Supplementary Material (ESI) for Chemical Communications


**Supporting Information**

# Induction in Urothermal Synthesis of Homochiral Porous Materials from Achiral Precursors

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All the syntheses were performed in polytetrafluoroethylene-lined stainless steel autoclaves under autogenous pressure. Reagents were purchased commercially and used without further purification. Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10 °C/min under nitrogen atmosphere. The adsorption experiments were performed on Micromeritics ASAP 2010 surface area and pore size analyzer. The sample was degassed at 200ºC for 2 days prior to the measurement.

Measurement of solid CD spectra: The mixture of about 1-mg sample and 200 mg dried KCl powder was well grounded and then pressed into a disk for use in the CD measurement, using a J-810 spectropolarimeter.

X-ray Crystallography. Data collections were performed on a Bruker Apex II CCD diffractometer equipped with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 293 K. All data sets were corrected for Lorentz and polarization factors. Absorption corrections by the multiscan method were applied. All structures were solved by the direct methods and refined by full-matrix least-squares fitting on F2 by SHELX-97.

**Synthesis:**

Synthesis of (±)-[Co(bdc)(e-urea)]·(e-urea) (**(±)-1**): 1,4-Benzenedicarboxlic acid ($H_2$bdc, 0.1167 g), ethyleneurea hemihydrate(2.2342 g), and $Co(NO_3)_2 \cdot 6H_2O$ (0.1978 g) were mixed in a 23-mL teflon cup. The vessel was then sealed and heated at 140 $^oC$ for 4 days. The autoclave was allowed to cool to room temperature. After washing by water and ethanol, the red crystals were obtained. Anal. Calcd for $C_{28}H_{32}Co_2N_8O_{12}$: C, 42.55; H, 4.08; N, 14.18. Found: C, 42.03; H, 3.79; N, 14.56.

Synthesis of (-)-[Co(bdc)(e-urea)]·(e-urea) (**(-)-1**): 1,4-Benzenedicarboxlic acid ($H_2$bdc, 0.1220 g, 0.7 mmol), ethyleneurea (1.9697 g), $Co(NO_3)_2 \cdot 6H_2O$ (0.2058 g, 0.7 mmol) and (-)-carvone (0.7331 g) were mixed in a 23-mL teflon cup. The vessel was then sealed and heated at 140 $^oC$ for 4 days. The autoclave was allowed to cool to room temperature. After washing by water and ethanol, the red crystals were obtained

at about 90 % yield. Anal. Calcd for $C_{28}H_{32}Co_2N_8O_{12}$: C, 42.55; H, 4.08; N, 14.18. Found: C, 42.33; H, 4.20; N, 14.44.

Synthesis of (+)-[Co(bdc)(e-urea)]·(e-urea) (**(+)-1**): 1,4-Benzenedicarboxlic acid ($H_2$bdc, 0.1234 g), ethyleneurea (2.0345 g), $Co(NO_3)_2 \cdot 6H_2O$ (0.2023 g) and (+)-carvone (0.7645 g) were mixed in a 23-mL teflon cup. The vessel was then sealed and heated at 140 $^oC$ for 4 days. The autoclave was allowed to cool to room temperature. After washing by water and ethanol, the red crystals were obtained at about 90 % yield. Anal. Calcd for $C_{28}H_{32}Co_2N_8O_{12}$: C, 42.55; H, 4.08; N, 14.18. Found: C, 42.25; H, 3.96; N, 14.25.

