Supplementary Information for

Framework-Flexibility Driven Selective Sorption of *p*-Xylene Over Other Isomers by a Dynamic Metal-Organic Framework

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Experimental Section:

Materials: All the reagents and solvents were commercially available and used as received, without further purification.

Synthesis of $\{[Zn_4O(L)_3(DMF)_2].xG\}_n$ (1⊃G): A mixture of H_2L (40 mg, 0.1 mmol), $Zn(NO_3)_2.6H_2O$ (29.7 mg, 0.1 mmol), DMF (1 mL) and 1-butanol (1 mL) was placed in a teflon capped glass vial. This was heated at 90 °C for 48h and then cooled to room temperature for 1day. Growth of colorless block-shaped crystals was observed upon cooling to RT, the desired product **1⊃G** appeared in ~ 72% yield.

Dehydrated phase **$Zn_4O(L)_3]_n$ (1)**: Shiny single crystals of **1⊃G** were heated at 160 °C under reduced pressure for 8h, to obtain the slightly pale colorless dehydrated crystals of compound **1**.

Resolvated phase **$\{[Zn_4O(L)_3(DMF)_2].(C_8H_{10})\}_n$ (1⊃PX'):** Colorless Single Crystals of **1⊃PX'** were obtained on exposing the crystals of **1** to the vapor of a solution of *p*-Xylene (2 mL) and DMF (1 mL) for 72h, without allowing any disturbance of the system.

Physical measurements: Powder X-ray diffraction (PXRD) patterns were measured on Bruker D8 Advanced X-Ray diffractometer at room temperature using Cu-Kα radiation (λ= 1.5406 Å) with a scan speed of 0.5° min^{-1} and a step size of 0.01° in 2 *theta*. Thermogravimetric analysis results were obtained in the temperature range of 30-600 ºC on Perkin-Elmer STA 6000 analyzer under N_2 atmosphere, at a heating rate of 10 ºC min^{-1}, The Fourier transform (FT-IR) infra-red spectra were recorded on NICOLET 6700 FT-IR Spectrophotometer using KBr Pellets.

X-ray Structural Studies: Single-crystal X-ray data of compound **1⊃G** and **1** were collected at 200K on a Bruker KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 30 mA) using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å), mounting on nylon CryoLoops (Hampton Research) with Paraton-N (Hampton Research) oil. Single-crystal X-Ray data of compound **1⊃PX'** crystals was collected at 100K on a Bruker KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 1 mA) using graphite-monochromated Cu Kα radiation (λ = 1.5418Å), mounting on nylon CryoLoop (Hampton Research) with Paraton-N (Hampton Research) oil. The data integration and reduction were processed with SAINT[S2] software. A multi-scan absorption correction was applied to the collected reflections. The structures were solved by the direct method using SHELXTL[S3] and were refined on F^2 by full-matrix least-squares technique using the SHELXL-97[S4] program

package within the WINGX[S5] programme. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were located in successive difference Fourier maps and they were treated as riding atoms using SHELXL default parameters. The structures were examined using the *Adsym* subroutine of PLATON[S6] to assure that no additional symmetry could be applied to the models. Tables S1, S2 and S3 contain crystallographic data for the compounds **1⊃G**, **1** and **1⊃PX** respectively.

Low Pressure Gas Sorption Measurements:- Low pressure gas and solvent sorption measurements were performed using BelSorpmax (Bel Japan). The sorption-recyclability experiments were recorded in BelAqua (Bel Japan). All the gases used were of 99.999% purity. As-synthesized crystals of compound **1⊃G** were heated at 180 °C under vacuum for 24 h, to get guest-free crystals of compound **1**. Prior to adsorption measurement, the guest free sample **1** was pretreated at 170 °C under vacuum for 2 h, using BelPrepvacII, and purged with N_2 on cooling.

Solvent exposure study: Crystalline solid powder of compound **1** taken in smaller glass vials were kept open inside larger capped closed glass vials containing different guest solvents (benzene, toluene, cyclohexane, *o*-xylene, *m*-xylene and *p*-xylene respectively) over a period of 48h to allow vapor-phase exposure of solvents and characterized by PXRD.

Synthesis of ligand (H_2L):- The asymmetric dicarboxylic acid ligand 4,4'-((4-(tert-butyl)-1,2-phenylene)bis(oxy))dibenzoic acid (**H_2L**) is synthesized in two steps according to the following reaction protocol:

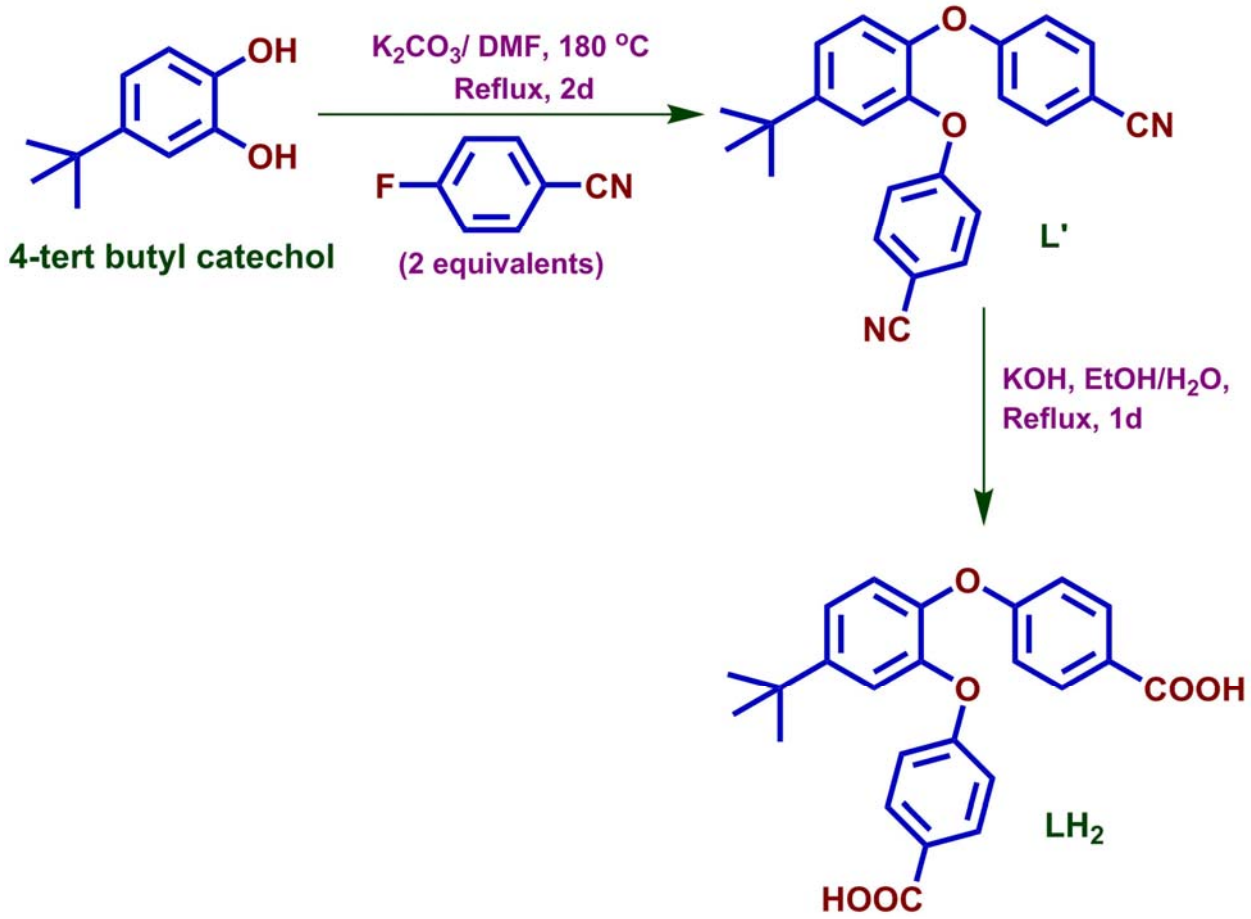

Figure S1: Synthesis of ligand LH_2 via intermediate L'.

Synthesis of Intermediate L'. 4-tert-butyl catechol (11 g, 0.0662 mole), 4-fluorobenzonitrile (16.029 g, 0.1324 mole) and potassium carbonate (~27.6 g, 0.2 mole) were refluxed at 180 °C in a mixture of N, N-dimethylformamide (DMF) and *p*-xylene (110 mL/55ml) for 2days. After cooling the reaction mixture to r.t., it was poured into ~100mL ice-cold water, followed by acidification with dil. HCl until pH~3. The reaction mixture was evaporated to dryness (maximum amount as possible) by rotary evaporation under reduced pressure, to get a reddish yellow product. This was extracted with Ethyl acetate (2 × 250mL), washed with brine/water

(twice each) and the resultant EtOAc layer was dried over anhydrous Na_2SO_4. Evaporation of this EtOAc layer, followed by drying under high vacuum yielded the intermediate compound L'.

Yield: 23.28 g, 95.48%. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 7.55-7.51 (m, 4H), 7.33 (dd, J=8.24 Hz, J= 2.28 Hz, 1H), 7.22 (d, J=2.28Hz, 1H), 7.14 (d, J=8.28Hz, 1H), 6.82-6.77 (m, 4H), 1.34 (s, 9H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ(ppm) : 161.1, 151.2, 145.2, 143.4, 134.2, 124.21, 122.9, 120.7, 119, 116.8, 106, 35, 31.5 ; HRMS (ESI) Calcd. for $C_{24}H_{20}N_2O_2$ 369.160 $[M+H]^+$, found 369.160 (Figures S3, S4 and S5).

Synthesis of ligand LH_2. A mixture of L' (10g, 0.0271 mole) and potassium hydroxide (9.138g, 0.163 mole) was refluxed in 200 mL water/ ethanol (1:1) solvent mixture for 1day. After the reaction mixture was allowed to cool to r.t., it was acidified by dil. HCl keeping on an ice bath till pH~1. The crude material that precipitated out was recrystallized from hot EtOH/water to get colorless crystalline product LH_2.

Yield: 9.56 g, 86.66%. ^{1}H NMR (400 MHz, DMSO-d_6) δ(ppm):7.87-7.84 (m, 4H), 7.36 (dd, J=8.7 Hz, J=2.28 Hz, 1H), 7.30 (d, J=2.28Hz, 1H), 7.22 (d, J=8.68Hz, 1H),6.87-6.83 (m, 4H), 1.29 (s, 9H) ; ^{13}C NMR (100 MHz, DMSO-d_6) δ(ppm): 167.1, 161.0, 150, 145.5, 144, 131.9, 125.3, 123.8, 122.6, 120.5, 116.4, 34.8, 31.4 : HRMS (ESI) Calcd. for $C_{24}H_{22}O_6$ 429.131$[M+Na]^+$, found 429.130 (Figures S6, S7 and S8).

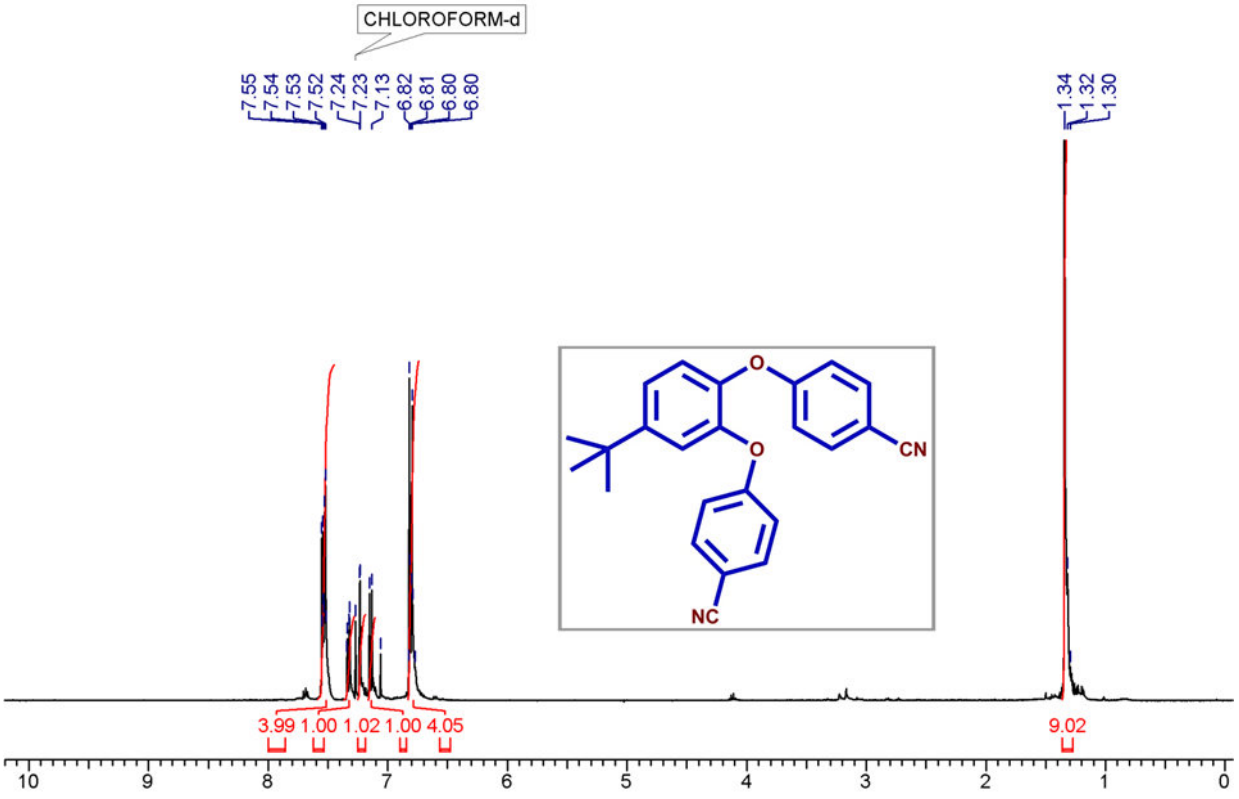

Figure S2: ^{1}H NMR spectrum of Ligand L'.

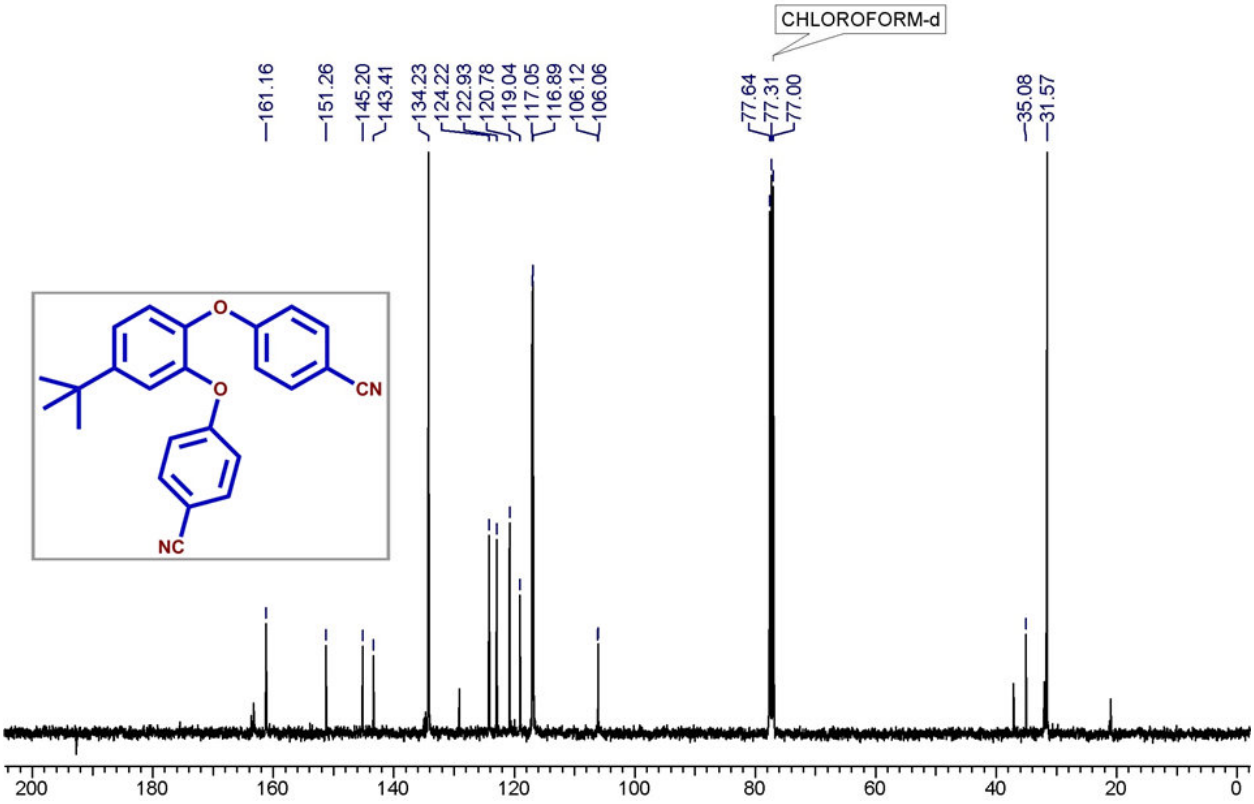

Figure S3: ^{13}C NMR spectrum of Ligand L'.

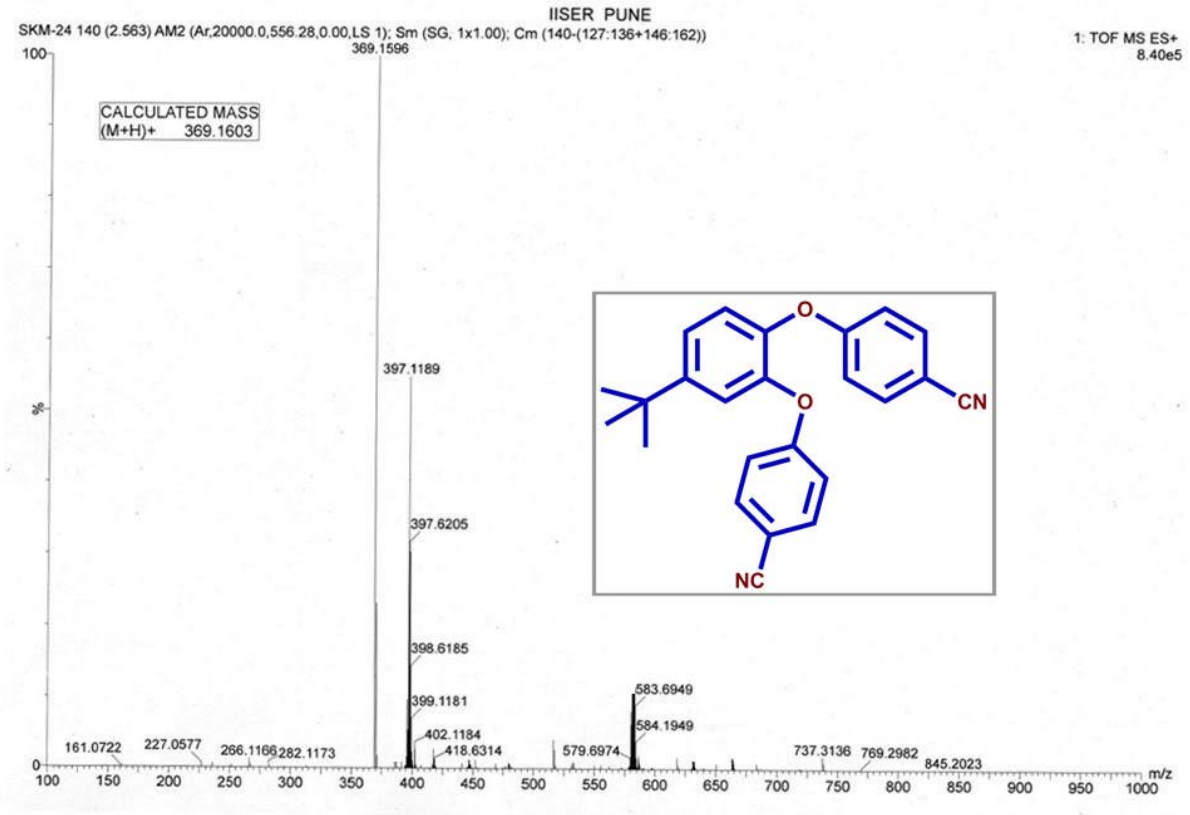

Figure S4: HRMS spectrum of Ligand L'.

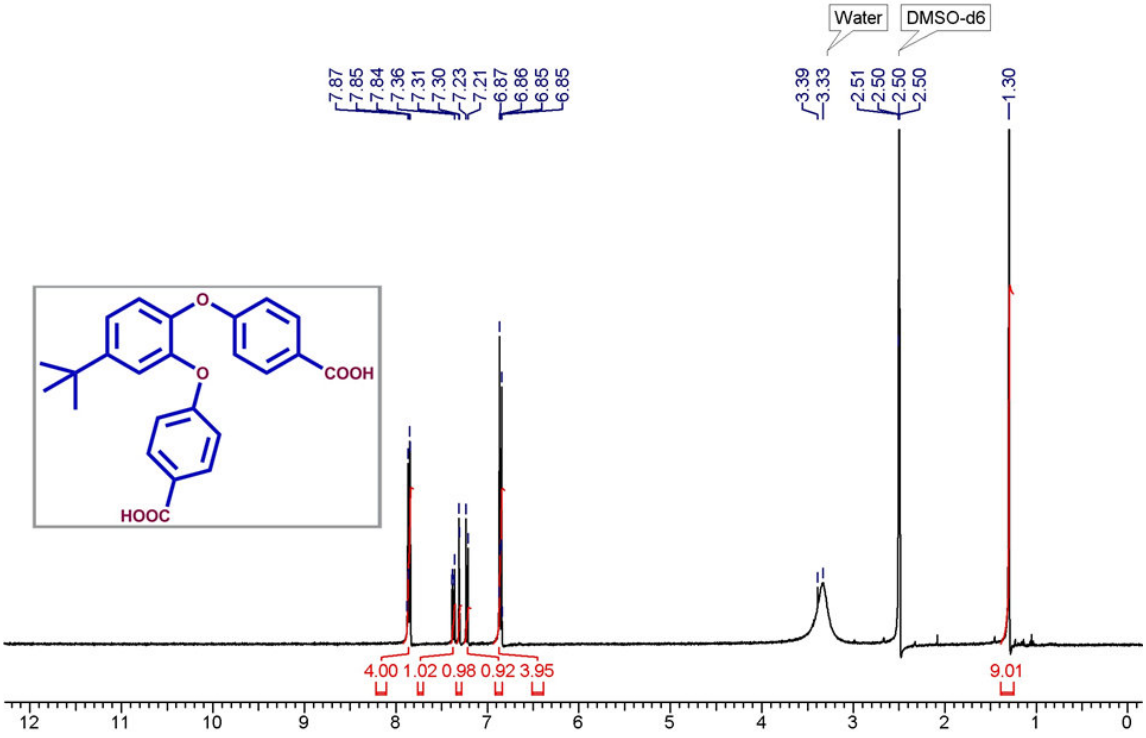

Figure S5: ^{1}H NMR spectrum of Ligand H_2L.

