The 4-pyridonyl group as a multifunctional electron donor in 1,8-naphthalimide-based photoluminescent and mechanically interlocked coordination compounds

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Supporting Information

1. Experimental Section	2
2. X-ray Crystallography	5
3. X-ray Powder Diffraction	7
4. Thermogravimetric Analysis	9
5. Spectroscopic data	11
6. Additional Gas Adsorption Data	13
7. NMR Spectra	15
8. References	19

1. Experimental Section

All starting materials, reagents and solvents were purchased from Sigma/Merck, Fluorochem, Acros Organics or Alfa Aesar, and were used as received without further purification. N-(4-picolyl)-4-nitro-1,8-naphthalimide and N-(4-carboxyphenylmethylene)-4-nitro-1,8-naphthalimide were prepared according to previous reports.^{S1-S2} NMR spectra were recorded using a Bruker AVANCE III instrument operating at 400 MHz for ¹H and 100 MHz for ¹³C, using CDCl₃ or d₆-DMSO solvents as specified. Chemical shifts are reported in ppm with the residual solvent and/or TMS as the calibrant. Mass spectra were acquired using a Micromass time of flight mass spectrometer (tof), interfaced to a Waters 2690 HPLC, with samples dissolved in HPLC-grade MeOH or MeCN. The instrument was operated in positive or negative mode as required. Leucine Enkephalin was used as an internal lock mass. Masses were recorded over the range 100-1000 m/z. Melting points were determined using an Electrothermal IA9000 digital melting point apparatus and are uncorrected. Infrared spectra were recorded on a PerkinElmer Spectrum One FTIR spectrometer in the range 4000 - 550 cm⁻¹. Thermogravimetric analysis was performed on a Perkin Elmer Pyris 1 TGA with a scan rate 5 °C min⁻¹ under a nitrogen atmosphere with N₂ flow rate 20 mL/min. All photophysical measurements were performed at 298 K in spectrophotometric grade solvents. UV-Vis absorption spectra were measured in 1 cm quartz cuvettes on a Varian Cary 50 spectrophotometer. Fluorescence spectra were measured on a Varian Cary Eclipse Fluorimeter. Quantum yields were calculated by comparison with quinine sulfate in 2M H₂SO₄ with excitation at 366 nm using an excitation slit width of 2.5 nm for all samples, and emission integrated across the range 380 - 600 nm. Solid-state emission spectra were measured with samples pressed into films between quartz plates which were then mounted in the beam path. Gas adsorption isotherms were measured using a Quantachrome Autosorb IQ gas sorption analyser. Chemically pure (CP, N4.5) grade He, N₂, H₂ and CO₂ gases from BOC gases were used for the measurements. The sample of methanolexchanged complex 4 was de-gassed under dynamic vacuum at 100 °C for 48 hours prior to the measurements.

X-ray powder diffraction patterns were recorded with a Bruker D2 Phaser instrument using Cu-K α ($\lambda = 1.5405$ Å) radiation at room temperature. Raw data were compared with the simulated patterns from the single crystal data collections carried out at 100 K. For the fresh complex **4**, X-ray powder diffraction was carried out at 120 K using a Bruker APEX-II Duo operating at Cu-K α wavelength ($\lambda = 1.5405$ Å). The crystals were ground together with a small quantity of NVH immersion oil and the resulting mass was immediately transferred to the cryostream of the instrument (T = 100 K). Data were collected using three 360 ° scans in φ covering the 2 θ range 3 – 55 °, which were subsequently merged and the Debye rings integrated in Bruker APEX-3, with baseline corrections then applied in DIFFRAC.EVA.^{S3,S4}

Synthesis of L1



To a solution of N-(4-picolyl)-4-nitro-1,8-naphthalimide (270 mg. 0.81 mmol) and potassium carbonate (240 mg, 1.7 mmol) in 7 mL of anhydrous DMSO was added 4hydroxypyridine (150 mg, 1.6 mmol). The mixture was heated at 115 °C under an argon atmosphere for 3 hours. On cooling to room temperature, H₂O (30 mL) was added and the resulting brown suspension was stirred for 15 minutes. The mixture was filtered and washed with 100 mL of H₂O, and the brown solid was air dried. The solids were extracted with PhMe (30 mL) followed by CHCl₃ (30 mL), and each organic phase was filtered and evaporated to dryness to give a total of 127 mg of orange solid, which was dried in air. Yield 41 %; m.p. 255-257 °C; ϵ (10³ L mol⁻¹ cm⁻¹) / λ_{max} (nm) 12.8 ± 0.8 (351); Found C, 66.82; H, 4.15; N, 10.26; Calculated for C₂₃H₁₅N₃O₃·1/3CHCl₃C, 66.54; H, 3.67; N, 9.98 %; δ_H(400 MHz, d₆-DMSO) 5.30 (s, 2H, H³), 6.35 (d, 2H, ${}^{3}J = 7.8$ Hz, H⁹), 7.34 (d, 2H, ${}^{3}J = 6.2$ Hz, H²), 7.95 - 8.07 (m, 4H, H¹⁰ + H⁵ +