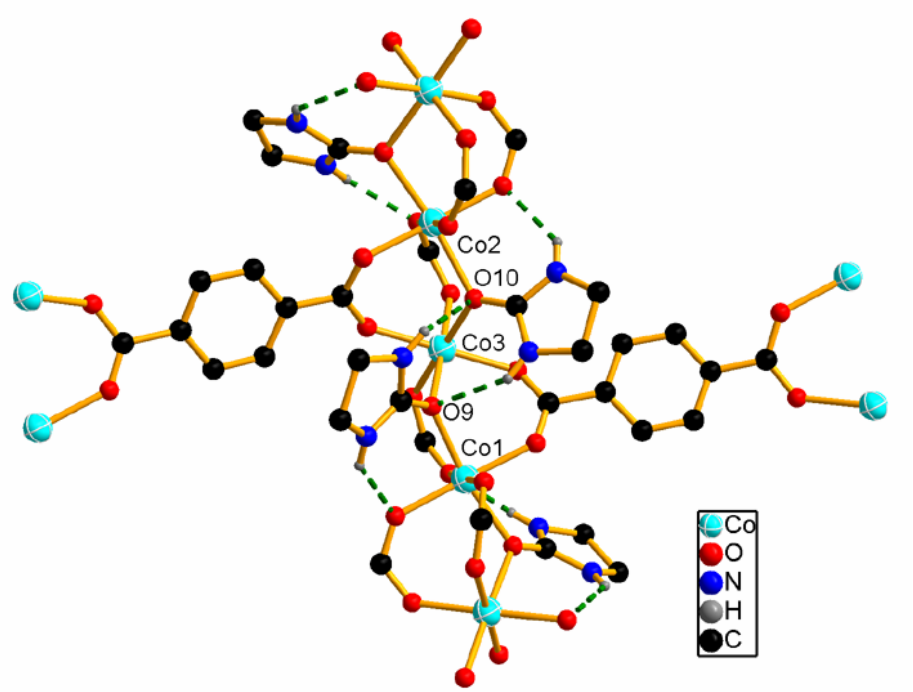


**Figure S1.** View of the coordination environment in **1** and the hydrogen bonding interactions (green dashed lines) between the e-urea ligands and the carboxylate groups.

