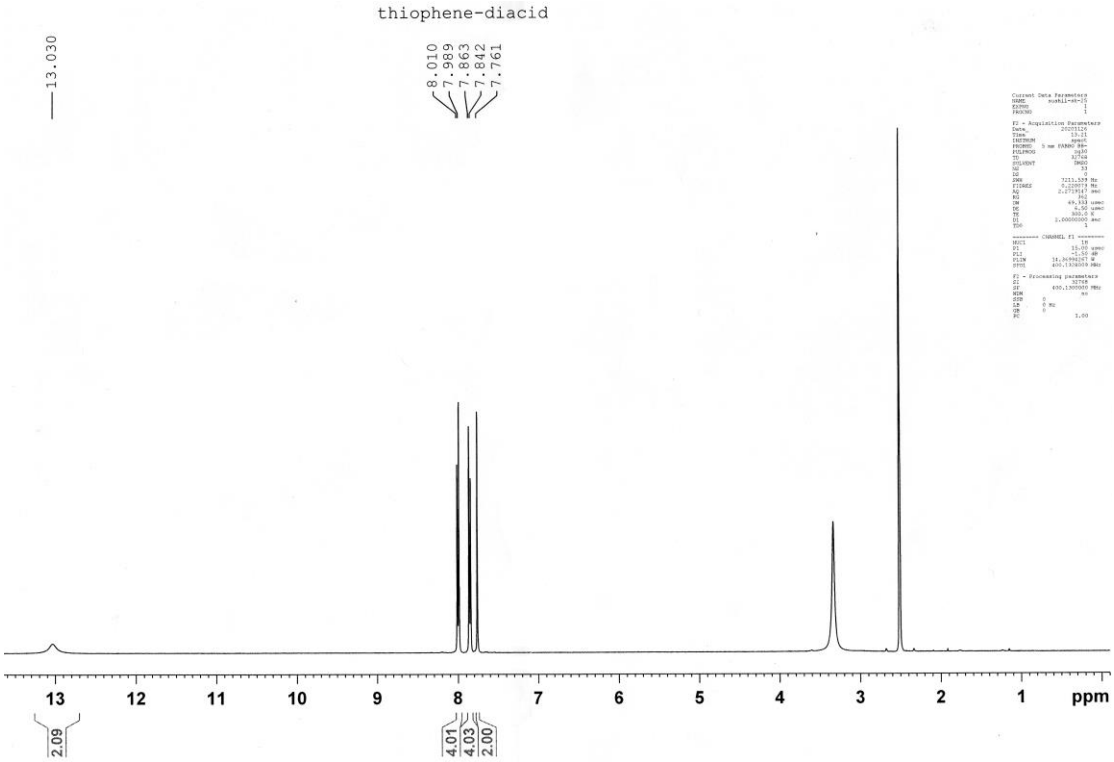

Fig. S4. ^{1}H NMR spectrum of H_2TDB in DMSO.