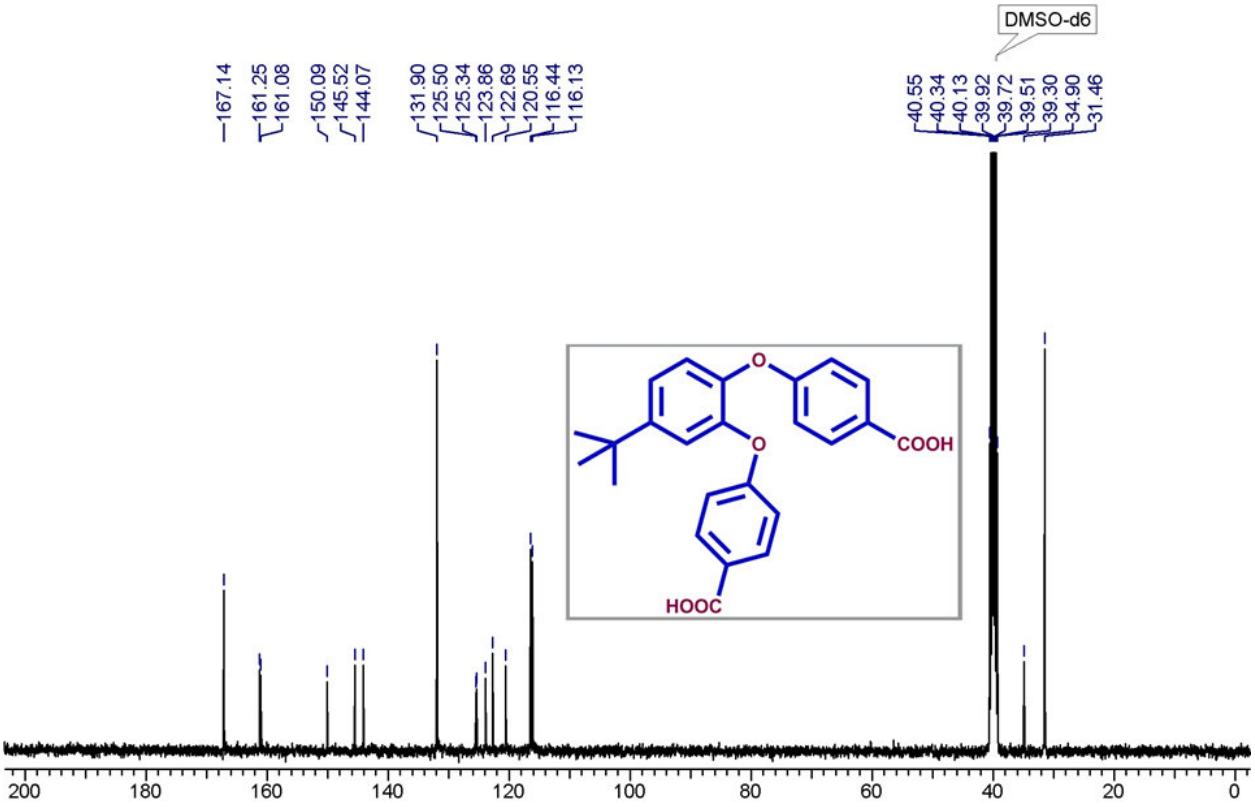

Figure S6: ^{13}C NMR spectrum of Ligand H_2L.

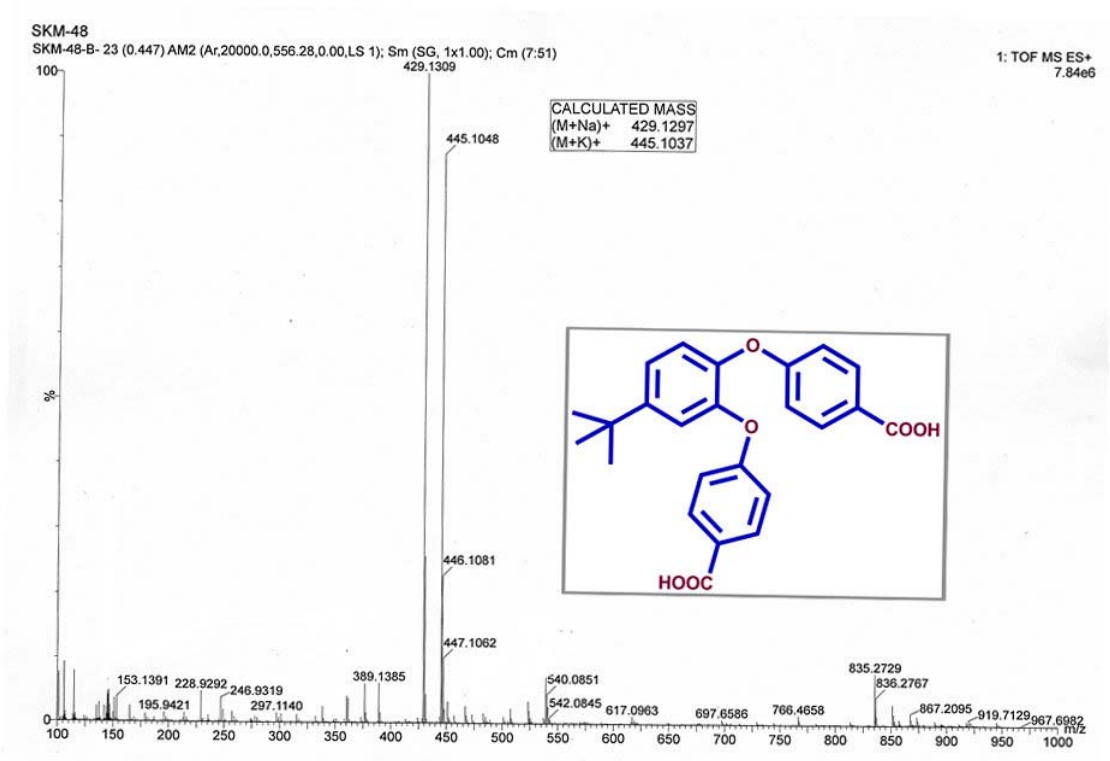

Figure S7: HRMS spectrum of Ligand H_2L.

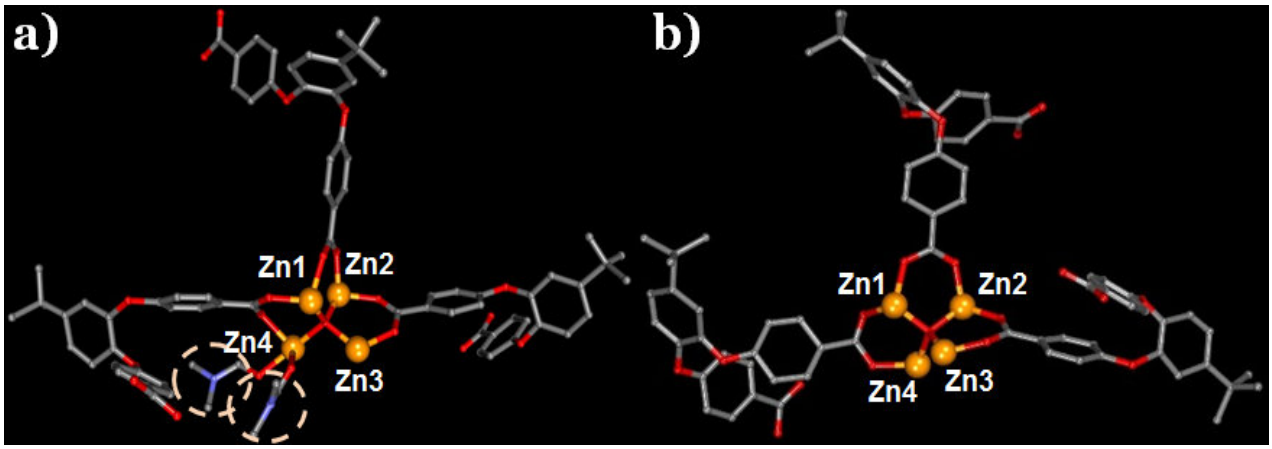

Figure S8: Asymmetric unit of the two phases: a) as-synthesized phase **1⊃G**; b) desolvated phase **1**; DMF molecules coordinated to Zn4 to make its environment octahedral are shown by dashed circle (water molecules are omitted for clarity for a)).

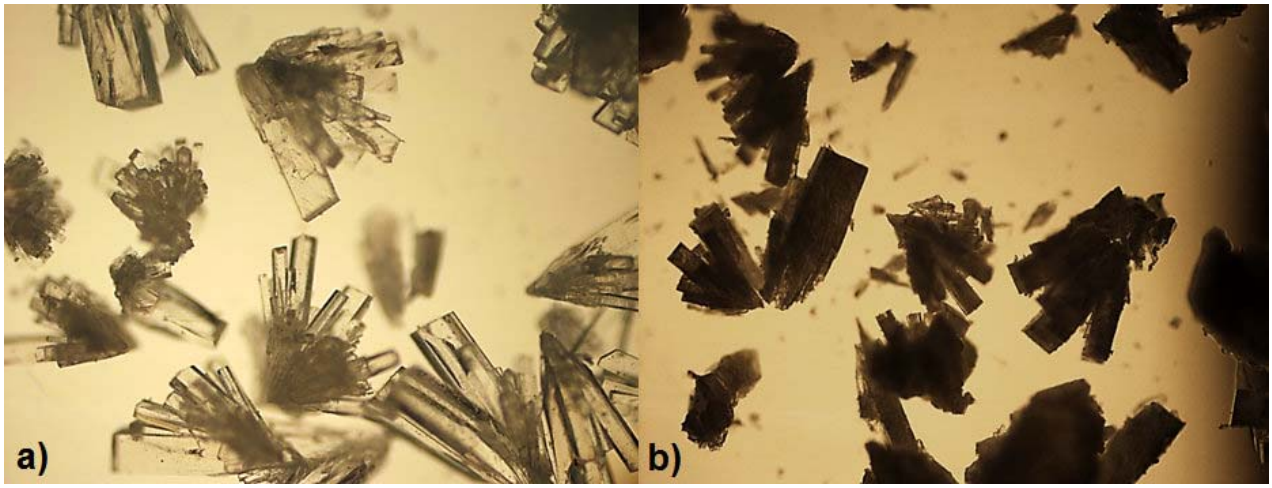

Figure S9: Microscopy images of the crystals for two different SCSC phases: a) compound **1⊃G** (as synthesized), b) compound **1** (desolvated).

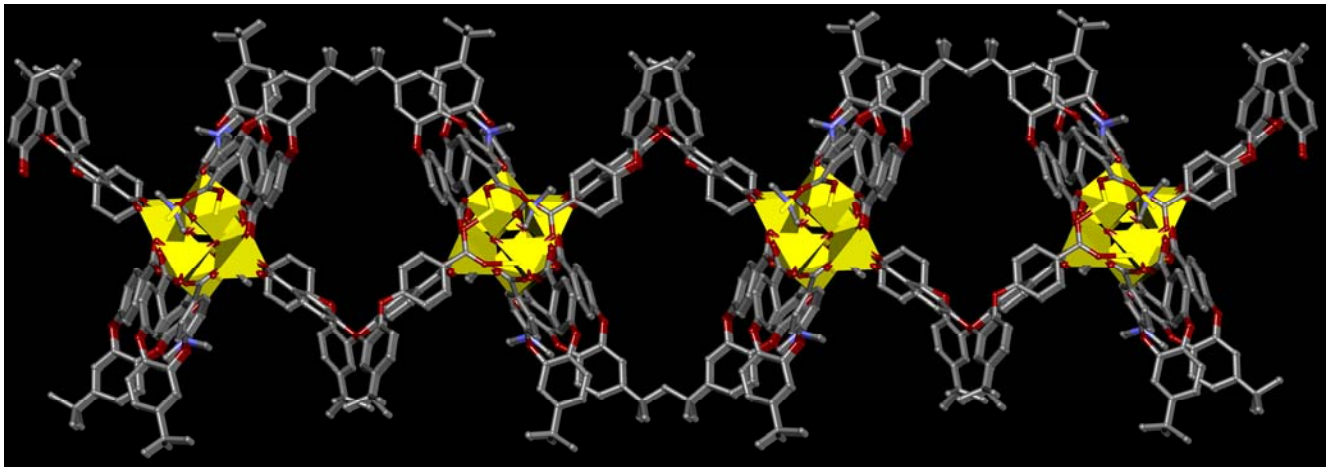

Figure S10: Progression of a single 2D-sheet (along *c*-axis) for the phase **1⊃G**.

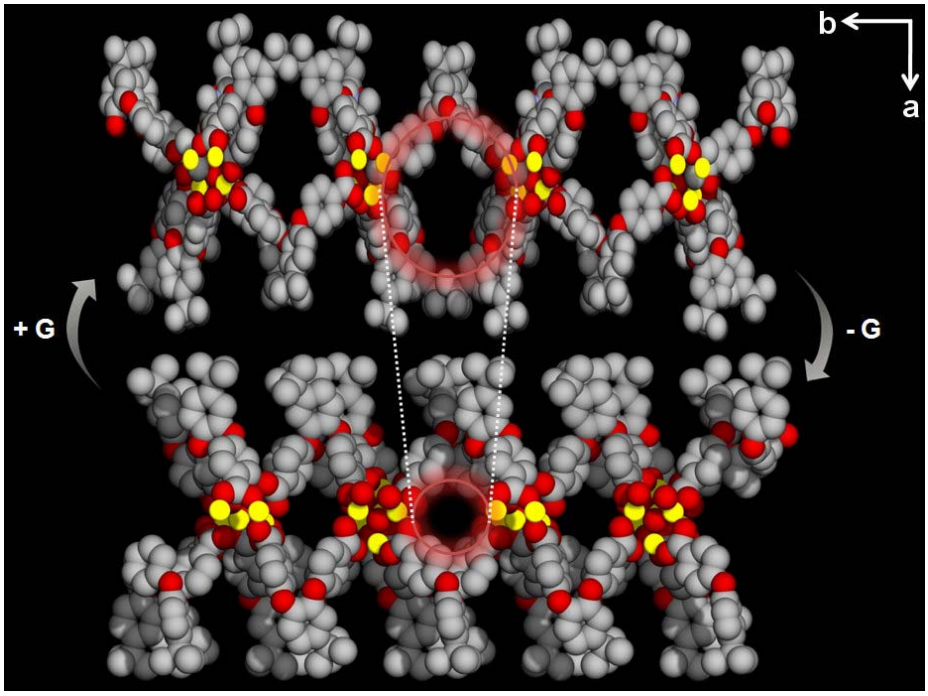

Figure S11: Squeezing of the channels of the single 2D-sheets (along *c*-axis) for the phases **1⊃G** and **1**.

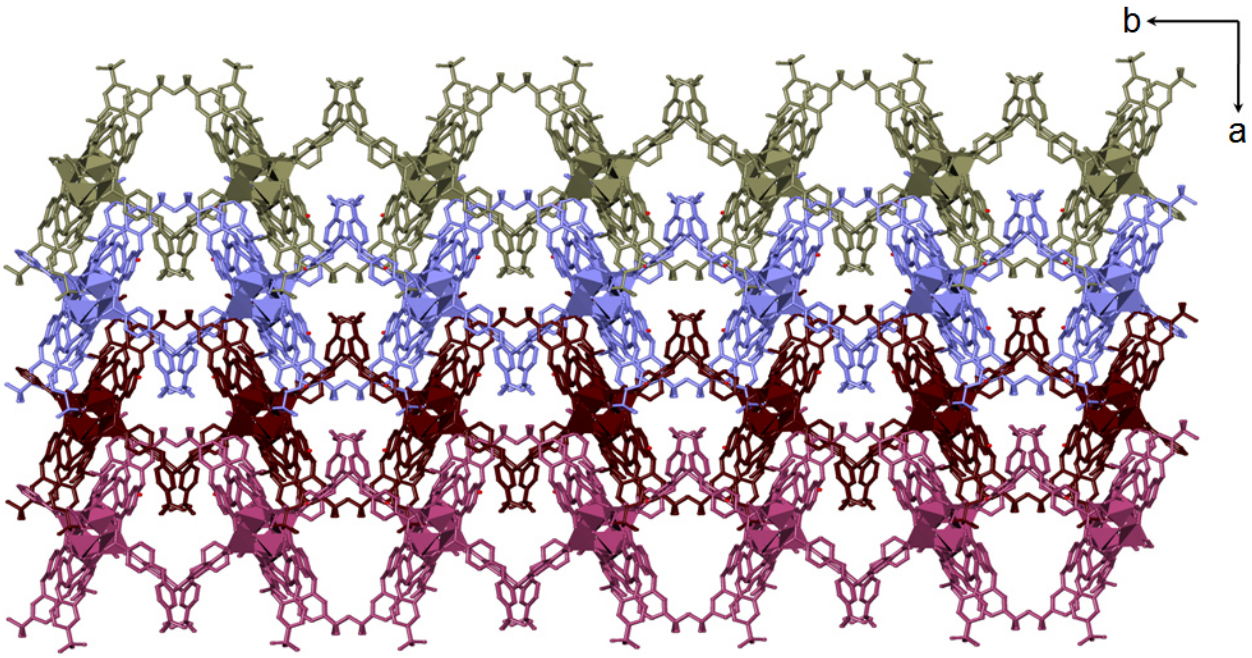

Figure S12: Perspective view along *c*-axis for the as-synthesized phase **1⊃G** (each color representing a 2D-sheet).

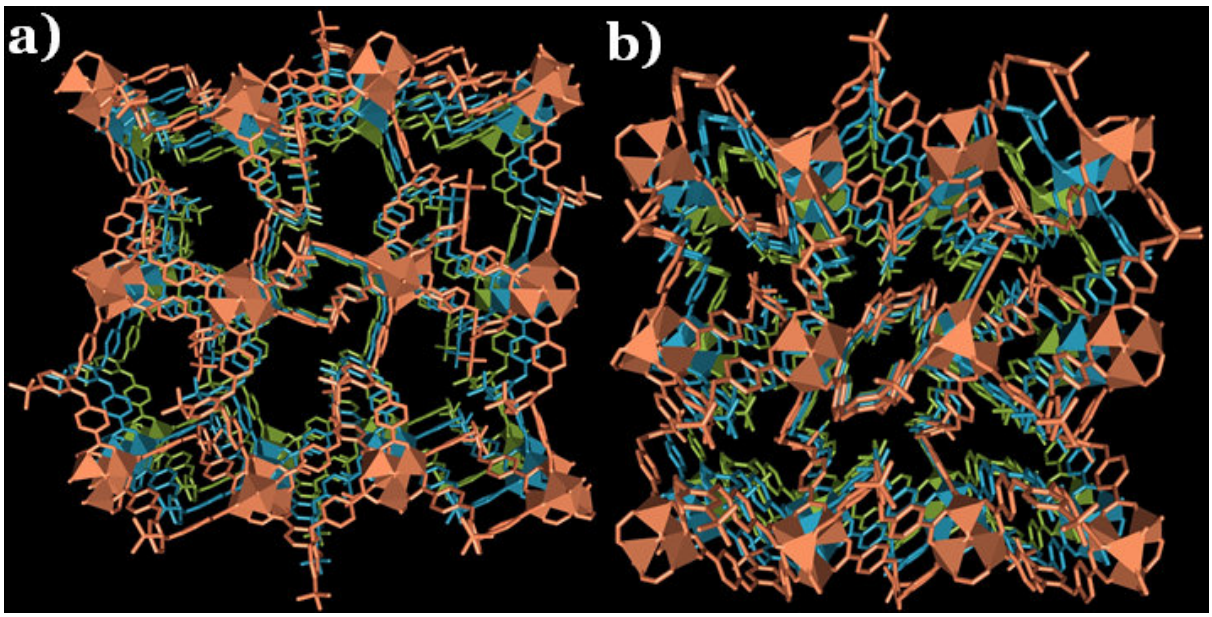

Figure S13: Perspective view along *a*-axis for the two phases: a) as-synthesized phase **1⊃G**; b) desolvated phase **1** (three nets shown in different colors) (guest molecules omitted for clarity).

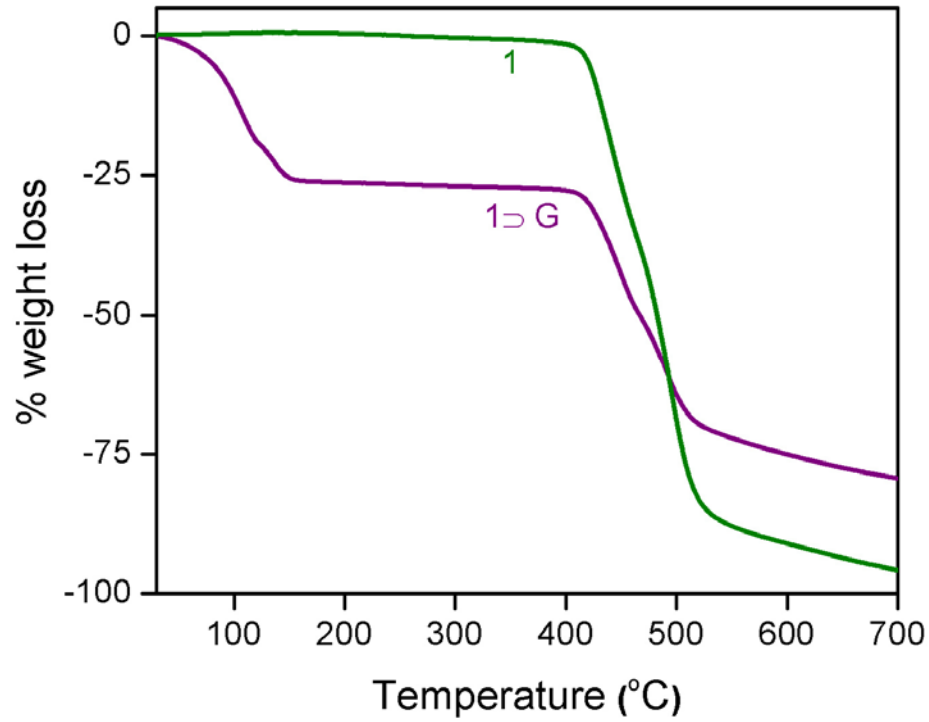

Figure S14: Thermogravimetric analysis (TGA) plots for the as-synthesized (**1⊃G**; purple color) and desolvated (**1**; olive color) compounds.