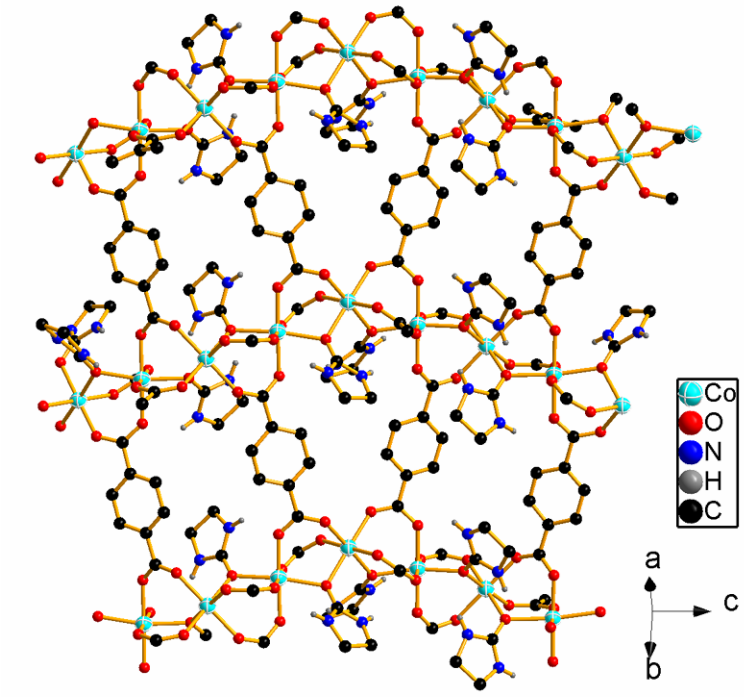


**Figure S2.** The layered substructure in **1**, showing the connectivity between the chains.

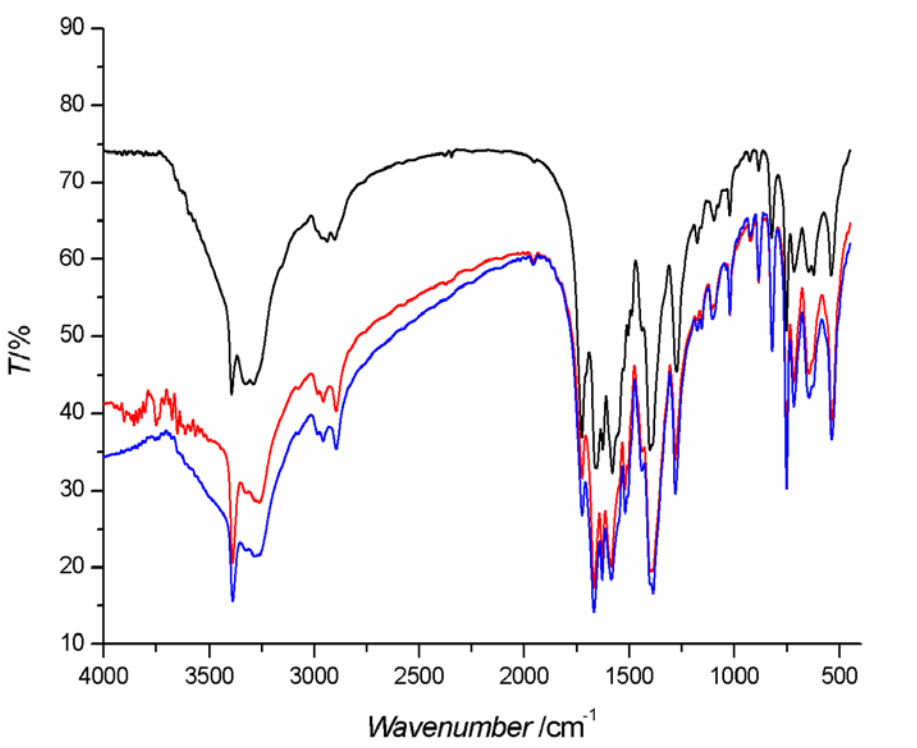


**Figure S3**. The IR spectra of **1** (blue line), (+)-**1** (red line) and (-)-**1** (black line).

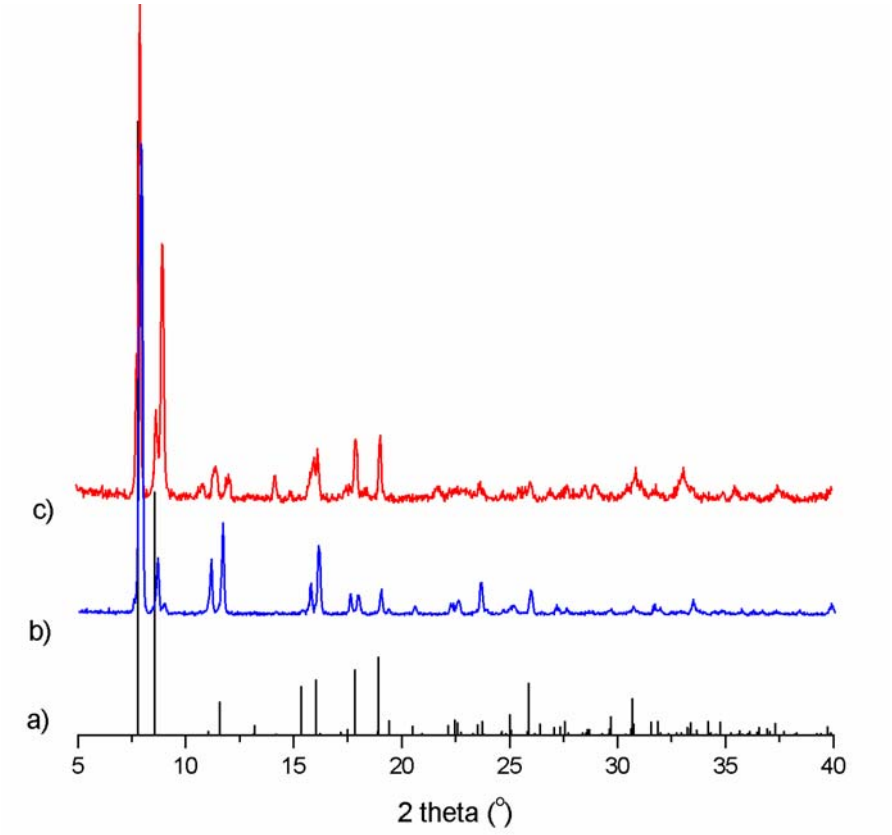


**Figure S4.** XPRD patterns: (a) simulated powder patterns of **1**; **(**b): powder sample of **1**; (c) powder sample of **1** after BET measurement.