H⁷), 8.14 (dd, 1H, ${}^{3}J = 8.2$ Hz, ${}^{4}J = 1.2$ Hz, H⁸), 8.49 (d, 2H, ${}^{3}J = 6.2$ Hz, H¹), 8.62 - 8.65 (m, 2H, H⁴ + H⁶); δ_c(100 MHz, d₆-DMSO) 42.40, 117.82, 122.00, 122.60, 122.63, 125.34, 128.91, 128.64, 128.91, 129.05, 131.16, 131.86, 141.57, 144.26, 146.00, 149.67, 162.76, 163.28, 177.44; m/z (ESMS) 382.1208 $([M+H]^+, \text{ calculated for } C_{23}H_{16}N_3O_3 382.1192); v_{max} (ATR, \text{ cm}^{-1}) 3387 \text{ w br}, 3076 \text{ w sh}, 1701 \text{ m}, 1658 \text{ s})$ br, 1564s sh, 1510m, 1465w, 1407m, 1383s, 1351s, 1318m, 1280m, 236s, 1197m, 1180s, 1128w, 1087w, 1002w, 957m sh, 852s, 788s, 754m, 730w.

Synthesis of HL2



To a mixture of N-(4-carboxyphenylmethylene)-4-nitro-1,8-naphthalimide (200 mg, 0.53 mmol) and potassium carbonate (290 mg, 2.1 mmol) in 5 mL of anhydrous DMSO was added 4-hydroxypyridine (100 mg, 1.1 mmol). The mixture was heated at 110 °C for 3 hours, and on cooling to room temperature 25 mL of H₂O was added. The mixture was acidified by dropwise addition of 0.5 mL of glacial acetic acid, causing the precipitation of a fine white solid. The mixture was filtered, and the solids were washed with 2×20 mL H₂O, 2×20 mL MeOH and 20 mL of Et₂O, and air-dried. Yield 193 mg (87 %); m.p. >300 °C; ε $(10^{3} \text{ L mol}^{-1} \text{ cm}^{-1}) / \lambda_{\text{max}}$ (nm) 12.8 ± 0.8 (357); Found C, 69.38; H, 3.57, N, 6.28; Calculated for C₂₅H₁₆N₂O₅· 1/2H₂O C, 69.28; H, 3.95; N, 6.46 %; δ_H (400 MHz, d_6 -DMSO) 5.34 (s, 2H, H³), 6.34 (d, 2H, ${}^{3}J = 7.9$ Hz, H⁹), 7.46 (d, 2H, ${}^{3}J = 8.1$ Hz, H²), 7.88 (d, 2H, ${}^{3}J = 8.3$ Hz, H¹), 7.96 (d, 2H, ${}^{3}J = 7.8$ Hz, H¹⁰), 7.98 - 8.14

(m, 3H, $H^5 + H^7 + H^8$), 8.62 – 8.65 (m, 2H, $H^4 + H^6$), 12.89 (br s, 1H, H^{11}); $\delta_C(100 \text{ MHz}, d_6\text{-DMSO})$ 43.02, 117.80, 122.57, 122.60, 125.34, 126.91, 127.32, 128.54, 129.04, 129.49 (overlapping), 129.60, 131.17, 131.85, 141.57, 142.10, 144.24, 162.72, 163.24, 167.03, 177.43; *m/z* (APCI) 423.0991 ([M-H]⁻ , calculated for C₂₅H₁₅N₂O₅ 423.0986); v_{max} (ATR, cm⁻¹) 3082w, 2949w, 1699s sh, 1658s, 1629m, 1587m, 1562m, 1513w, 1467w, 1403m, 1375m, 1430m, 1279s, 1236s, 1176s, 1117w, 1020w, 972w, 957w, 854s, 790s, 757s, 740m, 697w, 663w, 617s. A single crystal of the title compound as the DMF solvate was prepared by heating 10 mg of solid in 1 mL of DMF at 100 °C, and cooling to room temperature. This procedure proved inefficient for recrystallising bulk quantities and was not carried out on preparative scale. Instead, the as-synthesised material proved sufficiently pure for use in all analyses and further preparations.