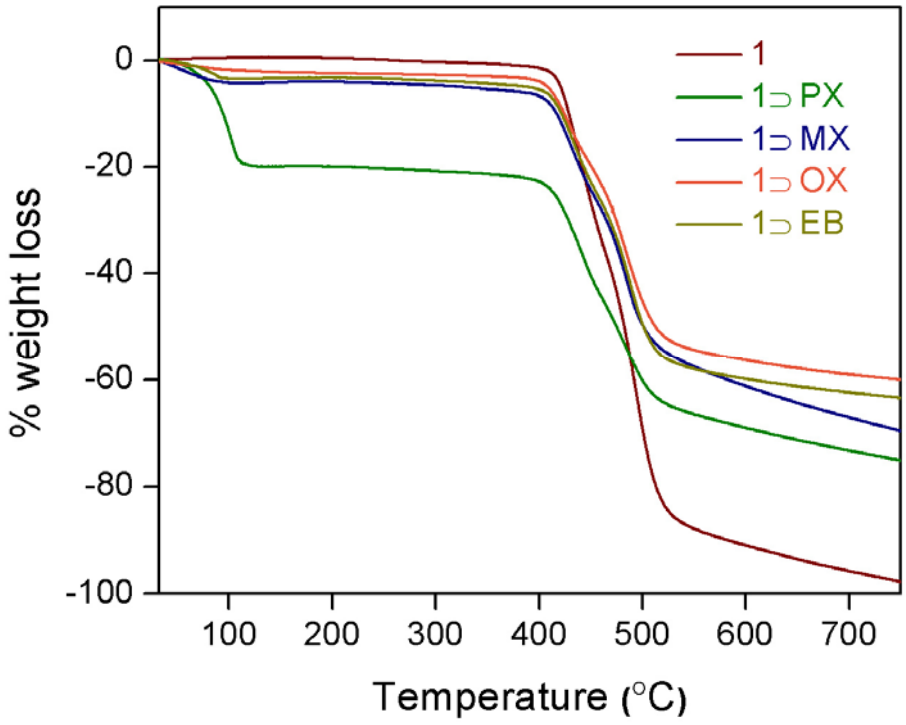

Figure S15: TGA plots for the guest-exposed phases of **1** (**1⊃ solvent**), compared with that of **1** (wine). Vapour of solvents like ***p*-xylene** (olive), ***m*-xylene** (orange), ***o*-xylene** (navy) and **ethyl benzene** (dark yellow) were exposed.

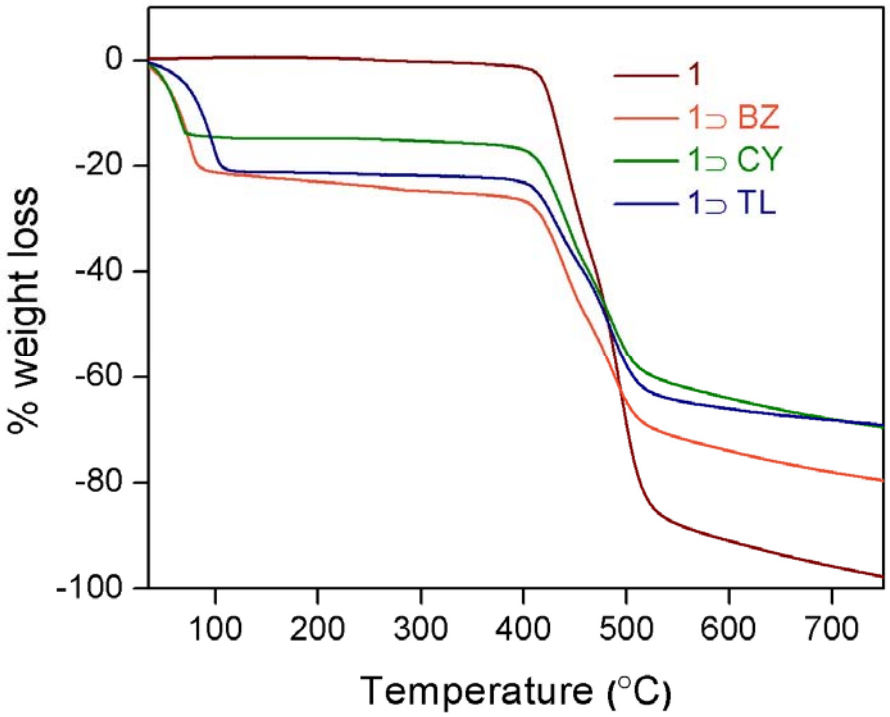

Figure S16: TGA plots for the guest-exposed phases of **1** (**1⊃ solvent**), compared with that of **1** (wine). Vapour of solvents like **Benzene** (orange), **Toluene** (olive), and **cyclohexane** (royal blue) were exposed.

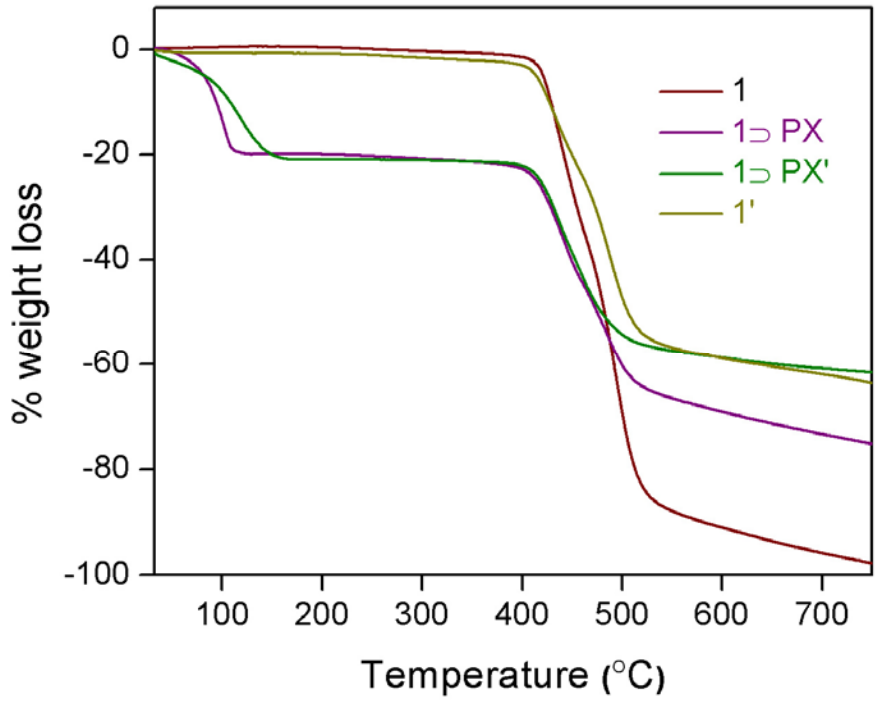

Figure S17: TGA plots for desolvated phase **1** (wine), compared with that of PX-exposed sample **1⊃PX** (purple), crystals **1⊃PX'**, along with the heated (redesolvated) phase **1'**.

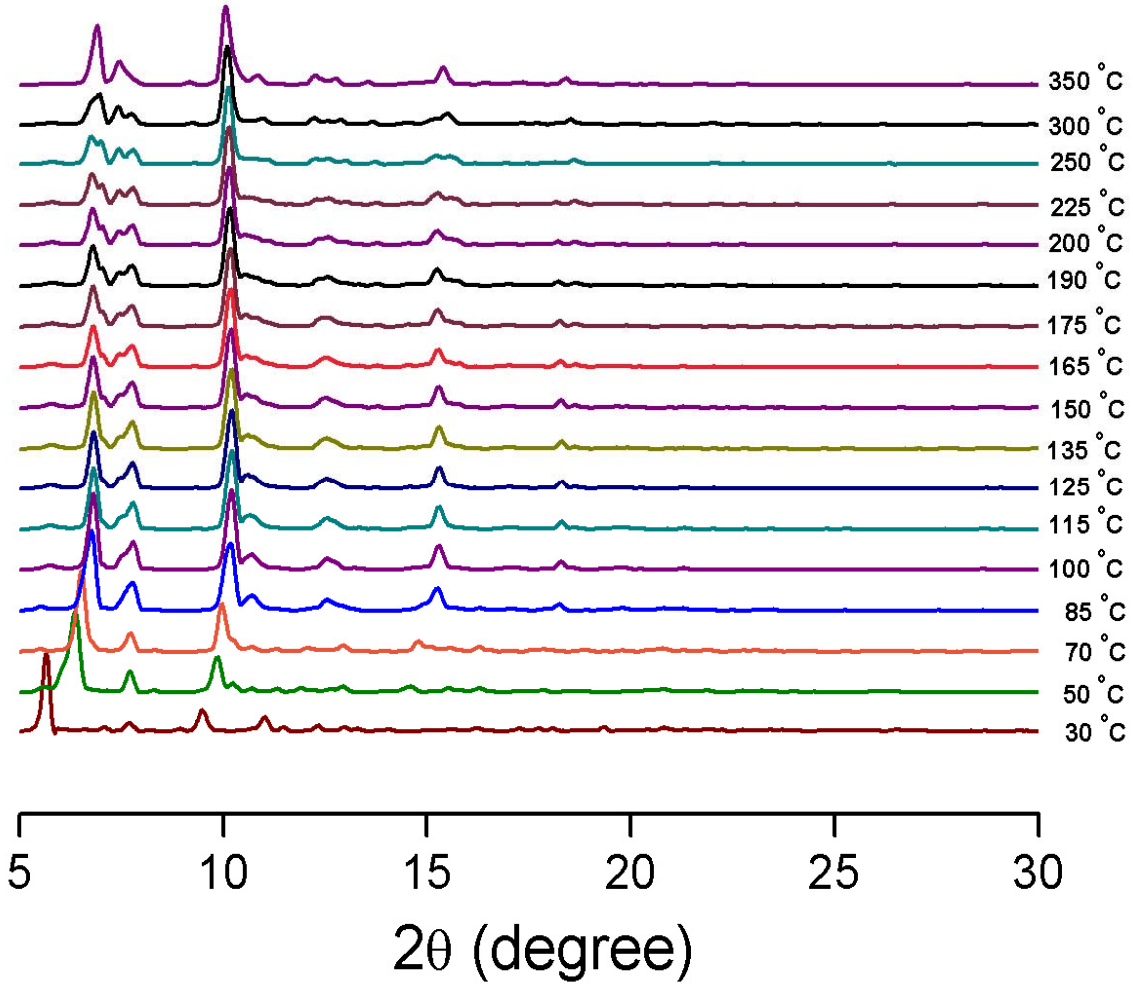

Figure S18: Variable temperature powder X-ray diffraction (PXRD) patterns of compound **1⊃G**.

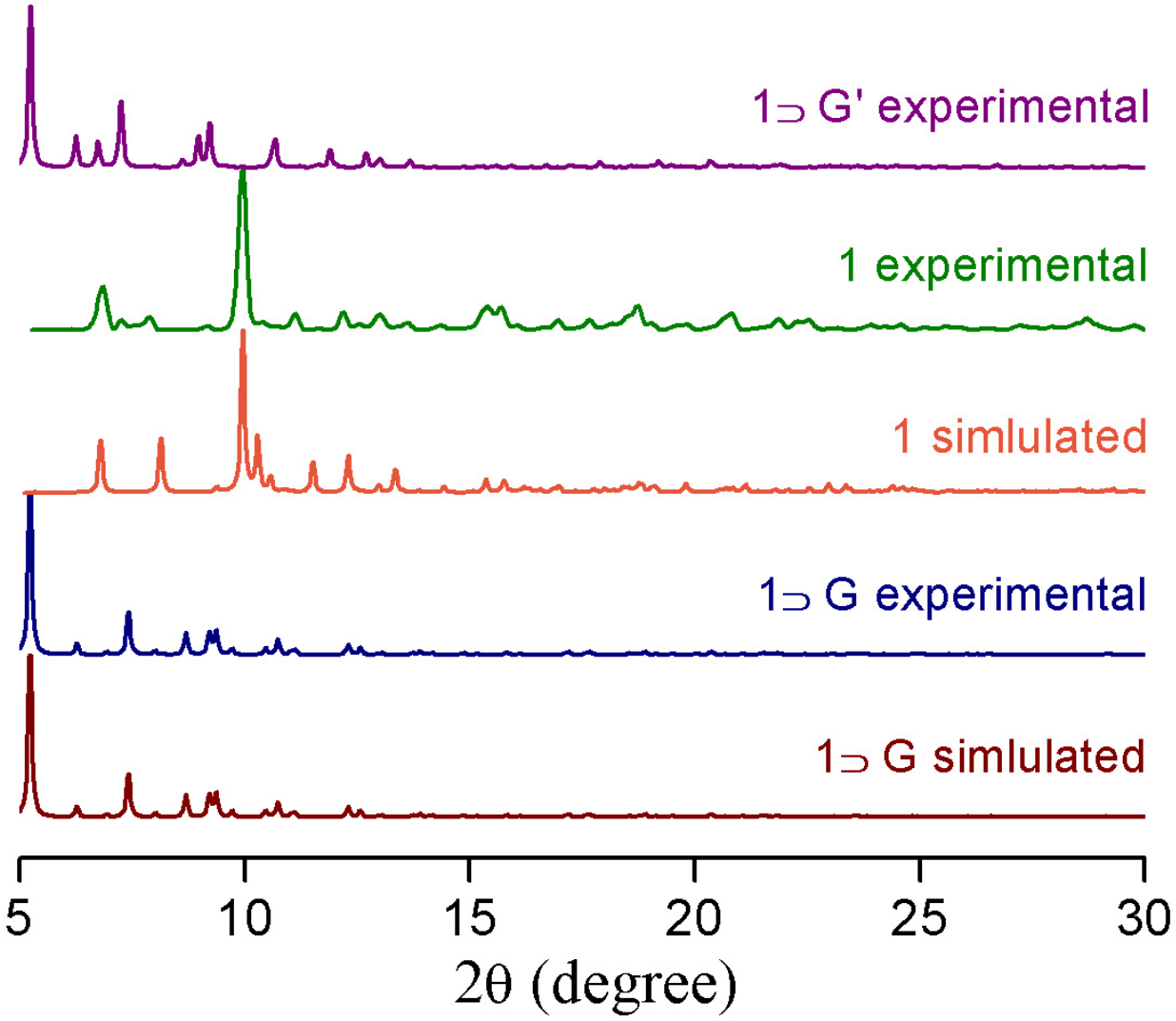

Figure S19: Powder X-ray diffraction (PXRD) patterns of compounds **1⊃G**, **1** and **1⊃G′**.

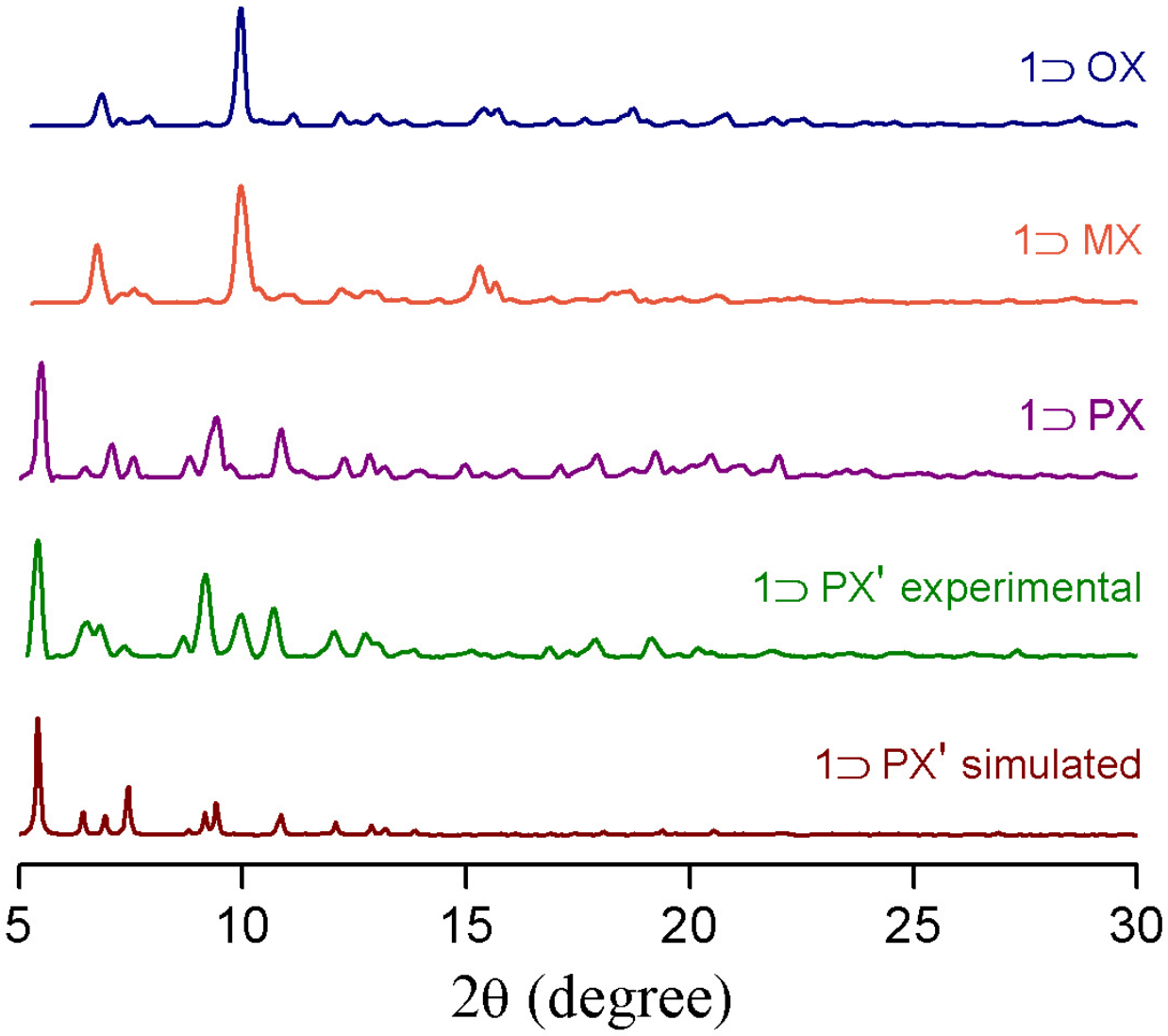

Figure S20: Simulated and experimental PXRD patterns of **1⊃PX'**, and experimental PXRD patterns for three different solvent exposed samples (**1⊃solvent**): **PX** (*p*-xylene), **MX** *(m*-xylene), **OX (***o*-xylene).

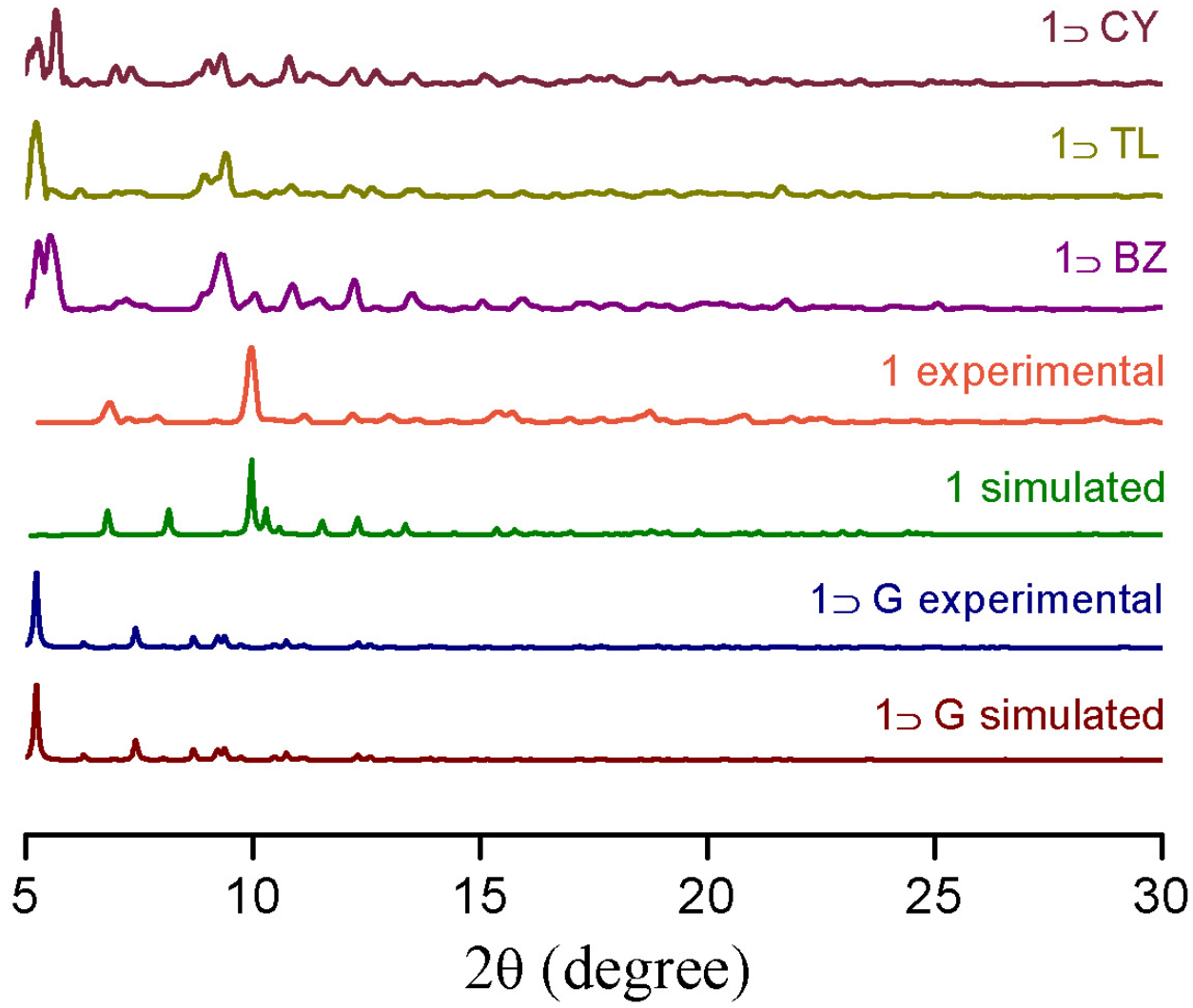

Figure S21: Simulated and experimental PXRD patterns of **1⊃G** and **1**, and experimental PXRD patterns for different solvent exposed samples (**1⊃solvent**); **BZ** (benzene), **TL** (toluene), and **CY** (cyclohexane).