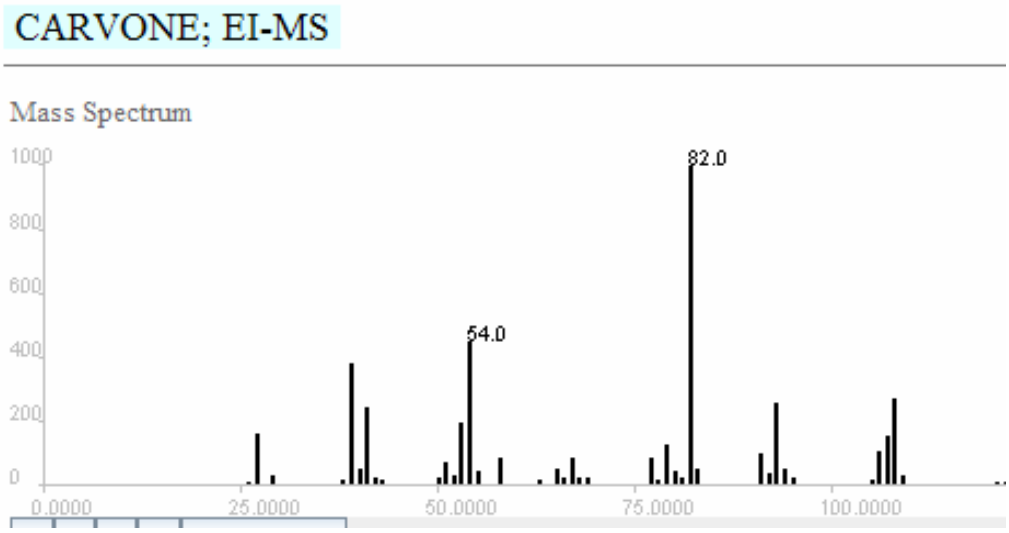


**Figure S5.** The EI-MS spectra of carvone. (from: http://www.massbank.jp/jsp/Dispatcher.jsp?type=disp&id=JP006601&site=10)