Synthesis of [Ag(L1)₂]SbF₆·3H₂O 1

To a solution of silver hexafluoroantimonate (10 mg, 29 µmol) in 3 mL of methanol was added L1 (10 mg, 26 µmol) in 3 mL of methanol. The mixture was sealed with ambient light excluded, yielding a crop of pale yellow crystals after 3 days. Yield 3.4 mg (22 % based on **L1**); m.p. 293 – 297 °C (decomp); Found C, 47.19; H, 2.47; N, 7.11; Calculated for $C_{46}H_{30}N_6O_6F_6AgSb\cdot 3(H_2O)$ C, 47.61; H, 3.13; N, 7.24 %; v_{max} (ATR, cm⁻¹) 3395w br, 3073w, 2940w, 1703m, 1656s, 1637m, 1546s sh, 1467w, 1403s, 1379s, 1354s sh, 1279m, 1235m, 1181s sh, 1128w, 1086w, 1069w, 1019w, 957m sh, 850s, 785s, 652s; Phase purity was confirmed by X-ray powder diffraction.

Synthesis of poly-[ZnL1(NO₃)₂]·0.5H₂O 2

To a suspension of **L1** (10 mg; 26 µmol) in 10 mL of acetonitrile was added zinc nitrate hexahydrate (32 mg; 107 µmol) in 10 mL of acetonitrile. The mixture was homogenised with sonication (10 seconds), capped and allowed to stand undisturbed for 5 days. After this time, the pale yellow crystals of the title compound were recovered by filtration. Yield 6.8 mg (45 % based on **L1**); m.p. > 300 °C; Found C, 47.51; H, 2.46; N, 12.38; calculated for $C_{23}H_{15}N_5O_9Zn \cdot 0.5H_2O$ C, 47.64; H, 2.78; N, 12.08 %; v_{max} (ATR, cm⁻¹) 3350w br, 3079w, 1701m, 1662s, 1634s, 1588s, 1547s, 1477s br, 1432w, 1397m, 1384m, 1353m, 1289s sh, 1229m, 1194m, 1180m sh, 1129w, 1088w, 1069m, 1015s, 961s, 924w, 851s, 808w, 785s, 755m, 677w, 634m, 615m. Phase purity was determined by X-ray powder diffraction.

Synthesis of poly-[Zn(L2)₂]·1.5DMF·0.5H₂O 3

In a 7 mL capacity glass vial with Teflon-lined screw cap, **HL2** (10 mg, 24 µmol) and zinc nitrate hexahydrate (14 mg, 47 µmol) were combined in 1 mL DMF. The mixture was homogenised by sonication (10 seconds), sealed, and heated at 100 °C for 4 days. Following this time, the mixture was filtered hot to recover colourless crystals which were washed with DMF and dried in air. Yield 7.7 mg (60 % based on **HL2**); m.p. > 300 °C; Found C, 63.16; H, 3.60; N, 7.39; Calculated for $C_{50}H_{30}N_4O_{10}Zn \cdot 1.5DMF \cdot 0.5H_2O$ C, 63.50; H, 4.06; N, 7.47; v_{max} (ATR, cm⁻¹) 3398w br, 3064m, 2932w, 1703s, 1658s, 1637s, 1586m, 1537s sh, 1370s sh, 1278w, 1232s, 1197w, 1179m sh, 1130w, 1102w, 1085w, 1017m, 972w, 955m, 926w, 858s, 813w, 787m, 756w, 737s, 712m, 652m, 621s. Phase purity was determined by X-ray powder diffraction.