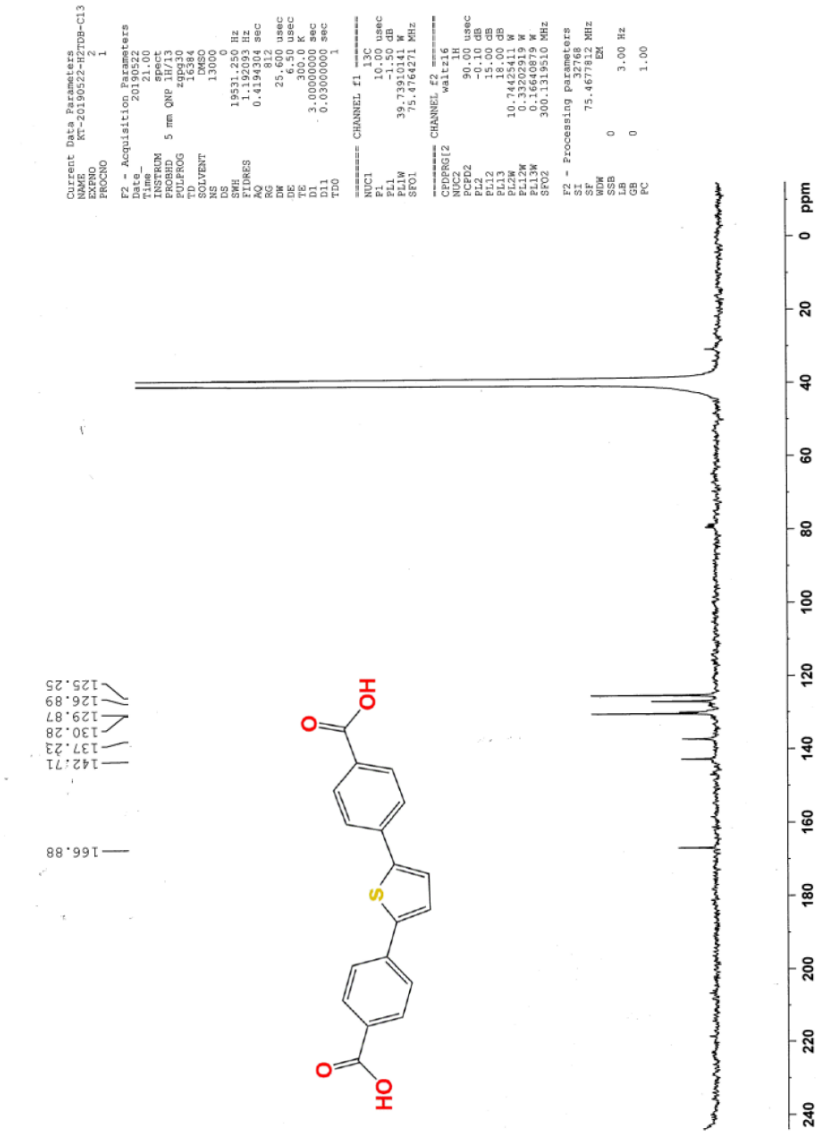

Fig. S5. ^{13}C NMR spectrum of H_2TDB in DMSO.

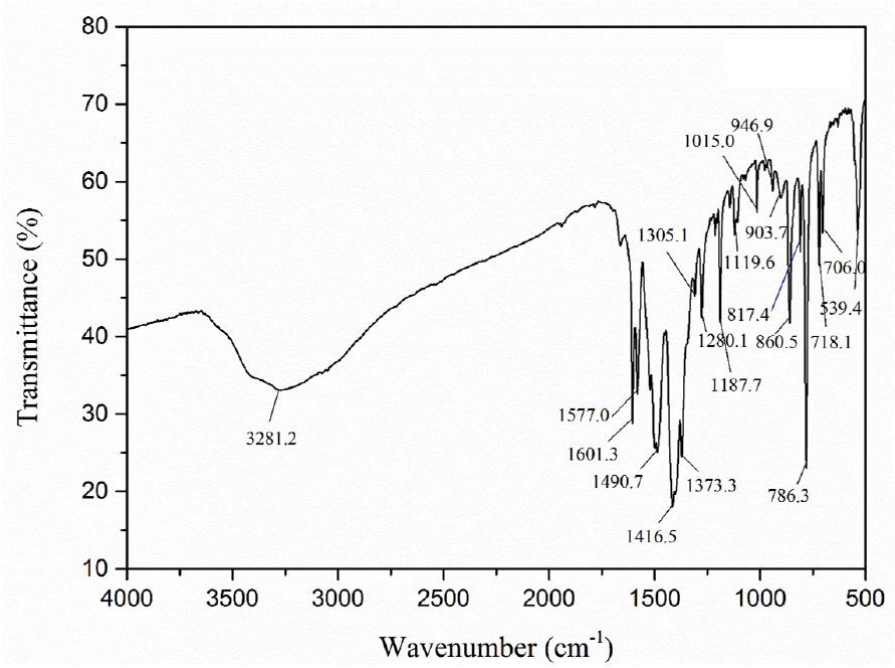

Fig. S6. FT-IR spectrum of compound **1**.