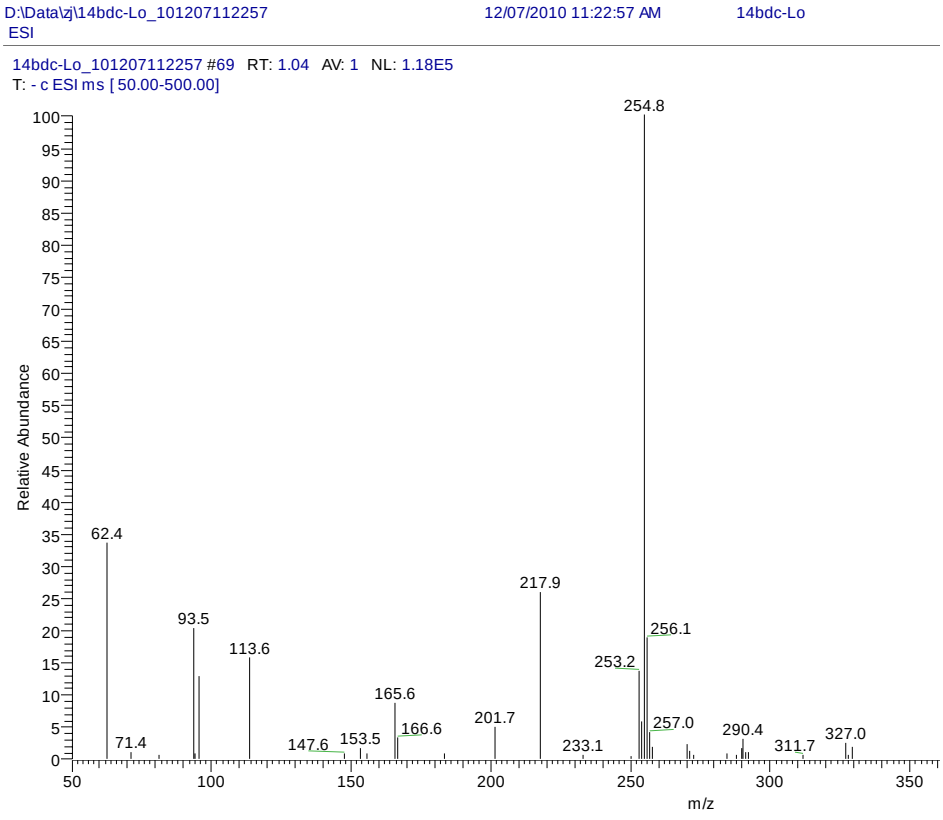


**Figure S6.** The EI-MS spectra of the digested sample of (-)-**1**. There are no peaks of carvone.

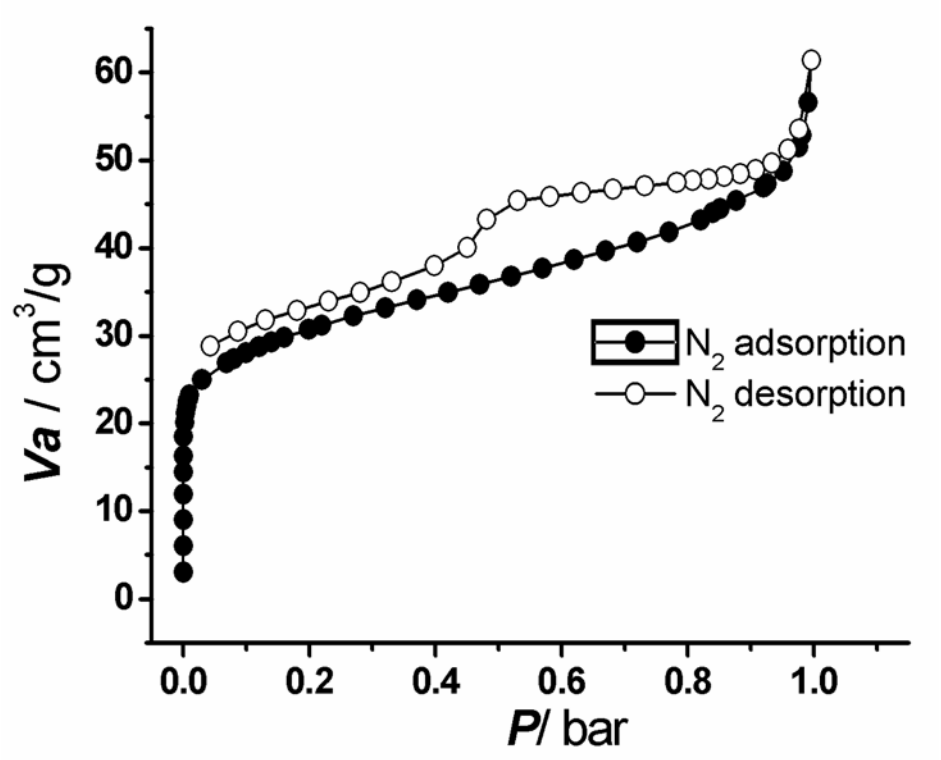


**Figure S7**. The $N_2$ adsorption isotherms of **1**(■adsorption; ●desorption).

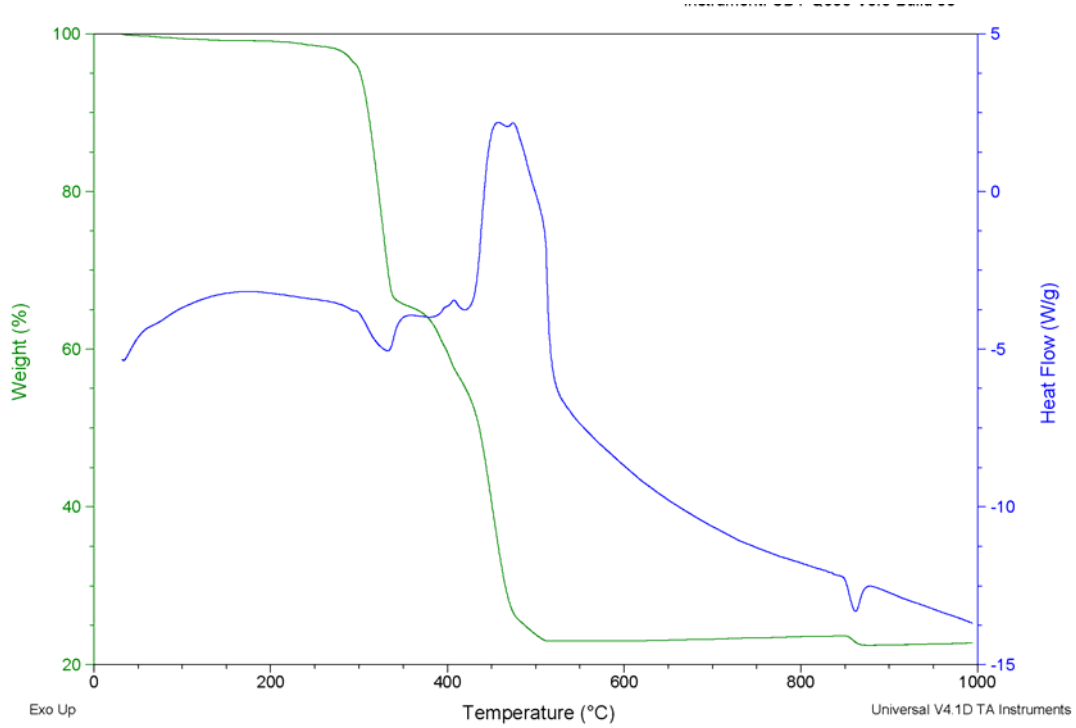


**Figure S8.** The TGA diagram of **1**.

**Table S1**: A summary of structure determinations of 5 randomly selected crystals in the products of **1** with chiral induction agent of (-)-carvone: the *R* factors and Flack absolute structure parameters for each refinement with space group ***P*4$_1$22**.

| | *a* | *c* | *R1* | $wR_2$ | Flack parameter |
|---|---|---|---|---|---|
| **1** | 11.3140(2) | 25.2429(10) | 0.0565 | 0.1499 | -0.01(6) |
| **2** | 11.3482(2) | 25.3182(10) | 0.0514 | 0.1428 | 0.01(5) |
| **3** | 11.3086(2) | 25.2555(14) | 0.0492 | 0.1437 | -0.02(5) |
| **4** | 11.3015(4) | 25.1676(18) | 0.0494 | 0.1406 | 0.02(5) |
| **5** | 11.3051(3) | 25.2097(16) | 0.0584 | 0.1491 | 0.02(5) |

**Table S2**: A summary of structure determinations of 2 randomly selected crystals in the products of **1** with chiral induction agent of (+)-carvone: the *R* factors and Flack absolute structure parameters for each refinement with space group ***P*4$_3$22**.

| | *a* | *c* | *R1* | $wR_2$ | Flack parameter |
|---|---|---|---|---|---|
| **6** | 11.2758(2) | 25.1488(10) | 0.0591 | 0.1657 | 0.02(5) |
| **7** | 11.3108(2) | 25.2380(12) | 0.0569 | 0.1532 | -0.02(6) |