Synthesis of poly-[Cu₃(L2)₄(NO₃)₂]·13H₂O·2DMF 4

In a 7 mL capacity glass vial with Teflon-lined screw cap, HL2 (10 mg, $24 \,\mu$ mol) was combined with copper nitrate hemipentahydrate (6 mg, 25 µmol) and DMF (1 mL). Best results were obtained when using freshly-opened analytical grade or anhydrous DMF for this procedure. The vial was sealed and heated at 100 °C for 8 hours, giving a pure phase of dark green crystals which were isolated by filtration. Yield 7.5 mg (53 % based on HL2). Found C, 53.23; H, 3.39; N, 6.68; Calculated for C₁₀₀H₆₀N₁₀O₂₆Cu₃·13H₂O·2DMF C, 53.30; H, 4.22; N, 7.04 %; v_{max} (ATR, cm⁻¹) 3329w br, 3070w, 2937w, 1702m, 1656s, 1632s, 1587s, 1532m sh, 1513m, 1470w, 1403w, 1376s, 1337s, 1278m, 1233s, 1177s, 1098m, 1017m, 957m sh, 850s, 785s, 756m, 739m, 707w, 617m. The crystals generated by this method were not of sufficient quality for structure determination by single crystal X-ray diffraction; for the diffraction study, the reaction was repeated using 1 mL of a 2:1 N,N-dimethylacetamide:ethanol mixture in place of DMF as the solvent. Although this reaction gave only a small quantity of crystalline material amongst large amounts of amorphous solids, these crystals showed greatly improved diffraction characteristics, and exhibited identical unit cell parameters to those obtained from the reaction with DMF. X-ray powder diffraction confirmed that the two phases were equivalent, differing only in the diffuse lattice solvent contribution. For this reason, the lattice solvent content of 4 is estimated entirely from bulk-phase methods (elemental analysis and TGA) and is not neccesarily expected to correlate with the electron count determined from SQUEEZE.^{S5}

2. X-ray Crystallography

Crystal and refinement data are presented in Table S1. CCDC 1831226-1831230. All datasets were collected on a Bruker APEX-II Duo dual-source instrument using Mo-K α radiation ($\lambda = 0.71073$ Å) for HL2 and complexes 1, 2 and 3, or microfocus Cu-K α radiation ($\lambda = 1.5405$ Å) for complex 4. All datasets were each collected using ω and φ scans. Single crystals were mounted on Mitegen micromounts in NVH immersion oil, and maintained at a temperature of 100 K using a Cobra cryostream. The diffraction data were reduced and processed using the Bruker APEX suite of programs.^{S3} Multi-scan absorption corrections were applied using SADABS.^{S6} The data were solved using the Intrinsic Phasing routine in SHELXT and refined with full-matrix least squares procedures using SHELXL-2015 within the OLEX-2 GUI.^{S7-S9} The functions minimized were $\Sigma w(F_0^2 - F_c^2)$, with $w = [\sigma^2(F_o^2) + aP^2 + bP]^{-1}$, where $P = [max(F_o)^2 + 2F_c^2]/3$. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions and refined with a riding model, with isotropic displacement parameters equal to either 1.2 or 1.5 times the isotropic equivalent of their carrier atoms. Specific refinement strategies are further outlined in the combined crystallographic information file (cif). The structures of HL2, complex 2 and complex 3 were refined to convergence with minimal restraints, only requiring DFIX and U_{ii} restraints for slight disorder of lattice DMF molecules or nitrato ligands. In complex 1, rotational disorder of a naphthalimide group was present and manifest as positional disorder of of the pyridone rings, which were fixed at a 2:1 ratio after free variable refinement suggested this distribution, and the lower occupancy of the two rings was constrained with an AFIX rigid hexagon constraint to maintain a reasonable geometry. One water molecule, split over three positions, was located within the lattice; while the oxygen sites could be modelled with an isotropic model, no reasonable position for the 6 1/3 occupancy hydrogen atoms could be ascertained; these were added to the crystallographic formula but not modelled explicitly.

In complex **4**, a similar rotational disorder was evident on one of the naphthalimide groups, however in this instance (probably due to anchoring of the pyridone oxygen atom by coordination) the naphthalimide carbon atoms were not coincident and required splitting of 20 non-hydrogen atoms in the C33-C50 fragment. Distance (DFIX and SIMU) and U_{ij} (RIGU) restraints were required to maintain appropriate chemical geometries, and a rigid hexagon AFIX constraint was employed for one of the two orientations of the pyridone ring. After modelling the framework atoms from the Fourier residuals and accounting for disorder, no further chemical species could be identified from the remaining residuals, and the diffuse electron density contribution was modelled with SQUEEZE.^{S5} The electron count provided, 316 electrons per Cu₃ formula unit, is higher than the *ca*. 210 electrons expected from supporting methods. However, as discussed in the text, the crystal used for single crystal measurements was prepared from a different solvent mixture than the pure bulk phase crystals used for other measurements (2:1 DMA/EtOH instead of DMF), so this discrepancy is not surprising.