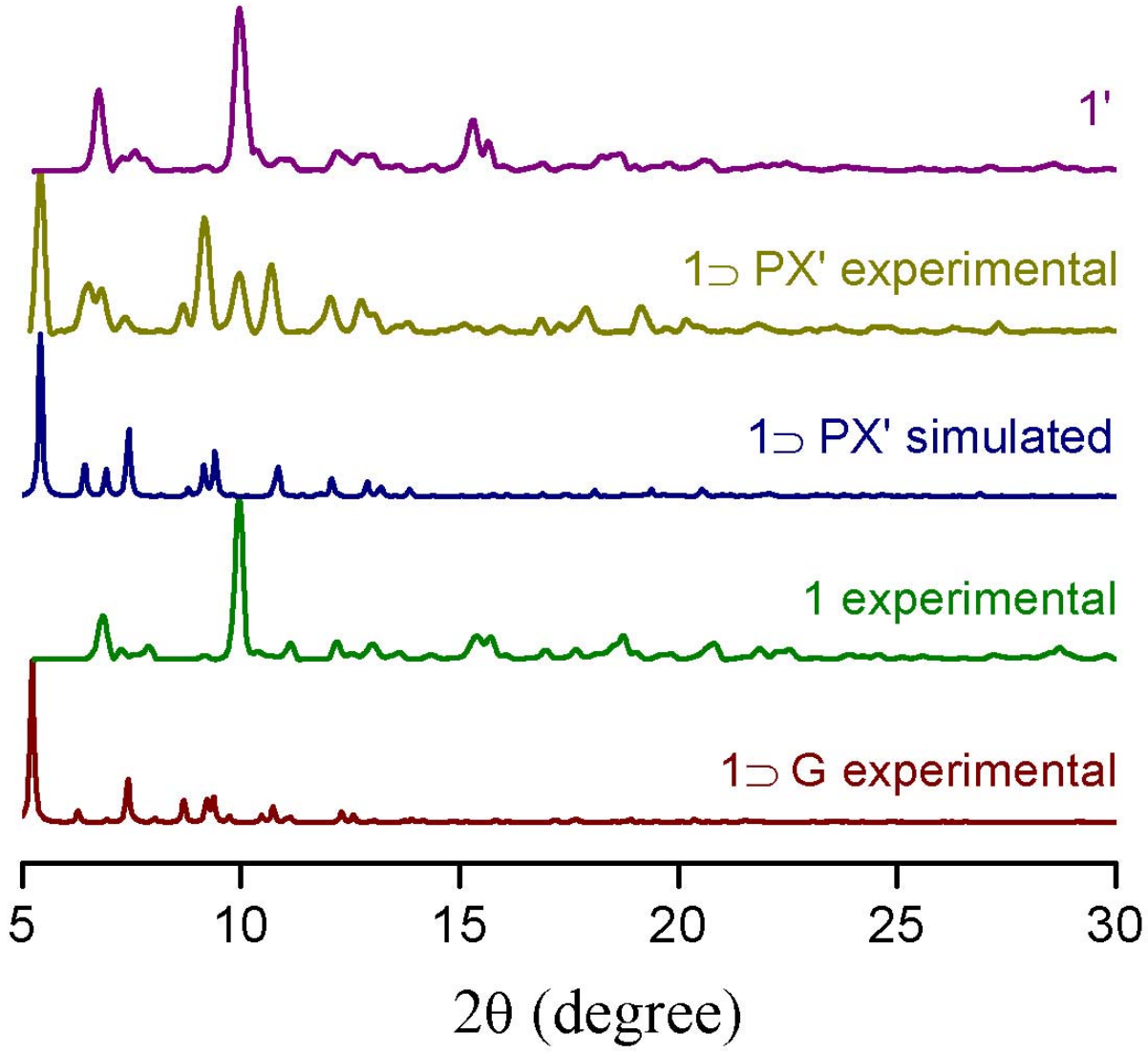

Figure S22: Powder X-ray diffraction (PXRD) patterns of compounds **1⊃G** (experimental), **1** (experimental), **1⊃PX'** (simulated), **1⊃PX'** (experimental) and **1'**(phase after heating phase **1⊃PX'**).

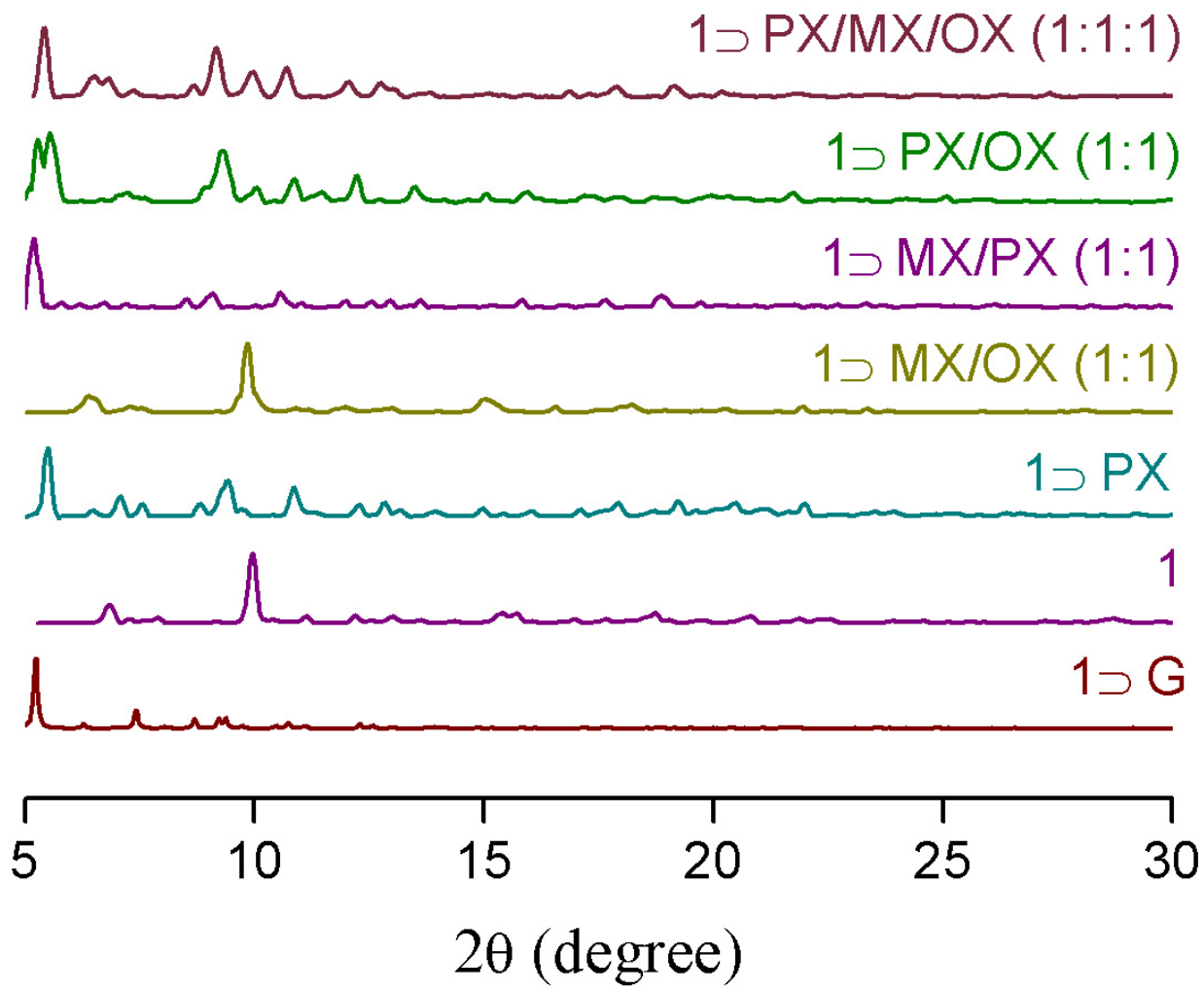

Figure S23: Experimental Powder X-ray diffraction (PXRD) patterns for compounds **1⊃G**, **1**, and the vapor-exposed phases: **1⊃PX** (only PX), **1⊃MX/OX** (binary mixture of 1:1 v/v MX and OX), **1⊃MX/PX** (binary mixture of 1:1 v/v MX and PX), **1⊃PX/OX** (binary mixture of 1:1 v/v PX and OX), **1⊃PX/MX/OX** (ternary mixture of 1:1:1 v/v PX, MX and OX).

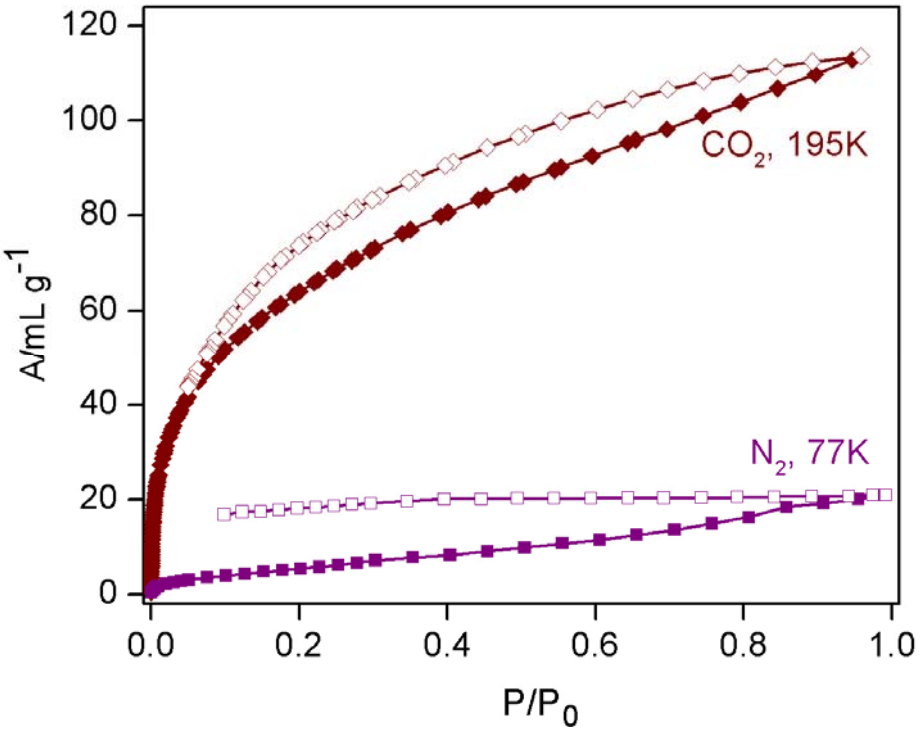

Figure S24: CO_2 and N_2 sorption isotherms of compound **1** at 195K and 77K respectively. Filled shapes = adsorption, hollow shapes = desorption.

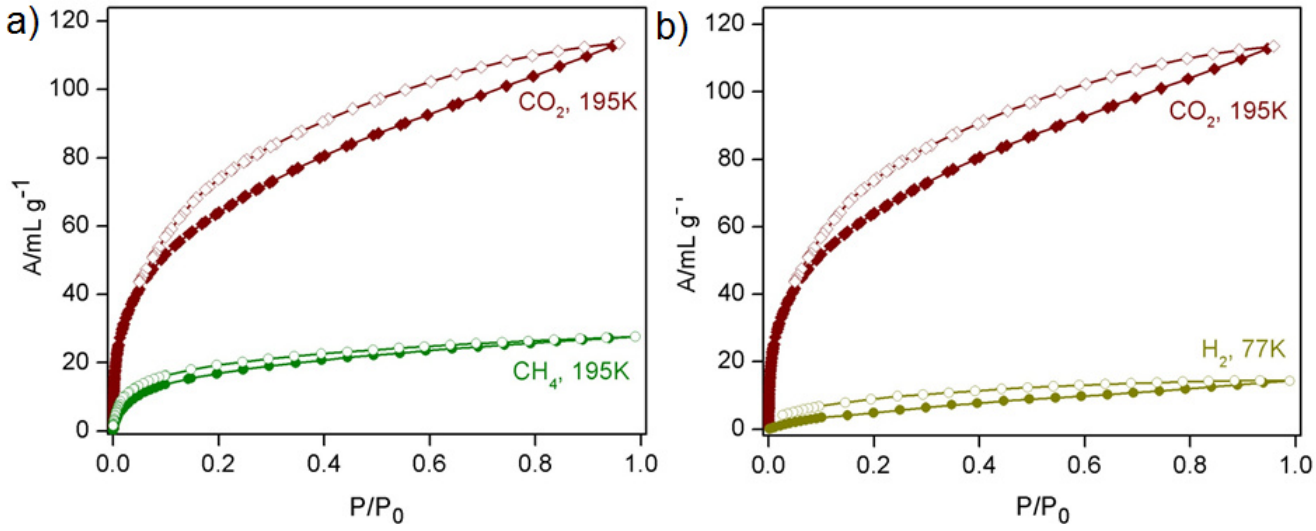

Figure S25: a) CO_2 and CH_4 sorption isotherms of compound **1** at 195K; b) CO_2 and H_2 sorption isotherms of compound **1** at 195K and 77K respectively. (Filled shapes = adsorption, hollow shapes = desorption).

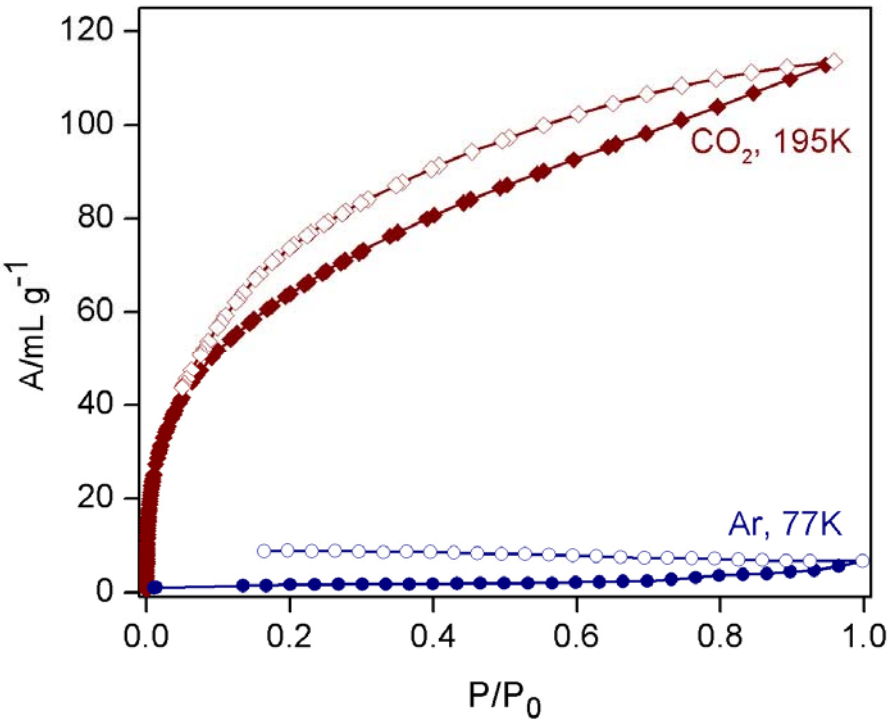

Figure S26: CO_2 and Ar sorption isotherms of compound **1** at 195K and 77K respectively. Filled shapes = adsorption, hollow shapes = desorption.

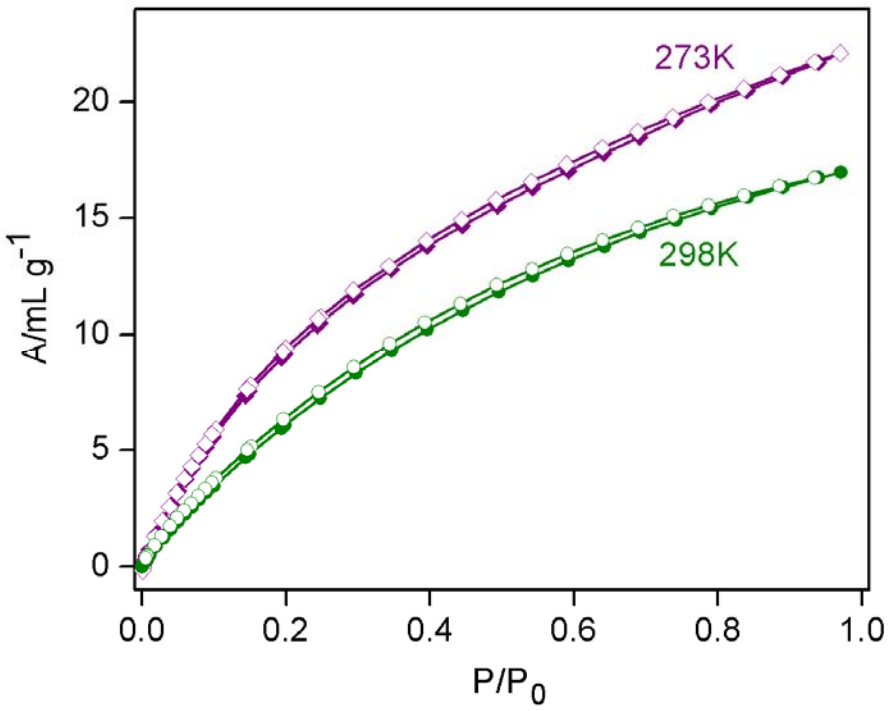

Figure S27: CO_2 sorption isotherms of compound **1** at 273K and 298K; filled shapes = adsorption, hollow shapes = desorption.

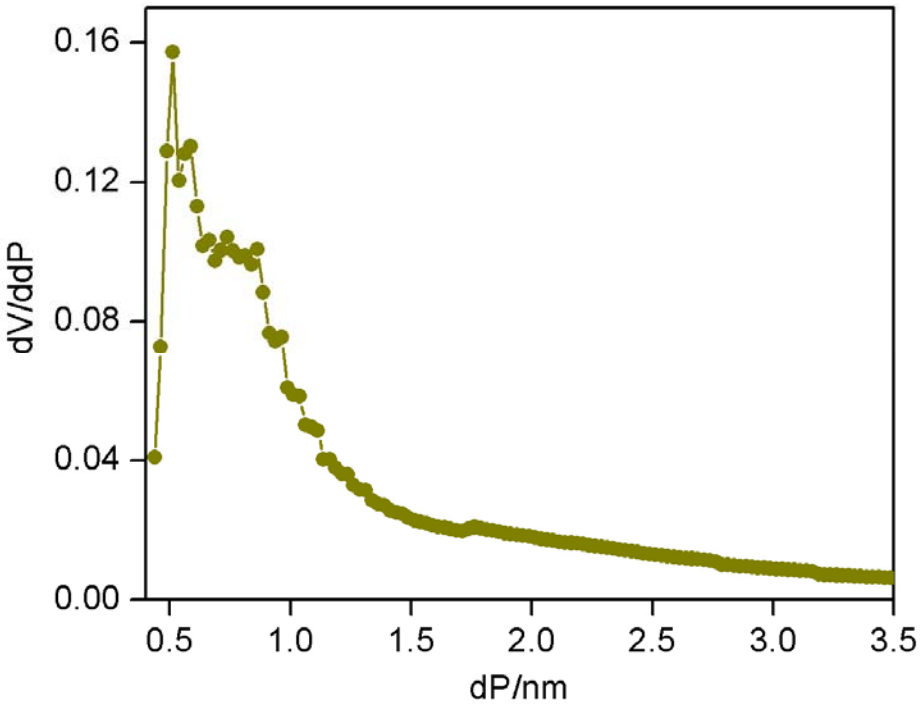

Figure S28: H-K (Horvath-Kawazoe) plot showing pore size distribution from CO_2 adsorption at 195K.

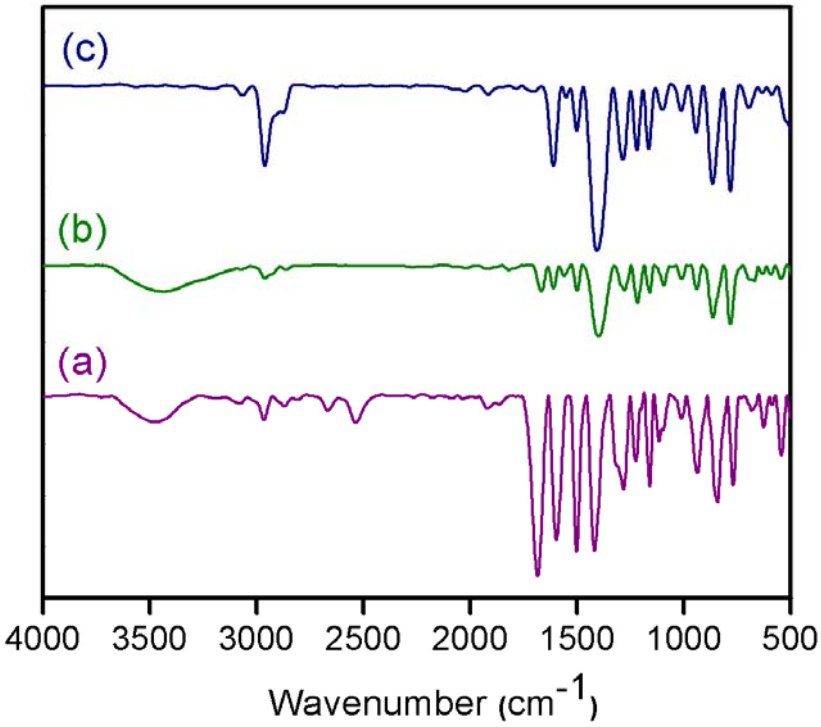

Figure S29: FTIR Spectra of (a) H_2L, (b) compound **1⊃G**, and (c) compound **1**.