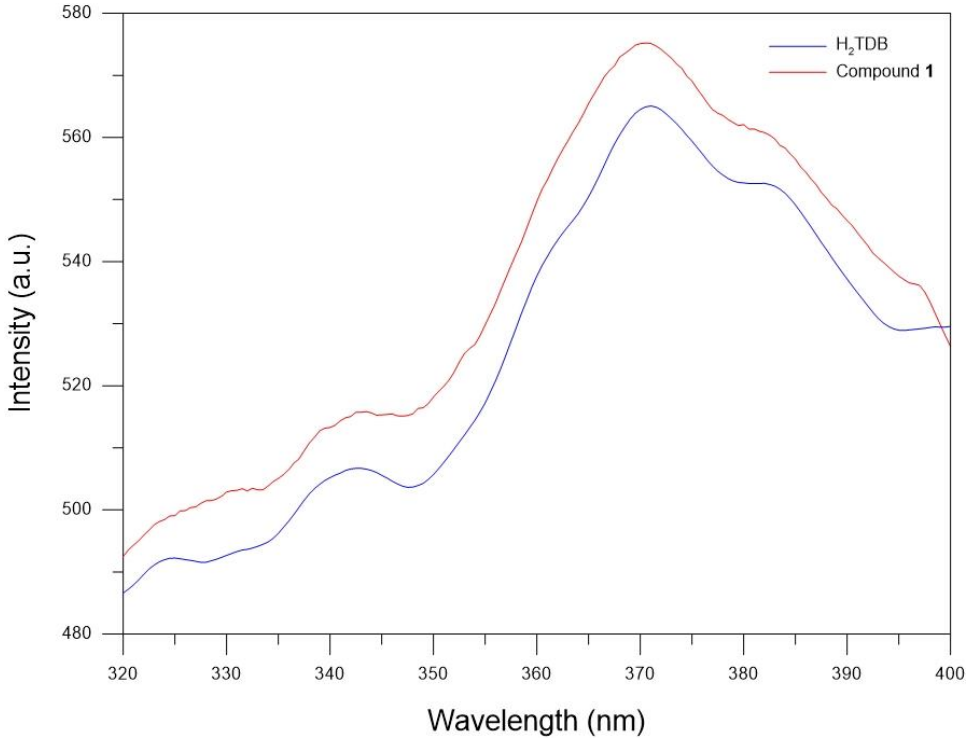

Fig. S7. Solid-state excitation spectra of the H_2TDB ligand and compound **1**.

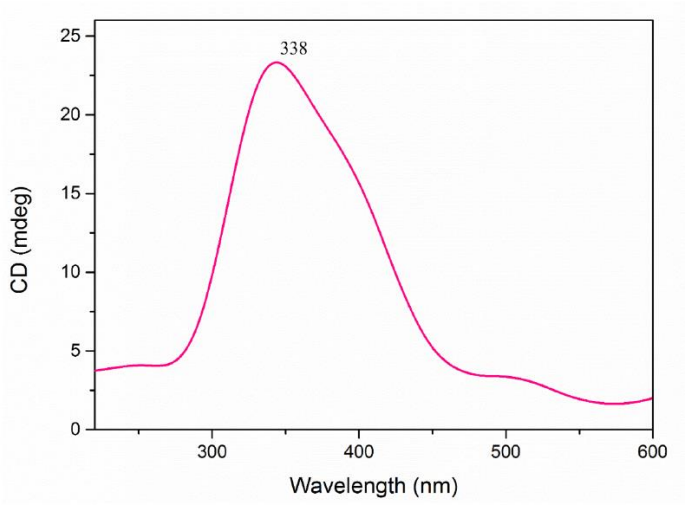

Fig. S8. Solid-state CD spectrum of compound **1**.

Table S1. Selected hydrogen bond geometry (Å,°).

Donor–H	Donor···Acceptor	H···Acceptor	Donor–H···Acceptor
O11–H11A 0.979 (0.000) 0.938	O11–O3 (7) 2.799 (0.000)	H11A–O3 (7) 2.082 (0.000) 2.108	O11–H11A···O3 (7) 128.53 (0.01) 129.41 (**)
O11–H11A 0.979 (0.000) 0.938	O11–O11 (8) 3.024 (0.000)	H11A–O11 (8) 2.680 (0.000) 2.688	O11–H11A···O11 (8) 100.97 (0.00) 101.84 (**)
O11–H11B 0.980 (0.000) 0.938	O11–O11 (8) 3.024 (0.000)	H11B–O11 (8) 2.797 (0.000) 2.800	O11–H11B···O11 (8) 93.77 (0.00) 94.63 (**)
O11–H11B 0.980 (0.000) 0.938	O11–O2 (9) 2.796 (0.000)	H11B–O2 (9) 2.070 (0.000) 2.097	O11–H11B···O2 (9) 129.34 (0.01) 130.23 (**)

(**) Values normalized following the refs. (a) G. A. Jeffrey and L. Lewis, *Carbohydr. Res.* **1978**, *60*,179; (b) R. Taylor and O. Kennard, *Acta Cryst.***1983**, *B39*, 133.

Equivalent positions:
(0) x, y, z
(1) -x+2, +y-1/2, -z
(2) x, +y-1, +z
(3) x, +y+1, +z
(4) x, +y+1, +z-1
(5) x, +y+1, +z+1
(6) x, +y, +z-1
(7) -x+1, +y+1/2, -z+2
(8) -x+1, +y-1/2, -z+1
(9) -x+1, +y+1/2, -z+1
(10) -x+2, +y+1/2, -z+1