Identification	HL2	1	2	3	4
Empirical		C48H39AgF6N6	C24H165N55O9		C100H60Cu3N10
formula	C ₂₈ H ₂₃ N ₃ O ₆	O ₉ Sb	Zn	C53H37N5O11Zn	O26
Formula weight	497.49	1187.47	591.3	985.24	2008.2
Temperature/K	100	100	100	100	100
Crystal system	monoclinic	monoclinic	triclinic	monoclinic	monoclinic
Space group	$P2_{1}/c$	C2/c	<i>P</i> -1	C2/c	C2/c
a/Å	10.0464(7)	39.611(2)	9.4661(14)	20.3079(18)	13.6882(7)
b/Å	17.5471(12)	8.5088(4)	10.7897(16)	17.8201(16)	34.3485(17)
c/Å	13.5425(9)	27.5544(15)	13.170(2)	12.0220(11)	26.2844(15)
α/°	90	90	69.199(2)	90	90
β/°	106.5660(10)	93.3010(10)	83.790(3)	91.431(2)	90.286(4)
γ/°	90	90	72.466(2)	90	90
Volume/Å ³	2288.2(3)	9271.5(8)	1199.0(3)	4349.3(7)	12358.0(11)
Z	4	8	2	4	4
pcalcg/cm ³	1.444	1.701	1.638	1.505	1.079
µ/mm⁻¹	0.103	1.094	1.092	0.639	1.135
F(000)	1040	4744	602	2032	4100
Crystal	0.32 imes 0.2 imes	0.12 imes 0.11 imes	0.13 imes 0.09 imes	0.12 imes 0.11 imes	0.17 imes 0.1 imes
size/mm ³	0.18	0.02	0.08	0.11	0.06
Radiation	$MoK\alpha (\lambda = 0.71073)$	$MoK\alpha (\lambda = 0.71073)$	$MoK\alpha (\lambda = 0.71073)$	MoK α ($\lambda = 0.71073$)	$CuK\alpha (\lambda = 1.54178)$
2\Overlap range for data collection/°	3.904 to 55.99	3.508 to 52.774	3.308 to 50.99	3.04 to 54.972	5.146 to 136.412
	$-13 \le h \le 13, -$	$-49 \le h \le 49, -8$	-11 ≤ h ≤ 11, -	$-26 \le h \le 26, -$	$-15 \le h \le 16, -$
Index ranges	$23 \le k \le 23, -$	\leq k \leq 10, -34 \leq	$13 \le k \le 13, -$	$23 \le k \le 23, -$	$36 \le k \le 41, -$
	$17 \le l \le 15$	$l \leq 34$	$15 \le l \le 14$	$15 \le l \le 13$	$29 \le l \le 31$
Reflections collected	33206	30813	12163	31047	28751
.	5515 [R _{int} =	9481 [R _{int} =	4455 [R _{int} =	4984 [R _{int} =	$11035 [R_{int} =$
Independent	0.0437, R _{sigma}	$0.0751, R_{sigma} =$	$0.0656, R_{sigma} =$	$0.0495, R_{sigma} =$	$0.0612, R_{sigma} =$
reflections	= 0.0317]	0.0911]	0.1024]	0.0364]	0.0803]
Reflections Observed [I>=2σ (I)]	4221	5824	2456	3936	5698
Data/restraints/p arameters	5515/0/340	9481/37/698	4455/12/392	4984/17/333	11035/358/778
Goodness-of-fit on F ²	1.017	1.008	0.988	1.034	1.009
Final R indexes	$R_1 = 0.0435,$	$R_1 = 0.0541,$	$R_1 = 0.0598,$	$R_1 = 0.0420,$	$R_1 = 0.0803,$
$[I \ge 2\sigma(I)]$	$wR_2 = 0.0973$	$wR_2 = 0.1026$	$wR_2 = 0.1378$	$wR_2 = 0.0983$	$wR_2 = 0.2281$
Final R indexes	$R_1 = 0.0649,$	$R_1 = 0.1112,$	$R_1 = 0.1300,$	$R_1 = 0.0611,$	$R_1 = 0.1292,$
[all data]	$wR_2 = 0.1079$	$wR_2 = 0.1208$	$wR_2 = 0.1632$	$wR_2 = 0.1075$	$wR_2 = 0.2657$
Largest diff. peak/hole / e Å ⁻³	0.44/-0.28	1.36/-1.36	0.70/-0.52	0.71/-1.07	0.50/-0.44
CCDC No.	1831226	1831227	1831228	1831229	1831230