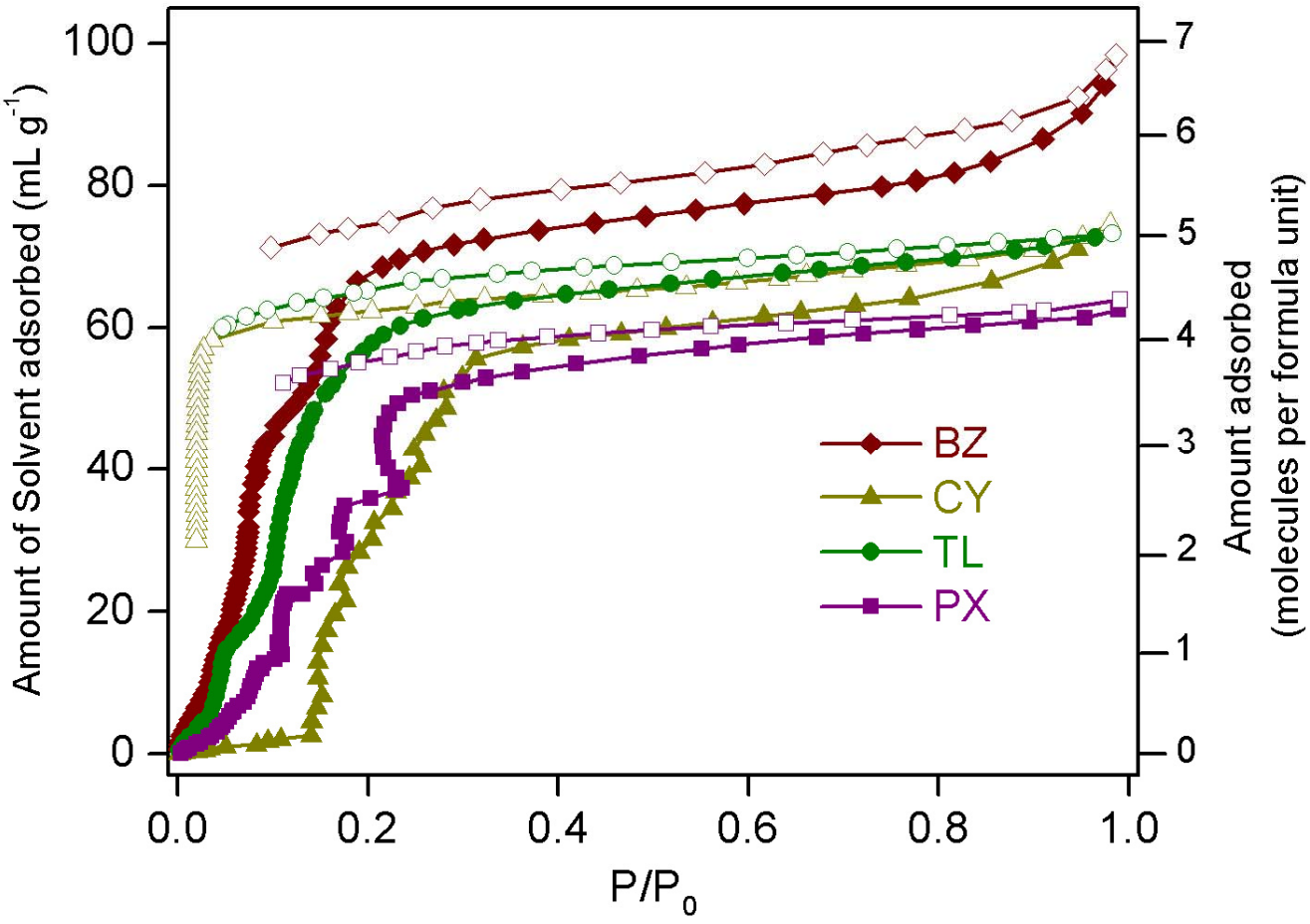

Figure S30: Solvent sorption isotherms for compound **1** recorded at 298K; color code: Benzene (wine red), toluene (olive), p-xylene (purple) and cyclohexane (dark yellow). Filled shapes: adsorption, hollow shapes: desorption.

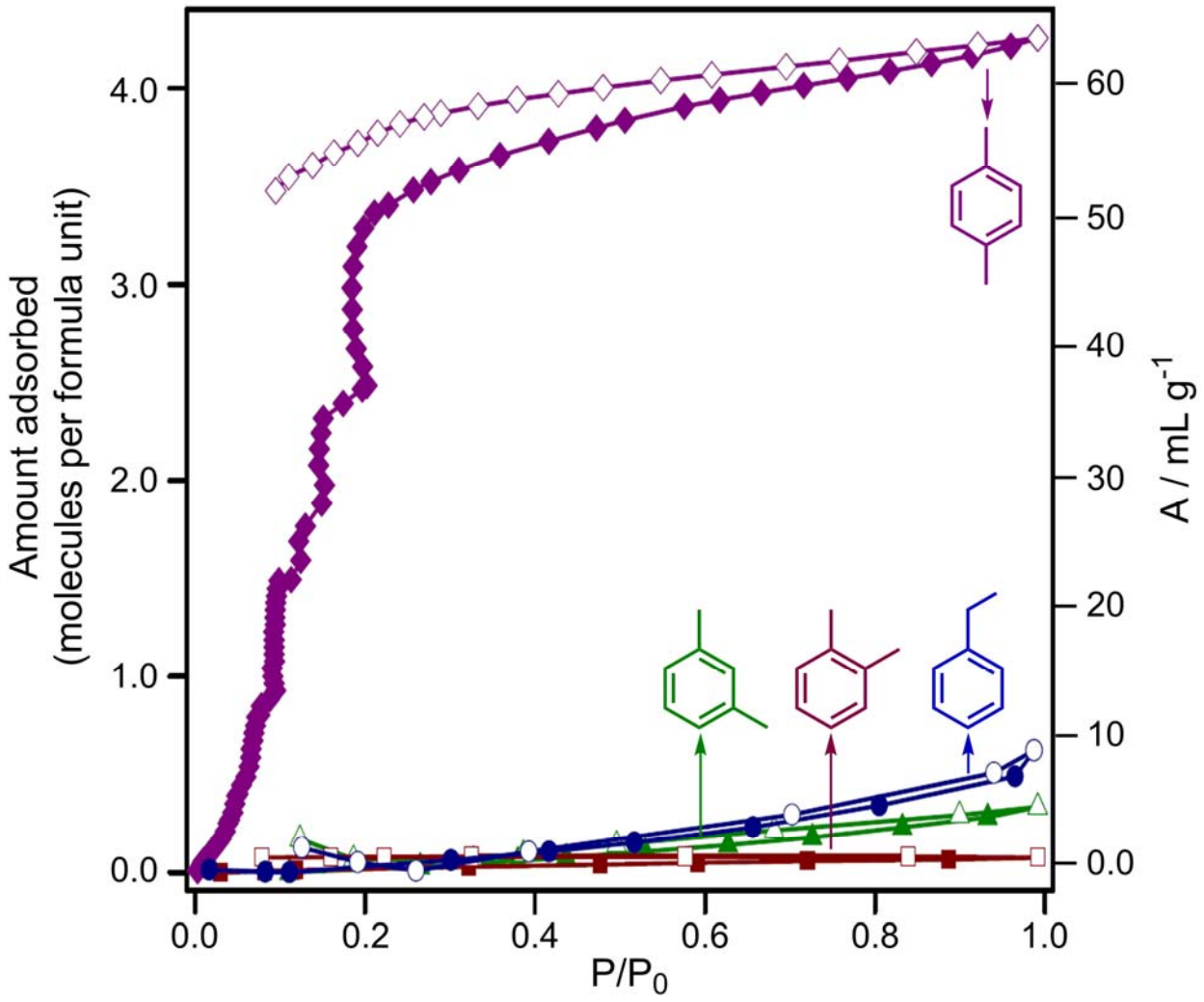

Figure S31. Solvent sorption isotherms for compound **1** at 298K for three xylene isomers along with isomeric ethyl benzene. Filled shapes: adsorption, hollow shapes: desorption.

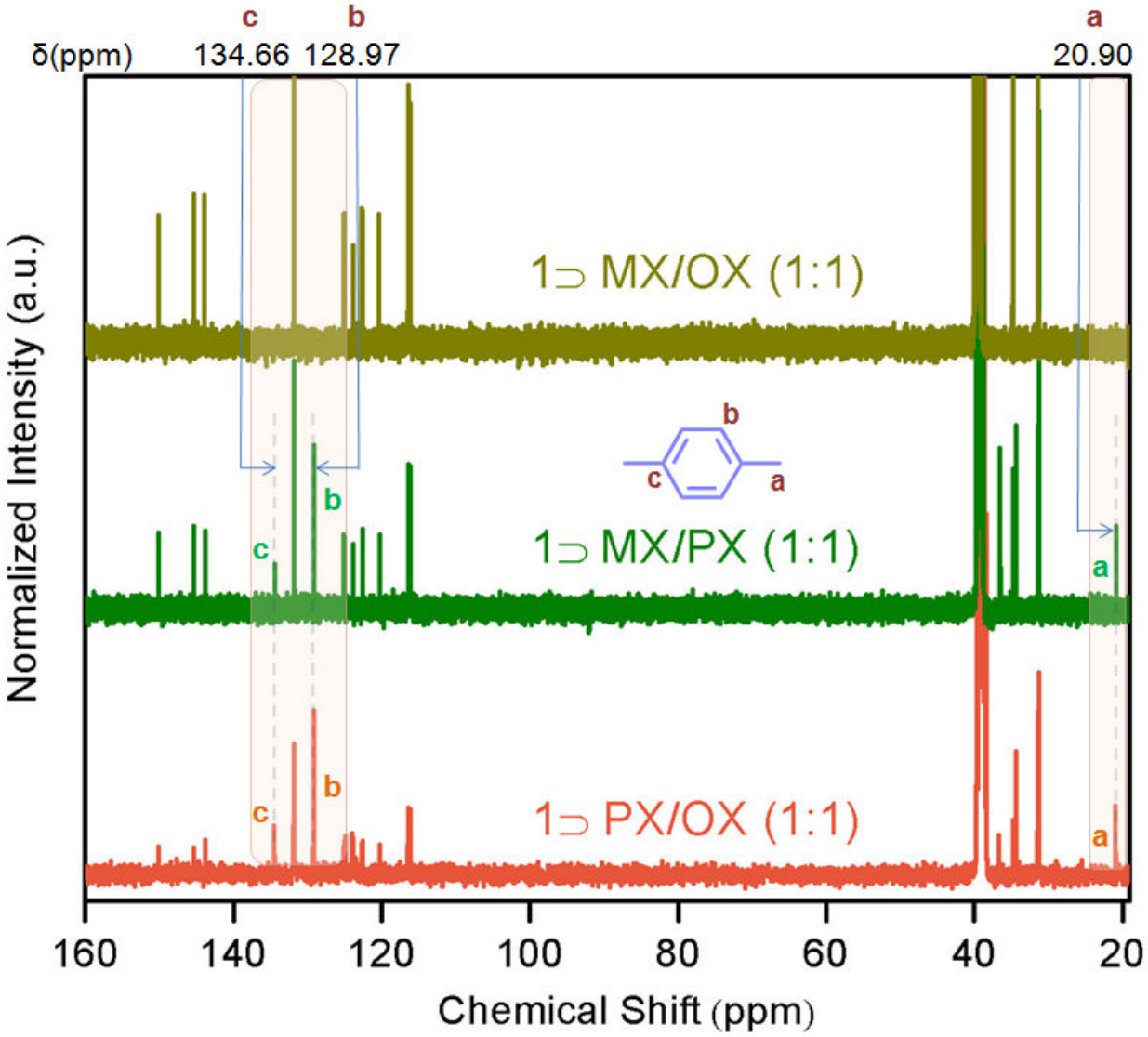

Figure S32. ^{13}C NMR spectra for different binary-xylene (1:1) mixture vapor-exposed phases of compound **1**. Vapor of each of the binary mixtures (1:1) exposed for 72h to the phase **1** before digesting in DCl/DMSO- d_6.

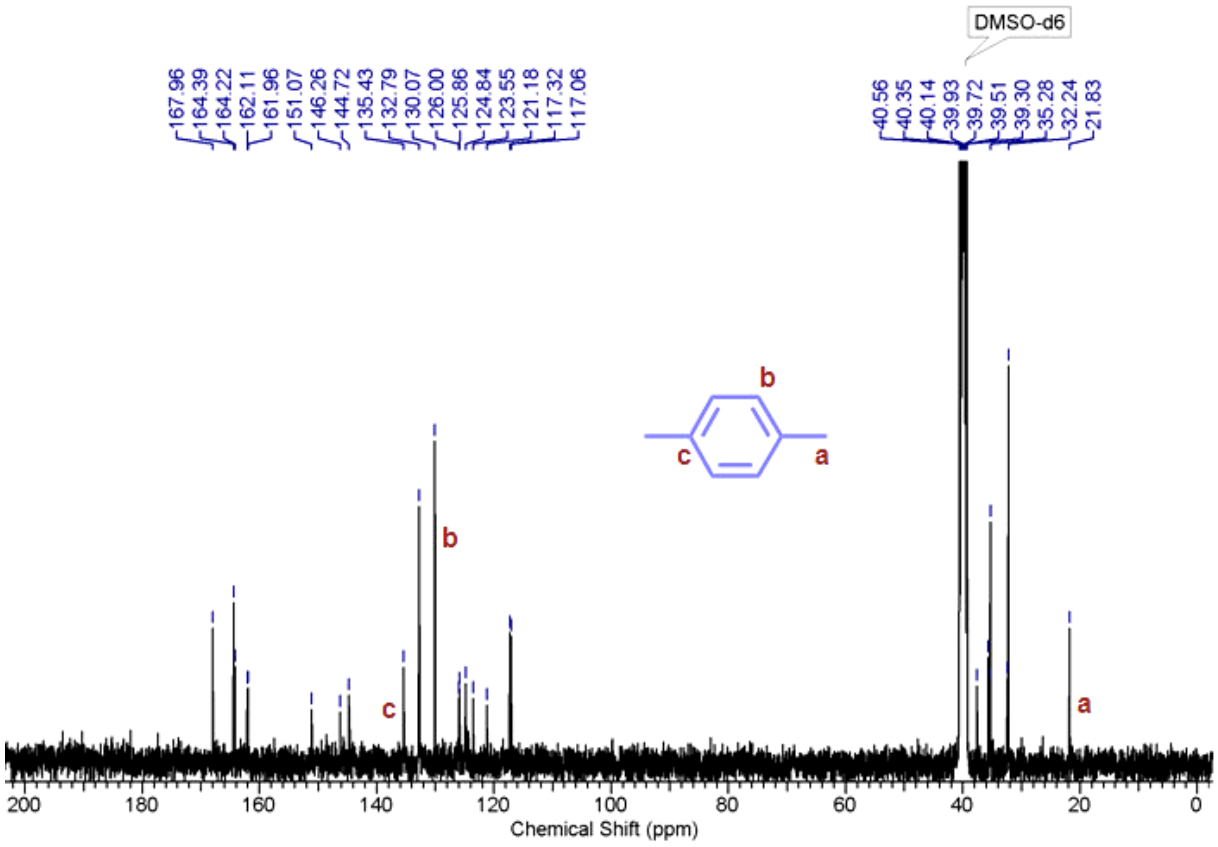

Figure S33: ^{13}C NMR spectrum of compound **1⊃PX'** digested in DCl/DMSO-d_6.

Table S1 Dimensions of Adsorptive molecules (Å) [8] (each atom surrounded by a van der Waals sphere)					
	x	***y***	**z**	**MIN-1**	**MIN-2**
BZ	6.628	7.337	3.277	3.277	6.628
TL	6.625	4.012	8.252	4.012	6.625
CY	7.168	6.580	4.982	4.982	6.580
PX	6.618	3.81	9.146	3.81	6.618
MX	8.994	3.949	7.315	3.949	7.258
OX	7.269	3.834	7.826	3.834	7.269
EB	6.625	5.285	9.361	5.285	6.625

MIN-1: Size of the adsorptive in the minimum dimension.

MIN-2: Second minimum dimension for molecular orientations that enable a molecule to enter the channel.

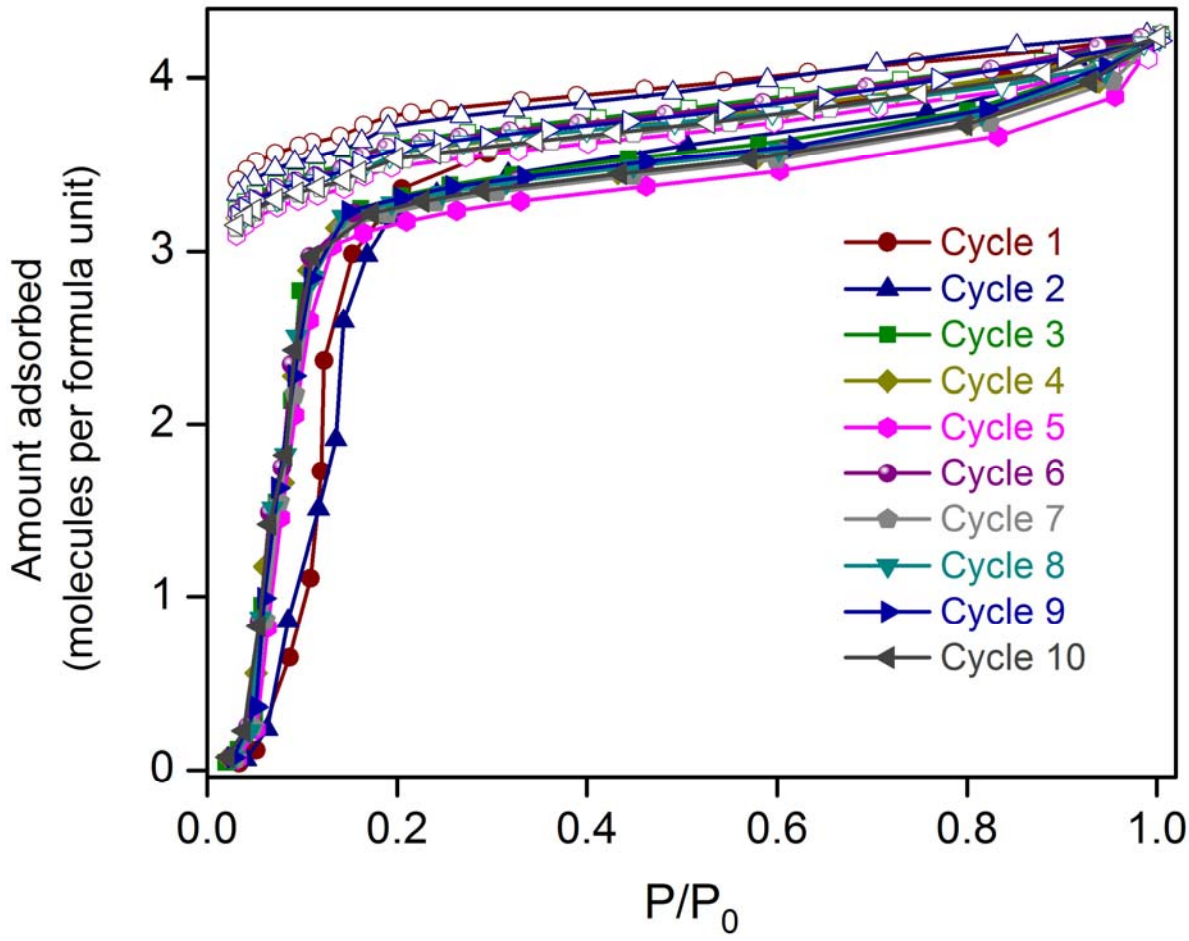

Figure S34: The recyclability of the PX adsorption behavior was confirmed by reproducing the same isotherm on unchanged desolvated sample **1** for ten consecutive cycles at 298 K. Filled shapes: adsorption, hollow shapes: desorption.

Figure S35: Bar diagram representation of the recyclability for the PX adsorption behavior as confirmed by reproducing the same isotherm on unchanged desolvated sample **1** for ten consecutive cycles at 298 K. Similar amounts of PX-uptake suggests the PX-sorption's recyclability behaviour for the material **1**.

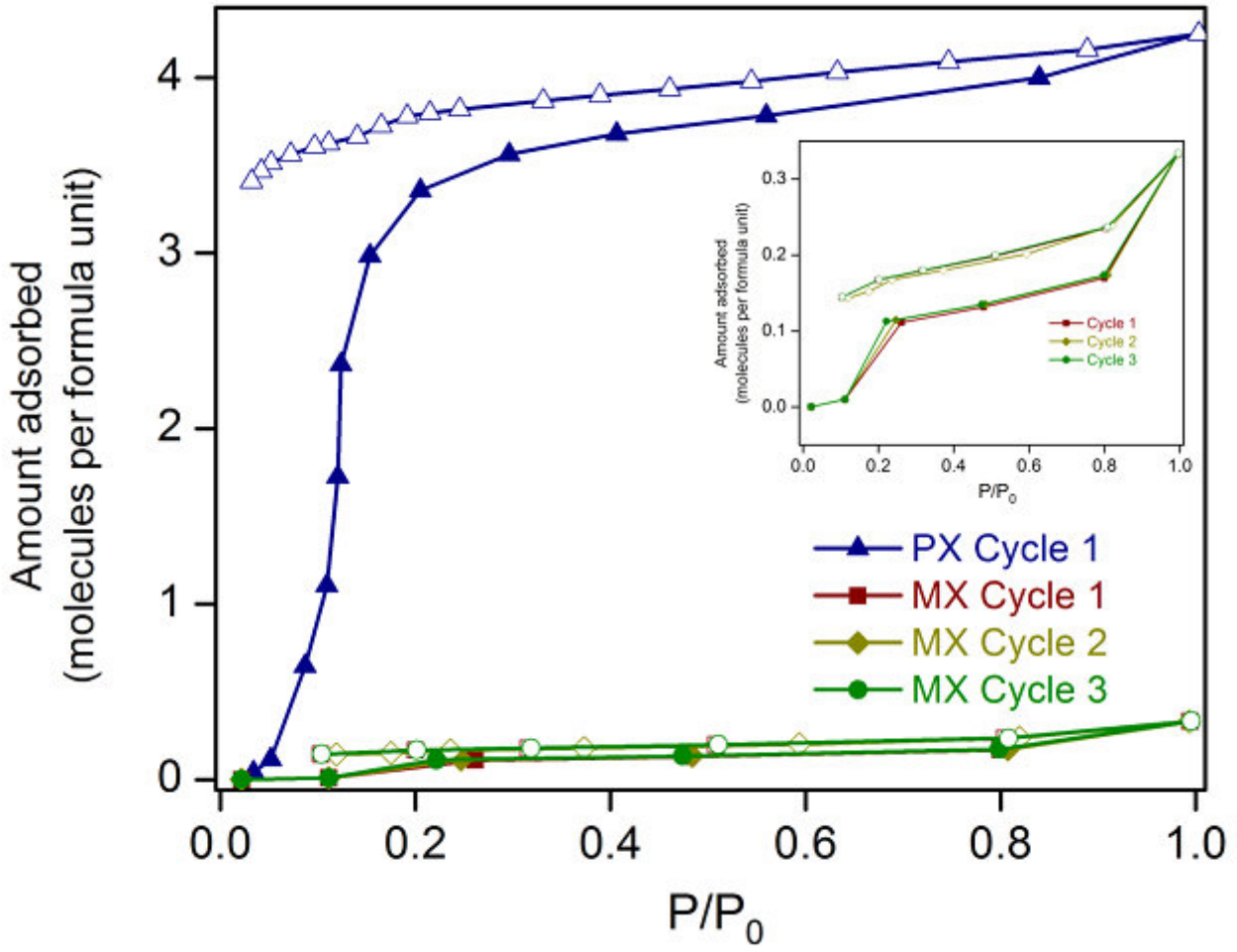

Figure S36: The recyclability of the MX adsorption behavior was confirmed by reproducing the same isotherm on unchanged desolvated sample **1** for three consecutive cycles at 298 K, as compared to the 'cycle 1' PX-sorption data; Inset: Plots for three consecutive recyclability cycles for MX. Filled shapes: adsorption, hollow shapes: desorption.