 Table S1 Crystal and refinement parameters for all structures

3. X-ray Powder Diffraction



Figure S1 X-ray powder diffraction pattern for complex **1** (blue, measured at room temperature) compared to the pattern simulated from single-crystal data (Red, 100 K)



Figure S2 X-ray powder diffraction pattern for complex **2** (blue, measured at room temperature) compared to the pattern simulated from single-crystal data (Red, 100 K)



Figure S3 X-ray powder diffraction pattern for complex **3** (blue, measured at room temperature) compared to the pattern simulated from single-crystal data (Red, 100 K)



Figure S4 X-ray powder diffraction pattern for complex **4** (blue, measured at 100 K) compared to the pattern simulated from single-crystal data (Red, 100 K) and the measured pattern from the MeOH-exchanged and air-exposed sample (green, room temperature)

4. Thermogravimetric Analysis



Figure S5 Thermogravimetric analysis trace for complex 1



Figure S6 Thermogravimetric analysis trace for complex 2



Figure S7 Thermogravimetric analysis trace for complex 3



Figure S8 Thermogravimetric analysis trace for complex **4** freshly isolated (blue) and following solvent exchange with MeOH (red).

5. Spectroscopic Data

The photoluminescence quantum yield for **L1** was determined by comparison with quinine sulfate (2M sulfuric acid, $\Phi = 0.546$).^{S10,S11} Absorbance (366 nm) and integrated emission (380 – 600 nm), were measured across a range of concentrations and plotted (Figure S9), and the quantum yield of the unknown was given by the following relation, where η is the refractive index of each solvent. Emission and excitation slits were held at 2.5 nm for all measurements.

 $\Phi_{\text{unknown}} = \Phi_{\text{standard}} (\text{Grad}_{\text{unknown}}/\text{Grad}_{\text{standard}}) (\eta^2_{\text{standard}}/\eta^2_{\text{unknown}})$

The measurements were carried out in quadruplicate and the average value of Φ , 0.29, is reported. The standard deviation of the four values was 0.027, providing good agreement within the accepted margin of error of $\pm 10\%$.



Figure S9 Comparative absorbance versus integrated emission plots for L1 compared to quinine sulfate



Figure S10 Overlaid absorption (black) and excitation (red, $\lambda_{em} = 450$ nm) spectra of L1 (CHCl₃, 9 μ M)

6. Additional Gas Adsorption Data

Isosteric Heat of Adsorption Calculations

The heat of adsorption of CO₂ for complex **4** was estimated by least-squares fitting of a virial thermal adsorption equation^{S12,S13}, modelling Ln(P) as a function of gas adsorbed. Datapoints were collected at 278, 288 and 298 K. The model function takes the form $ln(P) = \{ln(N) + (a_0 + a_1N + a_2N^2)/T + b\}$, where N represents the surface excess adsorption (mmol) at temperature T and a_0 , a_1 and a_2 are coefficients determined through least-squares fitting. The original parameter set of 5 parameters was sequentially reduced to maximise the data:parameter ratio. The enthalpy of adsorption is then given by the relation $Q(N) = -R(a_0 + a_1N + a_2N^2)$. Optimised coefficients and parameters are given below.

Table S2 Fitting parameters for CO₂ enthalpy of adsorption calculation

Temperatures (K)	278, 288, 298
a_0	-2699.23
a_1	67.6842
a_2	-2.19355
В	12.93888
\mathbb{R}^2	0.9989
Datapoints fitted	63



Figure S11 Calculated isosteric heat of adsorption of CO₂ for compound 4 as a function of loading.

BET summary				
Slope =	13.650			
Intercept =	-6.765e-02			
Correlation coefficient, $r = 0.999612$				
C constant=	-200.770			
Surface Area =	256.402 m²/g			

Table S3 Summary of BET isotherm parameters for compound 4 (N_2 , 77 K)



Figure S12 BET transformed isotherm plot for compound 4 (N_2 , 77 K).



Figure S13 ¹H NMR spectrum of L1 (400 MHz, d₆-DMSO)



Figure S14 13 C NMR spectrum of L1 (100 MHz, d₆-DMSO)



Figure S15 ¹H NMR spectrum of HL2 (400 MHz, d₆-DMSO)



Figure S16¹³C NMR spectrum of HL2 (100 MHz, d₆-DMSO)

8. References

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