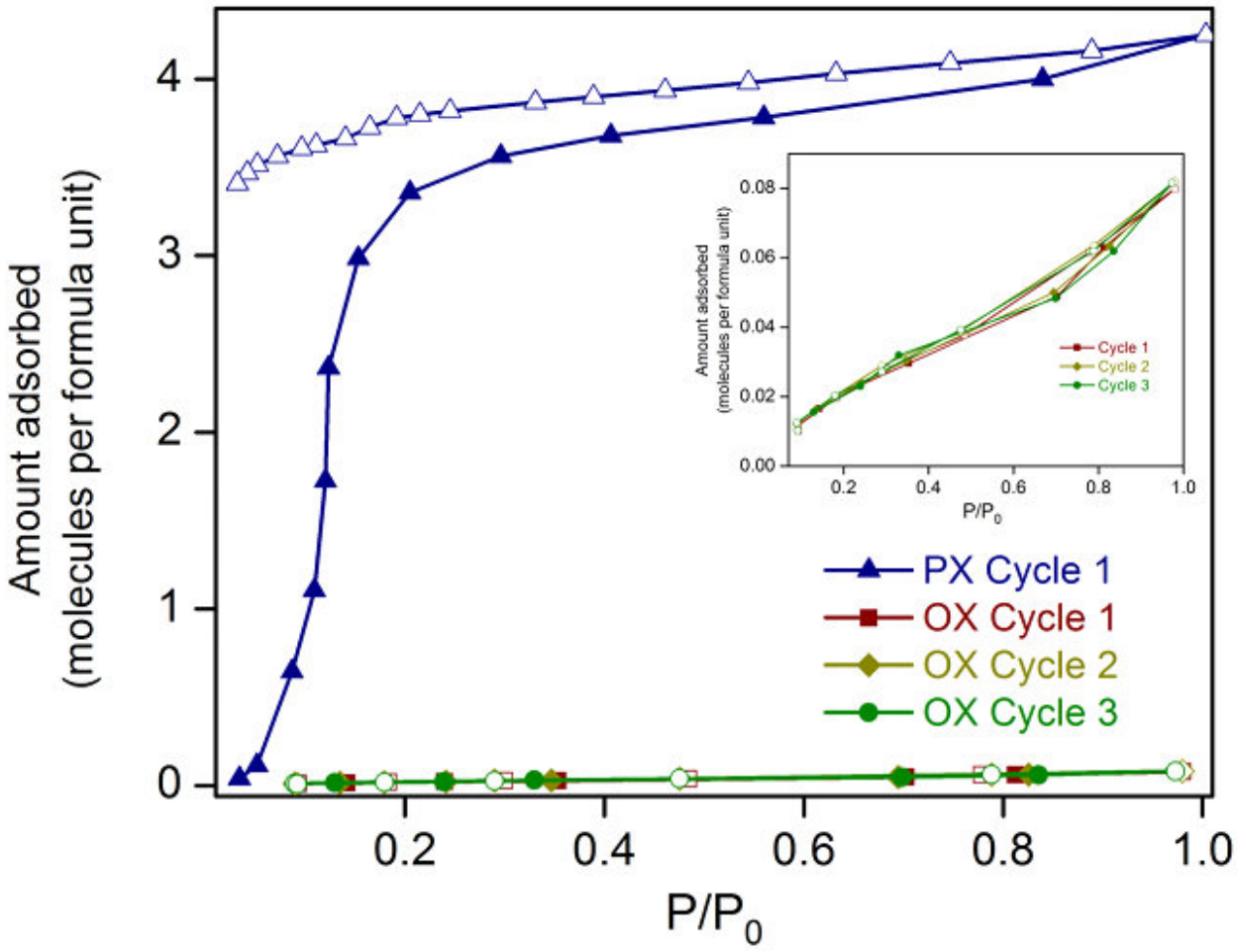

Figure S37: The recyclability of the OX adsorption behavior was confirmed by reproducing the same isotherm on unchanged desolvated sample **1** for three consecutive cycles at 298 K, as compared to the 'cycle 1' PX-sorption data; Inset: Plots for three consecutive recyclability cycles for OX. Filled shapes: adsorption, hollow shapes: desorption.

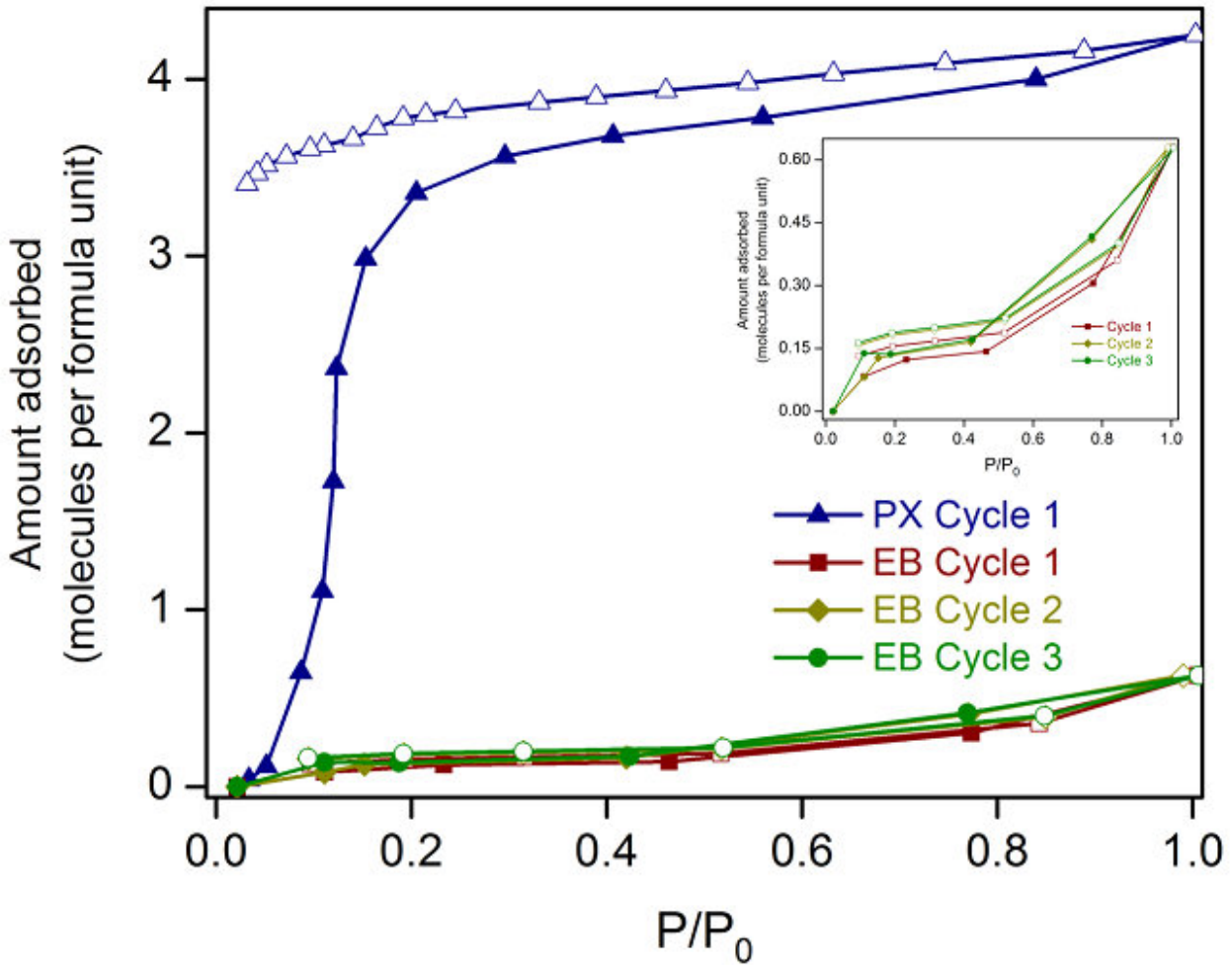

Figure S38: The recyclability of the EB adsorption behavior was confirmed by reproducing the same isotherm on unchanged desolvated sample **1** for three consecutive cycles at 298 K, as compared to the 'cycle 1' PX-sorption data; Inset: Plots for three consecutive recyclability cycles for EB. Filled shapes: adsorption, hollow shapes: desorption.

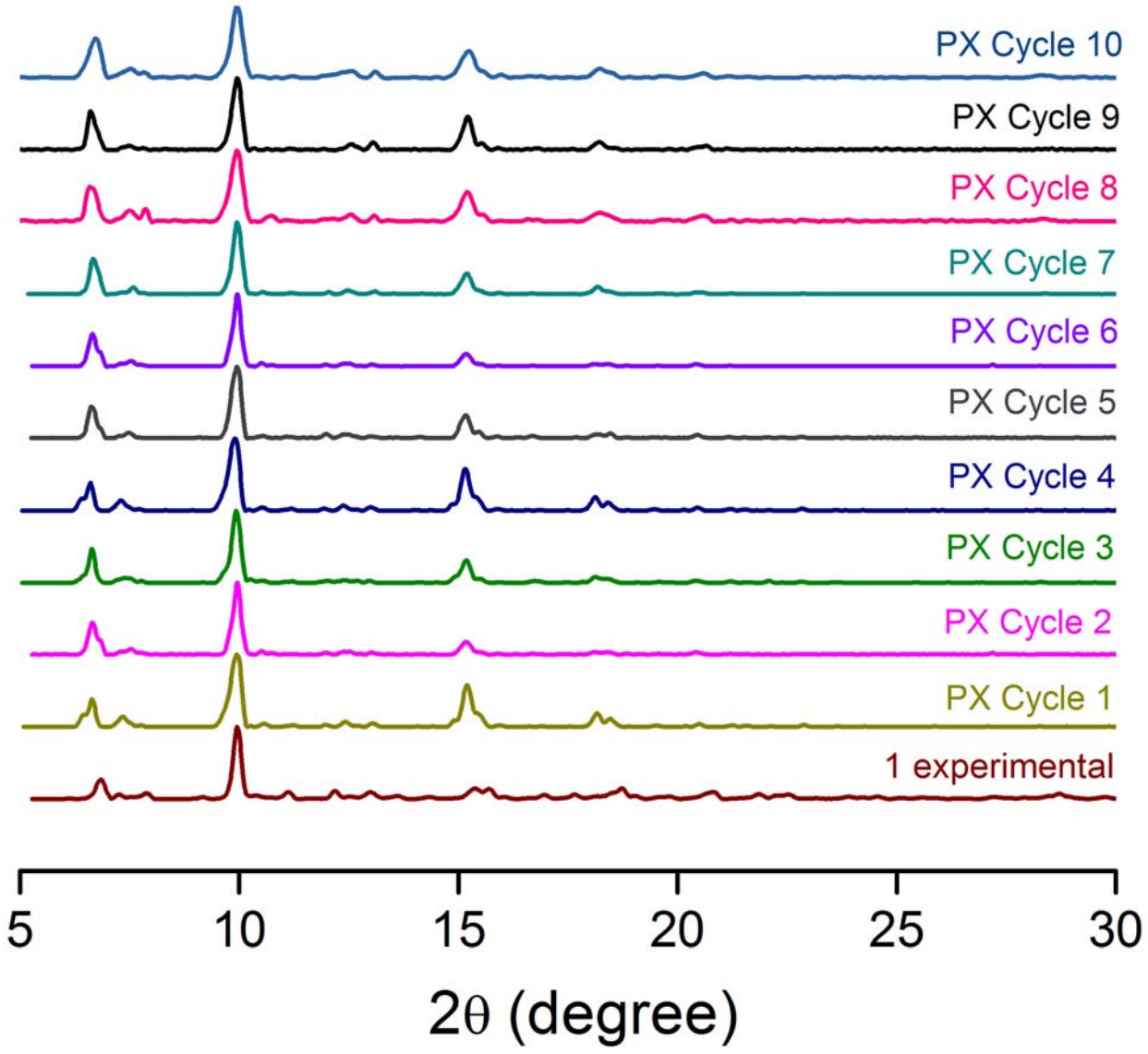

Figure S39: PXRD patterns for the post-desorption phases of the PX-recyclability experiments, plotted with the experimental PXRD pattern of **1**.

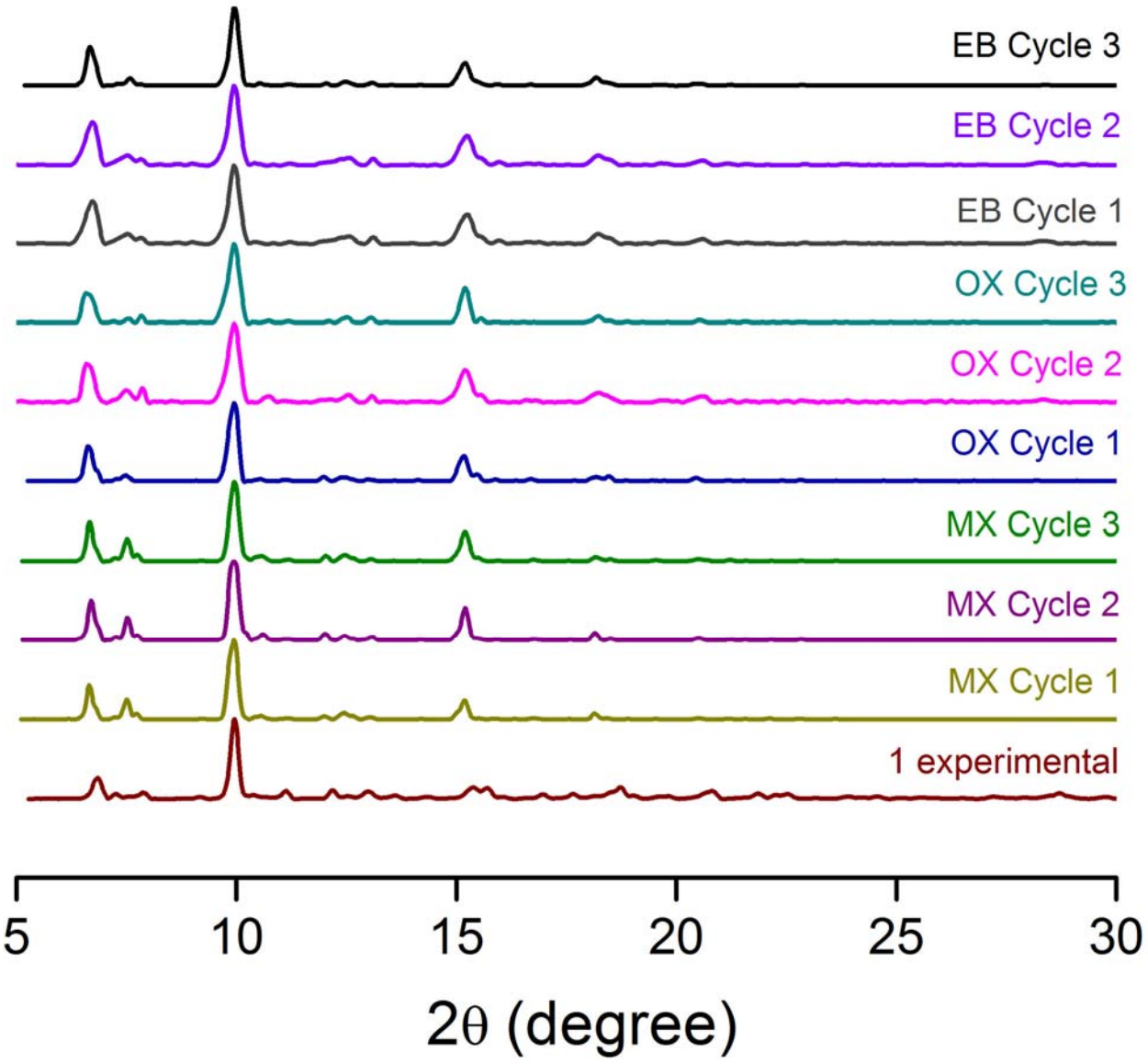

Figure S40: PXRD patterns for all the post-desorption phases of the MX-recyclability and OX-recyclability experiments, plotted with the experimental PXRD pattern of **1**.

GC Instrumentation: Materials and Methods:

GC-2014 Shimadzu Gas chromatograph (with AOC-20i Auto Injector) was used with the Column RTX-5 (Length: 30m, Inner diameter: 0.32 mm, Film thickness: 0.25 μm); Injection volume: 1 μL, Injection temperature: 200 °C, Initial Column temperature: 40 °C, Column heating range: 40-70 °C, heating at 1 °C/min. With this setup, we could not obtain separate retention times for PX and MX, rather both of them were giving GC signal at similar retention times. That is why, to support the observed decrease in the mixed (PX+MX) signal intensity with time when the MOF was immersed in a quaternary mixture of xylenes, two more experiments comprising of ternary combinations of xylenes (one excluding MX, and the other excluding PX) was performed. The results (Figures S42-S44) confirm that the observed decline in the signal intensity is solely in the presence of PX. The corresponding uptake times indicate convincingly fast kinetics of the process.

Table **S2.** Crystal data and structure refinement for compound **1⊃G**.

Identification code	Compound **1⊃G**	
Empirical formula	$C_{78}H_{78}N_2O_{23}Zn_4$	
Formula weight	1672.90	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.801(3) Å	α= 90°.
	b = 33.733(10) Å	β= 99.893(6)°.
	c = 25.650(8) Å	γ= 90°.
Volume	10,059(5) Å^3	
Z	4	
Density (calculated)	1.105 Mg/m^3	
Absorption coefficient	1.001 mm^{-1}	
F(000)	3456	
Crystal size	0.15 x 0.13 x 0.12 mm^3	
Theta range for data collection	1.01 to 25.00°.	
Index ranges	-11<=h<=14, -37<=k<=39, -30<=l<=16	
Reflections collected	28853	
Independent reflections	14814 [R(int) = 0.0772]	
Completeness to theta = 25.00°	83.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8893 and 0.8644	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14814 / 171 / 920	
Goodness-of-fit on F^2	0.809	
Final R indices [I>2sigma(I)]	R_1 = 0.0787, wR_2 = 0.1985	
R indices (all data)	R_1 = 0.1656, wR_2 = 0.2154	
Largest diff. peak and hole	0.628 and -0.672 e.Å^{-3}	

Table **S3.** Crystal data and structure refinement for compound **1**.

Identification code	Compound **1**	
Empirical formula	$C_{72}H_{60}O_{19}Zn_4$	
Formula weight	1490.68	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.306(9) Å	α = 90°.
	b = 26.370(18) Å	β= 96.549(13)°.
	c = 22.124(16) Å	γ = 90°.
Volume	7133(9) Å3	
Z	4	
Density (calculated)	1.388 Mg/m^3	
Absorption coefficient	1.398 mm^{-1}	
F(000)	3056	
Crystal size	0.15 x 0.12 x 0.10 mm^3	
Theta range for data collection	1.21 to 25.00°.	
Index ranges	-14<=h<=14, -31<=k<=31, -26<=l<=26	
Reflections collected	95666	
Independent reflections	12514 [R(int) = 0.2480]	
Completeness to theta = 25.00°	99.5 %	
Max. and min. transmission	0.8729 and 0.8177	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	12514 / 78 / 865	
Goodness-of-fit on F2	0.910	
Final R indices [I>2sigma(I)]	R_1 = 0.1106, wR_2 = 0.2622	
R indices (all data)	R_1 = 0.2897, wR_2 = 0.3313	
Largest diff. peak and hole	0.996 and -0.593 e.$Å^{-3}$	

Table **S4.** Crystal data and structure refinement for Compound **1⊃PX'**.

Identification code	Compound **1⊃PX'**	
Empirical formula	C_{86} H_{84} N_2 O_{21} Zn_4	
Formula weight	1743.03	
Temperature	200(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.080(5) Å	α= 90.000(5)°.
	b = 32.556(5) Å	β= 97.830(5)°.
	c = 25.722(5) Å	γ = 90.000(5)°.
Volume	10022(5) Å^3	
Z	4	
Density (calculated)	1.155 Mg/m^3	
Absorption coefficient	1.006 mm^{-1}	
F(000)	3608	
Crystal size	0.14 x 0.11 x 0.10 mm^3	
Theta range for data collection	1.48 to 16.80°.	
Index ranges	-9<=h<=9, -26<=k<=25, -19<=l<=20	
Reflections collected	28529	
Independent reflections	5363 [R(int) = 0.0419]	
Completeness to theta = 16.80°	94.9 %	
Max. and min. transmission	0.9061 and 0.8720	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5363 / 284 / 966	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R_1 = 0.0976, wR_2 = 0.2626	
R indices (all data)	R_1 = 0.1055, wR_2 = 0.2704	
Largest diff. peak and hole	1.480 and -0.674 e.Å^{-3}	

Table **S5**. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **1⊃G**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-1152(10)	4183(3)	3528(5)	61(3)
C(2)	-1943(9)	3994(3)	3855(4)	56(3)
C(3)	-3087(9)	3885(3)	3630(4)	71(3)
C(4)	-3848(11)	3723(3)	3909(4)	86(4)
C(5)	-3444(11)	3667(3)	4432(6)	77(4)
C(6)	-2326(13)	3768(3)	4670(4)	100(4)
C(7)	-1561(9)	3928(3)	4380(4)	73(3)
C(8)	-5326(13)	3536(4)	4655(5)	94(4)
C(9)	-5820(12)	3904(5)	4556(5)	99(5)
C(10)	-7090(10)	3930(5)	4459(4)	103(4)
C(11)	-7648(14)	3587(4)	4493(5)	127(6)
C(12)	-7217(11)	3204(4)	4584(5)	95(4)
C(13)	-6072(11)	3214(4)	4665(5)	116(3)
C(14)	-7994(11)	2887(4)	4603(5)	189(9)
C(15)	-8762(14)	2846(6)	4072(6)	249(12)
C(16)	-8760(14)	2934(6)	5007(7)	286(13)
C(17)	-7341(18)	2503(5)	4710(9)	400(20)
C(18)	1856(11)	3856(3)	2719(5)	81(3)
C(19)	2613(7)	3502(2)	2768(4)	136(3)
C(20)	2789(8)	3305(3)	2313(3)	153(3)
C(21)	3482(9)	2969(3)	2352(3)	164(3)
C(22)	3999(7)	2831(2)	2846(4)	198(5)
C(23)	3823(7)	3028(2)	3301(3)	80(3)
C(24)	3130(7)	3363(2)	3262(3)	82(3)
C(35)	2206(9)	5023(4)	1816(4)	75(4)
C(36)	3021(10)	5123(4)	1450(4)	86(4)
C(37)	4006(12)	5341(4)	1625(5)	129(5)
C(38)	4868(14)	5407(5)	1290(5)	163(7)
C(39)	4538(13)	5272(5)	786(5)	135(6)

C(40)	3589(11)	5060(4)	620(5)	108(5)
C(41)	2867(10)	4975(4)	959(4)	95(4)
C(42)	7343(9)	5467(2)	634(3)	138(6)
C(43)	6182(7)	5563(3)	513(4)	116(6)
C(44)	5847(6)	5944(4)	348(3)	121(4)
C(45)	6674(9)	6230(3)	304(3)	149(4)
C(46)	7836(8)	6134(3)	424(3)	146(5)
C(47)	8170(5)	5753(3)	589(3)	83(4)
C(67)	-1524(8)	6062(2)	2184(3)	88(4)
C(68)	-955(6)	6416(3)	2127(4)	130(5)
C(69)	-1578(10)	6751(2)	1941(5)	190(9)
C(70)	-2770(9)	6733(3)	1811(5)	213(11)
C(71)	-3339(6)	6379(3)	1868(5)	192(8)
C(72)	-2716(8)	6044(2)	2055(4)	134(6)
C(25)	5092(15)	2334(3)	3355(4)	193(5)
C(26)	6197(13)	2394(3)	3633(7)	204(9)
C(27)	6540(8)	2211(3)	4120(6)	201(10)
C(28)	5778(12)	1967(3)	4328(4)	235(8)
C(29)	4674(10)	1907(3)	4049(7)	240(7)
C(30)	4330(9)	2091(4)	3563(6)	245(8)
C(48)	9480(14)	5661(5)	667(6)	242(12)
C(49)	10106(17)	5980(5)	985(7)	264(11)
C(50)	9744(12)	5633(6)	117(5)	281(13)
C(51)	9540(20)	5271(6)	949(9)	380(20)
C(52)	-1757(8)	4399(3)	1583(5)	69(3)
C(53)	-2609(11)	4267(3)	1115(5)	101(4)
C(54)	-2208(12)	4117(4)	658(6)	128(5)
C(55)	-2956(14)	3995(5)	215(7)	167(7)
C(56)	-4136(13)	4039(4)	232(8)	143(6)
C(57)	-4582(11)	4210(5)	672(6)	128(5)
C(58)	-3800(9)	4344(3)	1074(5)	92(4)
C(59)	2300(8)	5132(4)	3749(4)	61(3)
C(60)	3135(9)	5313(3)	4199(4)	67(3)
C(61)	3834(9)	5625(3)	4131(4)	77(3)
C(62)	4593(9)	5770(3)	4561(5)	81(3)
C(63)	4557(10)	5615(4)	5037(5)	73(3)

C(64)	3899(10)	5318(4)	5123(4)	78(3)
C(65)	3186(9)	5155(3)	4723(4)	71(3)
C(66)	-892(9)	5688(3)	2352(4)	56(3)
C(73)	-1458(13)	5310(4)	3634(5)	106(5)
C(74)	-312(17)	5283(6)	4433(7)	270(13)
C(75)	-2081(15)	5691(5)	4327(7)	209(9)
C(76)	-3833(10)	4682(4)	2671(5)	84(4)
C(77)	-5676(9)	4386(4)	2717(6)	160(7)
C(78)	-5106(10)	5029(5)	3151(6)	151(6)
N(1)	-4848(8)	4709(3)	2833(4)	99(3)
N(2)	-1340(13)	5443(4)	4058(6)	130(5)
O(1)	-140(6)	4235(2)	3736(3)	68(2)
O(2)	-1574(6)	4286(2)	3065(3)	76(2)
O(3)	-4112(8)	3503(2)	4780(3)	99(2)
O(4)	-2090(5)	4568(2)	1957(3)	69(2)
O(5)	-720(6)	4315(2)	1554(3)	89(2)
O(6)	-1457(6)	5385(2)	2311(3)	88(2)
O(7)	2211(6)	5249(2)	2225(3)	80(2)
O(8)	1573(6)	4731(2)	1699(3)	78(2)
O(9)	5315(9)	5306(3)	424(4)	160(4)
O(10)	2143(5)	5343(2)	3347(3)	64(2)
O(11)	1882(6)	4805(2)	3831(3)	70(2)
O(12)	5289(6)	5755(2)	5489(3)	89(2)
O(13)	1411(7)	3967(2)	2278(3)	94(3)
O(14)	1815(5)	4040(2)	3131(3)	67(2)
O(15)	4749(12)	2510(3)	2904(5)	219(4)
O(16)	3258(12)	2079(3)	3364(9)	406(16)
O(17)	-3097(6)	4950(2)	2746(3)	82(2)
O(18)	-864(6)	5122(2)	3401(3)	85(2)
O(19)	280(4)	4752(2)	2688(2)	55(2)
O(20)	-4752(9)	3942(4)	-246(5)	202(6)
O(21)	166(6)	5722(2)	2507(3)	76(2)
Zn(1)	-1424(1)	4839(1)	2648(1)	59(1)
Zn(2)	843(1)	4482(1)	3319(1)	55(1)
Zn(3)	559(1)	4454(1)	2086(1)	60(1)
Zn(4)	1057(1)	5255(1)	2688(1)	59(1)

C(31)	7650(20)	2278(5)	4485(10)	305(15)
C(32)	8440(20)	2033(7)	4215(10)	306(15)
C(33)	8142(16)	2686(4)	4512(11)	357(19)
C(34)	7840(40)	2130(8)	5048(10)	720(60)
O(1W)	7685(17)	6329(6)	8948(5)	350(11)
O(2W)	3177(16)	6383(6)	2421(8)	361(11)

Table **S6**. Bond lengths [Å] and angles [°] for compound **1⊃G**.

C(1)-O(1)	1.233(12)
C(1)-O(2)	1.253(11)
C(1)-C(2)	1.502(13)
C(2)-C(7)	1.361(12)
C(2)-C(3)	1.423(12)
C(3)-C(4)	1.355(12)
C(3)-H(3)	0.9300
C(4)-C(5)	1.357(14)
C(4)-H(4)	0.9300
C(5)-C(6)	1.397(15)
C(5)-O(3)	1.403(12)
C(6)-C(7)	1.375(13)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.377(17)
C(8)-C(13)	1.400(14)
C(8)-O(3)	1.418(15)
C(9)-O(12)#1	1.324(14)
C(9)-C(10)	1.480(17)
C(10)-C(11)	1.343(14)
C(10)-H(10)	0.9300
C(11)-C(12)	1.392(17)
C(11)-H(11)	0.9300
C(12)-C(13)	1.331(16)
C(12)-C(14)	1.415(9)
C(13)-H(13)	0.9300
C(14)-C(16)	1.497(9)
C(14)-C(15)	1.508(9)
C(14)-C(17)	1.510(10)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600

C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-O(13)	1.221(12)
C(18)-O(14)	1.235(11)
C(18)-C(19)	1.484(12)
C(19)-C(20)	1.3900
C(19)-C(24)	1.3900
C(20)-C(21)	1.3900
C(20)-H(20)	0.9300
C(21)-C(22)	1.3900
C(21)-H(21)	0.9300
C(22)-C(23)	1.3900
C(22)-O(15)	1.390(10)
C(23)-C(24)	1.3900
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(35)-O(8)	1.241(12)
C(35)-O(7)	1.297(12)
C(35)-C(36)	1.494(13)
C(36)-C(41)	1.338(13)
C(36)-C(37)	1.383(14)
C(37)-C(38)	1.457(15)
C(37)-H(37)	0.9300
C(38)-C(39)	1.362(16)
C(38)-H(38)	0.9300
C(39)-C(40)	1.336(15)
C(39)-O(9)	1.418(12)
C(40)-C(41)	1.348(13)
C(40)-H(40)	0.9300
C(41)-H(41)	0.9300
C(42)-C(43)	1.3900
C(42)-C(47)	1.3900
C(42)-H(42)	0.9300
C(43)-O(9)	1.330(7)

C(43)-C(44)	1.3900
C(44)-O(20)#2	1.331(11)
C(44)-C(45)	1.3900
C(45)-C(46)	1.3900
C(45)-H(45)	0.9300
C(46)-C(47)	1.3900
C(46)-H(46)	0.9300
C(47)-C(48)	1.556(17)
C(67)-C(68)	1.3900
C(67)-C(72)	1.3900
C(67)-C(66)	1.490(11)
C(68)-C(69)	1.3900
C(68)-H(68)	0.9300
C(69)-C(70)	1.3900
C(69)-H(69)	0.9300
C(70)-O(16)#3	1.344(12)
C(70)-C(71)	1.3900
C(71)-C(72)	1.3900
C(71)-H(71)	0.9300
C(72)-H(72)	0.9300
C(25)-O(15)	1.301(13)
C(25)-C(26)	1.3900
C(25)-C(30)	1.3900
C(26)-C(27)	1.3900
C(26)-H(26)	0.9300
C(27)-C(28)	1.3900
C(27)-C(31)	1.49(2)
C(28)-C(29)	1.3900
C(28)-H(28)	0.9300
C(29)-C(30)	1.3900
C(29)-H(29)	0.9300
C(30)-O(16)	1.282(13)
C(48)-C(49)	1.469(10)
C(48)-C(51)	1.497(10)
C(48)-C(50)	1.498(9)
C(49)-H(49A)	0.9600

C(49)-H(49B)	0.9600
C(49)-H(49C)	0.9600
C(50)-H(50A)	0.9600
C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600
C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600
C(51)-H(51C)	0.9600
C(52)-O(4)	1.236(11)
C(52)-O(5)	1.271(10)
C(52)-C(53)	1.496(15)
C(53)-C(58)	1.414(14)
C(53)-C(54)	1.430(14)
C(54)-C(55)	1.376(17)
C(54)-H(54)	0.9300
C(55)-C(56)	1.409(18)
C(55)-H(55)	0.9300
C(56)-O(20)	1.355(17)
C(56)-C(57)	1.443(17)
C(57)-C(58)	1.338(15)
C(57)-H(57)	0.9300
C(58)-H(58)	0.9300
C(59)-O(10)	1.241(11)
C(59)-O(11)	1.243(12)
C(59)-C(60)	1.510(14)
C(60)-C(61)	1.368(12)
C(60)-C(65)	1.436(13)
C(61)-C(62)	1.385(13)
C(61)-H(61)	0.9300
C(62)-C(63)	1.335(14)
C(62)-H(62)	0.9300
C(63)-C(64)	1.310(13)
C(63)-O(12)	1.404(12)
C(64)-C(65)	1.330(13)
C(64)-H(64)	0.9300
C(65)-H(65)	0.9300

C(66)-O(6)	1.215(10)
C(66)-O(21)	1.248(11)
C(73)-N(2)	1.163(14)
C(73)-O(18)	1.180(13)
C(73)-H(73)	0.9300
C(74)-N(2)	1.512(10)
C(74)-H(74A)	0.9600
C(74)-H(74B)	0.9600
C(74)-H(74C)	0.9600
C(75)-N(2)	1.465(15)
C(75)-H(75A)	0.9600
C(75)-H(75B)	0.9600
C(75)-H(75C)	0.9600
C(76)-O(17)	1.246(11)
C(76)-N(1)	1.336(12)
C(76)-H(76)	0.9300
C(77)-N(1)	1.458(13)
C(77)-H(77A)	0.9600
C(77)-H(77B)	0.9600
C(77)-H(77C)	0.9600
C(78)-N(1)	1.418(13)
C(78)-H(78A)	0.9600
C(78)-H(78B)	0.9600
C(78)-H(78C)	0.9600
O(1)-Zn(2)	1.901(6)
O(2)-Zn(1)	2.175(7)
O(4)-Zn(1)	2.029(7)
O(5)-Zn(3)	1.912(7)
O(6)-Zn(1)	2.032(8)
O(7)-Zn(4)	1.954(6)
O(8)-Zn(3)	1.923(7)
O(10)-Zn(4)	1.962(7)
O(11)-Zn(2)	1.966(6)
O(12)-C(9)#1	1.324(14)
O(13)-Zn(3)	1.945(7)
O(14)-Zn(2)	1.988(6)

O(16)-C(70)#4	1.34(2)
O(17)-Zn(1)	2.067(6)
O(18)-Zn(1)	2.155(7)
O(19)-Zn(2)	1.875(6)
O(19)-Zn(3)	1.918(5)
O(19)-Zn(4)	1.931(5)
O(19)-Zn(1)	2.017(5)
O(20)-C(44)#2	1.33(7)
O(21)-Zn(4)	1.904(7)
Zn(2)-Zn(4)	3.1041(17)
Zn(2)-Zn(3)	3.1232(18)
Zn(3)-Zn(4)	3.1182(17)
C(31)-C(33)	1.493(10)
C(31)-C(32)	1.500(10)
C(31)-C(34)	1.508(9)
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600

O(1)-C(1)-O(2)	124.7(10)
O(1)-C(1)-C(2)	117.7(10)
O(2)-C(1)-C(2)	117.5(10)
C(7)-C(2)-C(3)	119.3(9)
C(7)-C(2)-C(1)	119.4(10)
C(3)-C(2)-C(1)	121.3(9)
C(4)-C(3)-C(2)	123.9(10)
C(4)-C(3)-H(3)	118.0
C(2)-C(3)-H(3)	118.0
C(3)-C(4)-C(5)	115.2(11)
C(3)-C(4)-H(4)	122.4

C(5)-C(4)-H(4)	122.4
C(4)-C(5)-C(6)	122.9(11)
C(4)-C(5)-O(3)	122.9(11)
C(6)-C(5)-O(3)	114.2(12)
C(7)-C(6)-C(5)	121.2(11)
C(7)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4
C(2)-C(7)-C(6)	117.5(10)
C(2)-C(7)-H(7)	121.2
C(6)-C(7)-H(7)	121.2
C(9)-C(8)-C(13)	117.0(15)
C(9)-C(8)-O(3)	119.5(11)
C(13)-C(8)-O(3)	123.3(15)
O(12)#1-C(9)-C(8)	127.4(13)
O(12)#1-C(9)-C(10)	114.5(15)
C(8)-C(9)-C(10)	118.0(14)
C(11)-C(10)-C(9)	115.5(15)
C(11)-C(10)-H(10)	122.2
C(9)-C(10)-H(10)	122.2
C(10)-C(11)-C(12)	129.9(16)
C(10)-C(11)-H(11)	115.0
C(12)-C(11)-H(11)	115.0
C(13)-C(12)-C(11)	109.6(12)
C(13)-C(12)-C(14)	131.3(14)
C(11)-C(12)-C(14)	119.1(13)
C(12)-C(13)-C(8)	129.9(15)
C(12)-C(13)-H(13)	115.0
C(8)-C(13)-H(13)	115.0
C(12)-C(14)-C(16)	114.6(12)
C(12)-C(14)-C(15)	109.4(12)
C(16)-C(14)-C(15)	107.1(9)
C(12)-C(14)-C(17)	110.0(13)
C(16)-C(14)-C(17)	108.4(10)
C(15)-C(14)-C(17)	107.1(10)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5

H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(13)-C(18)-O(14)	124.4(10)
O(13)-C(18)-C(19)	118.8(9)
O(14)-C(18)-C(19)	116.4(11)
C(20)-C(19)-C(24)	120.0
C(20)-C(19)-C(18)	119.2(8)
C(24)-C(19)-C(18)	120.8(8)
C(19)-C(20)-C(21)	120.0
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(22)-C(21)-C(20)	120.0
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(23)-C(22)-C(21)	120.0
C(23)-C(22)-O(15)	117.9(8)
C(21)-C(22)-O(15)	122.0(8)
C(22)-C(23)-C(24)	120.0
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(19)	120.0
C(23)-C(24)-H(24)	120.0

C(19)-C(24)-H(24)	120.0
O(8)-C(35)-O(7)	125.6(9)
O(8)-C(35)-C(36)	116.9(11)
O(7)-C(35)-C(36)	117.5(11)
C(41)-C(36)-C(37)	118.3(11)
C(41)-C(36)-C(35)	120.7(11)
C(37)-C(36)-C(35)	120.8(11)
C(36)-C(37)-C(38)	121.5(11)
C(36)-C(37)-H(37)	119.2
C(38)-C(37)-H(37)	119.2
C(39)-C(38)-C(37)	113.2(13)
C(39)-C(38)-H(38)	123.4
C(37)-C(38)-H(38)	123.4
C(40)-C(39)-C(38)	124.7(12)
C(40)-C(39)-O(9)	115.8(11)
C(38)-C(39)-O(9)	119.0(13)
C(39)-C(40)-C(41)	119.8(11)
C(39)-C(40)-H(40)	120.1
C(41)-C(40)-H(40)	120.1
C(36)-C(41)-C(40)	121.9(12)
C(36)-C(41)-H(41)	119.1
C(40)-C(41)-H(41)	119.1
C(43)-C(42)-C(47)	120.0
C(43)-C(42)-H(42)	120.0
C(47)-C(42)-H(42)	120.0
O(9)-C(43)-C(42)	125.9(9)
O(9)-C(43)-C(44)	112.4(10)
C(42)-C(43)-C(44)	120.0
O(20)#2-C(44)-C(43)	122.8(11)
O(20)#2-C(44)-C(45)	117.1(11)
C(43)-C(44)-C(45)	120.0
C(46)-C(45)-C(44)	120.0
C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0
C(47)-C(46)-C(45)	120.0
C(47)-C(46)-H(46)	120.0

C(45)-C(46)-H(46)	120.0
C(46)-C(47)-C(42)	120.0
C(46)-C(47)-C(48)	116.5(9)
C(42)-C(47)-C(48)	123.2(9)
C(68)-C(67)-C(72)	120.0
C(68)-C(67)-C(66)	122.0(8)
C(72)-C(67)-C(66)	117.9(8)
C(69)-C(68)-C(67)	120.0
C(69)-C(68)-H(68)	120.0
C(67)-C(68)-H(68)	120.0
C(68)-C(69)-C(70)	120.0
C(68)-C(69)-H(69)	120.0
C(70)-C(69)-H(69)	120.0
O(16)#3-C(70)-C(69)	113.6(10)
O(16)#3-C(70)-C(71)	126.4(10)
C(69)-C(70)-C(71)	120.0
C(72)-C(71)-C(70)	120.0
C(72)-C(71)-H(71)	120.0
C(70)-C(71)-H(71)	120.0
C(71)-C(72)-C(67)	120.0
C(71)-C(72)-H(72)	120.0
C(67)-C(72)-H(72)	120.0
O(15)-C(25)-C(26)	120.8(16)
O(15)-C(25)-C(30)	119.2(16)
C(26)-C(25)-C(30)	120.0
C(25)-C(26)-C(27)	120.0
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(28)-C(27)-C(26)	120.0
C(28)-C(27)-C(31)	113.8(15)
C(26)-C(27)-C(31)	125.9(14)
C(27)-C(28)-C(29)	120.0
C(27)-C(28)-H(28)	120.0
C(29)-C(28)-H(28)	120.0
C(30)-C(29)-C(28)	120.0
C(30)-C(29)-H(29)	120.0

C(28)-C(29)-H(29)	120.0
O(16)-C(30)-C(29)	117.3(17)
O(16)-C(30)-C(25)	121.7(16)
C(29)-C(30)-C(25)	120.0
C(49)-C(48)-C(51)	113.3(12)
C(49)-C(48)-C(50)	113.7(10)
C(51)-C(48)-C(50)	113.5(11)
C(49)-C(48)-C(47)	108.7(14)
C(51)-C(48)-C(47)	101.7(15)
C(50)-C(48)-C(47)	104.7(12)
C(48)-C(49)-H(49A)	109.5
C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(48)-C(51)-H(51A)	109.5
C(48)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(48)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
O(4)-C(52)-O(5)	125.9(10)
O(4)-C(52)-C(53)	120.1(9)
O(5)-C(52)-C(53)	114.0(11)
C(58)-C(53)-C(54)	117.9(12)
C(58)-C(53)-C(52)	121.9(10)
C(54)-C(53)-C(52)	119.5(11)
C(55)-C(54)-C(53)	121.7(13)
C(55)-C(54)-H(54)	119.1

C(53)-C(54)-H(54)	119.1
C(54)-C(55)-C(56)	116.1(15)
C(54)-C(55)-H(55)	121.9
C(56)-C(55)-H(55)	121.9
O(20)-C(56)-C(55)	109.0(17)
O(20)-C(56)-C(57)	126.4(14)
C(55)-C(56)-C(57)	124.2(15)
C(58)-C(57)-C(56)	116.1(11)
C(58)-C(57)-H(57)	121.9
C(56)-C(57)-H(57)	121.9
C(57)-C(58)-C(53)	122.8(12)
C(57)-C(58)-H(58)	118.6
C(53)-C(58)-H(58)	118.6
O(10)-C(59)-O(11)	130.1(11)
O(10)-C(59)-C(60)	112.9(11)
O(11)-C(59)-C(60)	117.1(10)
C(61)-C(60)-C(65)	118.4(10)
C(61)-C(60)-C(59)	122.8(11)
C(65)-C(60)-C(59)	118.9(10)
C(60)-C(61)-C(62)	119.4(10)
C(60)-C(61)-H(61)	120.3
C(62)-C(61)-H(61)	120.3
C(63)-C(62)-C(61)	118.3(10)
C(63)-C(62)-H(62)	120.9
C(61)-C(62)-H(62)	120.9
C(64)-C(63)-C(62)	124.5(11)
C(64)-C(63)-O(12)	114.6(12)
C(62)-C(63)-O(12)	120.8(12)
C(63)-C(64)-C(65)	120.0(11)
C(63)-C(64)-H(64)	120.0
C(65)-C(64)-H(64)	120.0
C(64)-C(65)-C(60)	119.3(11)
C(64)-C(65)-H(65)	120.3
C(60)-C(65)-H(65)	120.3
O(6)-C(66)-O(21)	127.5(10)
O(6)-C(66)-C(67)	116.5(10)

O(21)-C(66)-C(67)	116.0(10)
N(2)-C(73)-O(18)	134.1(17)
N(2)-C(73)-H(73)	113.0
O(18)-C(73)-H(73)	113.0
N(2)-C(74)-H(74A)	109.5
N(2)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
N(2)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
N(2)-C(75)-H(75A)	109.5
N(2)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
N(2)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
O(17)-C(76)-N(1)	122.7(10)
O(17)-C(76)-H(76)	118.6
N(1)-C(76)-H(76)	118.6
N(1)-C(77)-H(77A)	109.5
N(1)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
N(1)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
N(1)-C(78)-H(78A)	109.5
N(1)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
N(1)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(76)-N(1)-C(78)	121.6(11)
C(76)-N(1)-C(77)	119.4(12)
C(78)-N(1)-C(77)	118.8(10)
C(73)-N(2)-C(75)	132.6(18)
C(73)-N(2)-C(74)	114.2(15)

C(75)-N(2)-C(74)	112.6(13)
C(1)-O(1)-Zn(2)	117.2(7)
C(1)-O(2)-Zn(1)	130.5(7)
C(5)-O(3)-C(8)	118.8(10)
C(52)-O(4)-Zn(1)	139.3(6)
C(52)-O(5)-Zn(3)	123.6(7)
C(66)-O(6)-Zn(1)	139.0(8)
C(35)-O(7)-Zn(4)	126.2(7)
C(35)-O(8)-Zn(3)	131.4(7)
C(43)-O(9)-C(39)	120.3(9)
C(59)-O(10)-Zn(4)	127.8(7)
C(59)-O(11)-Zn(2)	126.9(7)
C(9)#1-O(12)-C(63)	116.9(10)
C(18)-O(13)-Zn(3)	128.0(7)
C(18)-O(14)-Zn(2)	133.9(8)
C(25)-O(15)-C(22)	123.0(11)
C(30)-O(16)-C(70)#4	120(5)
C(76)-O(17)-Zn(1)	120.3(7)
C(73)-O(18)-Zn(1)	125.1(8)
Zn(2)-O(19)-Zn(3)	110.8(3)
Zn(2)-O(19)-Zn(4)	109.3(3)
Zn(3)-O(19)-Zn(4)	108.2(3)
Zn(2)-O(19)-Zn(1)	108.5(2)
Zn(3)-O(19)-Zn(1)	110.1(3)
Zn(4)-O(19)-Zn(1)	109.9(3)
C(44)#2-O(20)-C(56)	117(3)
C(66)-O(21)-Zn(4)	118.8(6)
O(19)-Zn(1)-O(4)	102.2(2)
O(19)-Zn(1)-O(6)	95.8(3)
O(4)-Zn(1)-O(6)	93.5(3)
O(19)-Zn(1)-O(17)	170.0(3)
O(4)-Zn(1)-O(17)	87.3(3)
O(6)-Zn(1)-O(17)	86.5(3)
O(19)-Zn(1)-O(18)	82.5(2)
O(4)-Zn(1)-O(18)	174.9(3)
O(6)-Zn(1)-O(18)	87.7(3)

O(17)-Zn(1)-O(18)	87.8(3)
O(19)-Zn(1)-O(2)	90.8(3)
O(4)-Zn(1)-O(2)	89.4(3)
O(6)-Zn(1)-O(2)	172.0(3)
O(17)-Zn(1)-O(2)	86.2(3)
O(18)-Zn(1)-O(2)	88.7(3)
O(19)-Zn(2)-O(1)	122.5(3)
O(19)-Zn(2)-O(11)	113.3(3)
O(1)-Zn(2)-O(11)	103.7(3)
O(19)-Zn(2)-O(14)	106.8(2)
O(1)-Zn(2)-O(14)	104.0(3)
O(11)-Zn(2)-O(14)	104.9(3)
O(19)-Zn(2)-Zn(4)	35.97(17)
O(1)-Zn(2)-Zn(4)	140.7(2)
O(11)-Zn(2)-Zn(4)	77.6(2)
O(14)-Zn(2)-Zn(4)	113.71(18)
O(19)-Zn(2)-Zn(3)	35.03(16)
O(1)-Zn(2)-Zn(3)	126.0(2)
O(11)-Zn(2)-Zn(3)	129.8(2)
O(14)-Zn(2)-Zn(3)	72.48(19)
Zn(4)-Zn(2)-Zn(3)	60.10(4)
O(5)-Zn(3)-O(19)	118.6(2)
O(5)-Zn(3)-O(8)	103.6(3)
O(19)-Zn(3)-O(8)	111.7(3)
O(5)-Zn(3)-O(13)	106.5(3)
O(19)-Zn(3)-O(13)	113.0(3)
O(8)-Zn(3)-O(13)	101.6(3)
O(5)-Zn(3)-Zn(4)	128.6(2)
O(19)-Zn(3)-Zn(4)	36.04(16)
O(8)-Zn(3)-Zn(4)	75.7(2)
O(13)-Zn(3)-Zn(4)	124.2(2)
O(5)-Zn(3)-Zn(2)	131.6(2)
O(19)-Zn(3)-Zn(2)	34.14(18)
O(8)-Zn(3)-Zn(2)	122.7(2)
O(13)-Zn(3)-Zn(2)	78.9(2)
Zn(4)-Zn(3)-Zn(2)	59.65(4)

O(21)-Zn(4)-O(19)	119.0(3)
O(21)-Zn(4)-O(7)	106.0(3)
O(19)-Zn(4)-O(7)	111.8(3)
O(21)-Zn(4)-O(10)	109.6(3)
O(19)-Zn(4)-O(10)	111.9(3)
O(7)-Zn(4)-O(10)	96.0(3)
O(21)-Zn(4)-Zn(2)	136.9(2)
O(19)-Zn(4)-Zn(2)	34.77(17)
O(7)-Zn(4)-Zn(2)	115.8(2)
O(10)-Zn(4)-Zn(2)	77.1(2)
O(21)-Zn(4)-Zn(3)	123.1(2)
O(19)-Zn(4)-Zn(3)	35.76(15)
O(7)-Zn(4)-Zn(3)	77.4(2)
O(10)-Zn(4)-Zn(3)	126.7(2)
Zn(2)-Zn(4)-Zn(3)	60.26(4)
C(27)-C(31)-C(33)	117.7(18)
C(27)-C(31)-C(32)	100.1(17)
C(33)-C(31)-C(32)	105.0(15)
C(27)-C(31)-C(34)	122(3)
C(33)-C(31)-C(34)	105.5(15)
C(32)-C(31)-C(34)	104.9(16)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5

C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+1,-z #3 -x,y+1/2,-z+1/2

#4 -x,y-1/2,-z+1/2

Table **S7**. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1⊃G**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	64(8)	68(8)	53(7)	-21(6)	17(8)	-16(6)
C(2)	65(7)	66(7)	39(6)	-9(5)	9(7)	-16(5)
C(3)	76(8)	81(8)	57(7)	-2(6)	18(7)	-26(6)
C(4)	96(10)	113(10)	50(7)	9(7)	15(8)	-34(7)
C(5)	72(9)	69(8)	98(11)	-11(7)	33(10)	-26(6)
C(6)	144(13)	109(10)	50(7)	6(7)	20(10)	-4(9)
C(7)	70(8)	94(9)	57(7)	3(6)	18(7)	-18(6)
C(8)	99(9)	112(9)	67(7)	-24(7)	5(7)	-75(7)
C(9)	89(11)	150(14)	64(8)	-49(9)	31(9)	-60(11)
C(10)	68(9)	180(15)	52(7)	-33(8)	-12(8)	-28(9)
C(11)	156(15)	148(15)	90(10)	-33(11)	59(11)	-56(12)
C(12)	88(8)	124(8)	71(7)	-18(7)	11(8)	-67(8)
C(13)	125(8)	143(8)	78(6)	-25(6)	13(8)	-56(7)
C(14)	190(17)	260(20)	119(13)	-52(14)	25(13)	-179(16)
C(15)	230(20)	320(30)	200(20)	-20(18)	20(20)	-200(20)
C(16)	270(20)	380(30)	250(20)	-20(20)	180(20)	-190(20)
C(17)	630(60)	140(20)	490(50)	-90(20)	290(50)	-190(20)
C(18)	96(8)	86(7)	61(6)	-24(6)	11(7)	24(6)
C(19)	174(6)	116(6)	109(5)	-36(5)	1(6)	65(5)
C(20)	195(7)	131(6)	120(5)	-36(5)	-9(6)	79(5)
C(21)	207(7)	140(6)	129(6)	-33(5)	-15(6)	85(5)
C(22)	275(11)	168(9)	134(8)	-22(8)	-12(9)	161(8)
C(23)	81(8)	56(8)	92(9)	-15(6)	-16(7)	-16(6)
C(24)	97(7)	59(7)	97(7)	-22(6)	32(7)	5(6)
C(35)	46(7)	140(12)	47(7)	10(7)	29(7)	9(7)
C(36)	65(8)	134(11)	59(8)	-17(7)	12(8)	-23(7)
C(37)	102(11)	206(15)	84(10)	-47(10)	33(10)	-63(10)
C(38)	143(15)	280(20)	69(9)	-48(11)	42(12)	-90(13)
C(39)	95(11)	267(18)	57(8)	-36(10)	55(10)	-80(11)

C(40)	83(10)	182(14)	63(8)	-35(8)	20(9)	-25(9)
C(41)	74(9)	159(12)	53(7)	-41(7)	18(8)	-15(8)
C(42)	111(12)	156(14)	167(15)	29(11)	79(13)	9(10)
C(43)	45(8)	203(17)	109(12)	-70(12)	36(9)	-44(10)
C(44)	78(9)	196(13)	80(8)	-32(9)	-12(8)	-41(8)
C(45)	110(9)	233(12)	100(7)	20(8)	9(9)	-22(8)
C(46)	98(9)	239(13)	103(8)	29(9)	25(9)	-10(10)
C(47)	57(8)	159(12)	34(6)	3(7)	7(7)	15(8)
C(67)	75(9)	65(9)	119(10)	-44(7)	-2(9)	-5(7)
C(68)	87(10)	81(11)	197(16)	-5(10)	-39(11)	12(9)
C(69)	132(15)	69(12)	330(30)	7(12)	-78(16)	-9(10)
C(70)	102(13)	63(12)	420(30)	-17(14)	-92(17)	29(10)
C(71)	77(10)	74(10)	380(20)	-22(13)	-94(13)	-19(9)
C(72)	61(9)	64(10)	257(19)	-30(9)	-28(11)	0(7)
C(25)	265(12)	157(11)	144(11)	9(9)	-5(10)	155(9)
C(26)	200(15)	92(13)	320(30)	60(14)	47(14)	76(12)
C(27)	90(11)	64(11)	400(30)	35(13)	-102(14)	-18(8)
C(28)	122(11)	110(10)	420(20)	41(11)	-94(13)	-6(9)
C(29)	116(10)	113(10)	430(20)	44(10)	-122(11)	11(8)
C(30)	127(11)	108(11)	430(20)	38(10)	-145(12)	29(8)
C(48)	170(18)	280(20)	330(20)	-170(20)	200(20)	-91(16)
C(49)	239(14)	277(14)	273(14)	-40(9)	34(10)	-16(9)
C(50)	63(11)	630(40)	160(17)	-10(20)	57(15)	-8(17)
C(51)	370(20)	380(20)	380(20)	12(10)	64(11)	14(10)
C(52)	34(6)	78(8)	89(9)	-13(7)	-10(7)	-9(6)
C(53)	74(9)	121(10)	100(10)	-83(8)	-5(9)	5(7)
C(54)	83(10)	183(15)	110(11)	-67(11)	-11(11)	14(9)
C(55)	96(13)	221(18)	166(17)	-112(14)	-28(13)	14(12)
C(56)	73(10)	165(13)	164(14)	-81(11)	-58(11)	23(9)
C(57)	44(8)	222(17)	105(11)	-39(11)	-25(10)	5(9)
C(58)	40(7)	141(11)	83(9)	-22(8)	-25(8)	6(7)
C(59)	33(6)	102(10)	47(7)	-16(7)	5(6)	11(6)
C(60)	47(7)	94(9)	58(7)	-33(6)	0(7)	-5(6)
C(61)	64(7)	107(9)	59(7)	-22(7)	12(7)	-45(7)
C(62)	58(8)	113(10)	71(8)	-21(8)	9(8)	-40(7)
C(63)	50(8)	99(10)	59(8)	-43(8)	-22(7)	-6(7)

C(64)	73(9)	116(10)	41(6)	-37(7)	-3(7)	-14(7)
C(65)	60(7)	98(9)	47(7)	-27(6)	-16(7)	-1(6)
C(66)	54(8)	54(8)	57(7)	0(6)	3(7)	16(6)
C(73)	115(12)	124(12)	80(9)	-62(9)	21(10)	-34(9)
C(74)	360(40)	320(30)	136(18)	-122(19)	50(20)	10(30)
C(75)	260(20)	192(17)	218(19)	-77(14)	170(20)	7(15)
C(76)	50(7)	115(10)	86(9)	-30(7)	8(8)	6(7)
C(77)	43(7)	201(16)	219(19)	56(13)	-25(10)	-58(9)
C(78)	77(10)	236(18)	150(14)	-61(13)	49(11)	28(10)
N(1)	43(6)	142(9)	108(9)	-4(7)	4(7)	4(6)
N(2)	163(14)	143(11)	90(9)	-26(9)	32(11)	20(9)
O(1)	45(4)	101(5)	55(5)	1(4)	-3(4)	-8(4)
O(2)	68(5)	90(6)	76(5)	-16(4)	26(5)	-28(4)
O(3)	99(7)	115(7)	86(6)	1(5)	26(6)	-20(5)
O(4)	45(4)	100(6)	58(4)	-23(4)	-7(4)	-3(4)
O(5)	47(5)	134(7)	77(5)	-48(4)	-19(5)	23(4)
O(6)	75(5)	65(5)	113(7)	7(5)	-16(5)	-5(4)
O(7)	64(5)	132(6)	46(4)	-26(4)	15(4)	-8(4)
O(8)	63(5)	104(6)	66(5)	-22(4)	9(5)	-24(4)
O(9)	166(10)	214(11)	114(8)	-54(7)	68(9)	-60(8)
O(10)	45(4)	93(5)	50(4)	-8(4)	-4(4)	-16(4)
O(11)	61(5)	84(6)	61(5)	-20(4)	1(4)	-22(4)
O(12)	69(5)	113(7)	73(5)	-29(5)	-20(5)	-20(5)
O(13)	122(7)	98(6)	49(4)	-24(4)	-24(5)	50(5)
O(14)	55(4)	76(5)	70(5)	-28(4)	11(4)	-1(3)
O(15)	292(10)	189(9)	157(8)	-26(7)	-13(8)	173(7)
O(16)	204(14)	87(9)	780(40)	-23(14)	-320(20)	7(9)
O(17)	42(4)	95(6)	107(6)	-34(5)	13(5)	-8(4)
O(18)	72(5)	104(6)	84(5)	-43(4)	26(5)	-3(4)
O(19)	33(3)	78(4)	53(4)	-20(3)	4(4)	0(3)
O(20)	89(8)	317(15)	165(10)	-161(10)	-78(8)	60(8)
O(21)	56(5)	74(5)	91(6)	-13(4)	-13(5)	-2(4)
Zn(1)	35(1)	73(1)	67(1)	-15(1)	4(1)	-4(1)
Zn(2)	39(1)	74(1)	51(1)	-18(1)	3(1)	-5(1)
Zn(3)	42(1)	82(1)	53(1)	-19(1)	-3(1)	0(1)
Zn(4)	41(1)	75(1)	57(1)	-16(1)	0(1)	-7(1)

C(31)	190(20)	180(20)	480(40)	-80(30)	-120(20)	-24(18)
C(32)	288(17)	301(17)	323(17)	-9(10)	29(10)	5(10)
C(33)	200(20)	89(14)	700(60)	0(20)	-180(30)	-4(14)
C(34)	540(70)	710(80)	740(80)	450(70)	-400(70)	-400(60)
O(1W)	450(30)	500(30)	129(11)	97(14)	120(16)	140(20)
O(2W)	320(20)	450(30)	350(20)	-122(19)	150(20)	-75(18)

Table **S8**. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8038(13)	6106(6)	7785(8)	67(5)
C(2)	7308(13)	6497(7)	8024(7)	74(5)
C(3)	7760(11)	6907(6)	8333(7)	65(5)
C(4)	7100(10)	7256(6)	8553(7)	66(5)
C(5)	6020(14)	7183(5)	8459(7)	62(4)
C(6)	5510(13)	6777(6)	8154(7)	70(4)
C(7)	6145(13)	6414(6)	7904(7)	76(5)
C(8)	4280(13)	7610(5)	8495(8)	54(4)
C(9)	3959(11)	7733(6)	7947(8)	62(4)
C(10)	2857(12)	7806(5)	7747(8)	73(5)
C(11)	2074(10)	7729(5)	8143(8)	56(4)
C(12)	2443(14)	7600(6)	8714(9)	88(6)
C(13)	3500(14)	7523(6)	8912(7)	73(5)
C(14)	879(11)	7804(6)	7929(7)	64(4)
C(15)	418(13)	7384(7)	7527(10)	131(8)
C(16)	186(13)	7863(10)	8405(10)	169(12)
C(17)	692(13)	8293(9)	7574(15)	226(17)
C(18)	5549(12)	8110(6)	7553(7)	56(4)
C(19)	6348(11)	8018(5)	7149(7)	62(4)
C(20)	7198(10)	8351(5)	7137(7)	58(4)
C(21)	7311(10)	8751(5)	7547(7)	53(4)
C(22)	6568(11)	8812(6)	7971(7)	66(4)
C(23)	5660(12)	8502(6)	7948(6)	59(4)
C(24)	14612(14)	6492(7)	6431(8)	80(5)
C(25)	13729(16)	6827(7)	6578(9)	105(6)
C(26)	12776(15)	6573(8)	6665(8)	105(6)
C(27)	12599(14)	6046(7)	6566(7)	72(5)

C(28)	13409(12)	5751(7)	6360(8)	88(6)
C(29)	14423(14)	5978(7)	6320(7)	87(5)
C(30)	11534(11)	5787(8)	6644(7)	68(5)
C(31)	8235(15)	4659(6)	6177(6)	62(4)
C(32)	7495(13)	4324(6)	5788(7)	63(4)
C(33)	6335(15)	4505(7)	5650(7)	82(5)
C(34)	5578(17)	4211(9)	5337(9)	124(8)
C(35)	5835(16)	3724(9)	5119(7)	82(6)
C(36)	6953(19)	3560(6)	5211(7)	85(6)
C(37)	7748(15)	3876(7)	5546(7)	82(5)
C(38)	4100(20)	3502(9)	4636(11)	130(9)
C(39)	3312(17)	3656(10)	5022(10)	158(10)
C(40)	2223(18)	3756(10)	4705(12)	142(6)
C(41)	1874(19)	3723(9)	4094(12)	147(6)
C(42)	2717(17)	3520(9)	3826(11)	147(6)
C(43)	3806(13)	3441(7)	4047(11)	98(6)
C(45)	1897(17)	4556(7)	5385(10)	149(8)
C(46)	322(17)	4120(11)	4681(12)	213(15)
C(47)	1193(17)	3670(7)	5609(9)	142(9)
C(48)	11716(11)	4110(6)	7416(11)	65(5)
C(49)	8127(15)	4322(6)	8270(8)	73(5)
C(50)	7397(13)	4028(7)	8598(9)	83(5)
C(51)	12136(14)	6237(7)	10886(11)	116(7)
C(52)	12744(17)	6522(7)	10533(10)	119(8)
C(53)	13840(20)	6541(7)	10745(11)	101(7)
C(54)	14345(16)	6288(8)	11247(9)	100(7)
C(55)	13662(15)	6025(6)	11564(7)	83(5)
C(56)	15472(16)	6802(8)	10376(8)	91(6)
C(57)	16200(20)	7221(9)	10387(9)	148(11)
C(58)	17133(17)	7258(11)	10370(11)	147(9)
C(59)	17743(15)	6810(9)	10276(9)	111(6)
C(60)	17109(13)	6331(8)	10222(8)	115(5)
C(61)	16035(13)	6378(10)	10299(9)	103(5)
C(62)	18960(16)	6824(7)	10285(8)	139(8)
C(63)	19362(17)	7324(8)	10019(12)	188(12)
C(64)	19489(15)	6836(10)	10954(8)	163(11)

C(65)	19347(17)	6368(10)	9920(10)	191(14)
C(66)	14495(15)	5791(8)	9847(10)	83(5)
C(67)	13862(15)	5388(6)	9970(8)	79(5)
C(68)	12943(14)	5303(6)	9590(9)	81(5)
C(69)	12671(16)	5613(7)	9078(9)	85(5)
C(70)	13368(15)	5992(7)	8956(8)	86(5)
C(71)	14282(15)	6089(7)	9340(10)	92(6)
C(72)	11689(16)	5515(9)	8639(11)	94(7)
O(1)	9019(8)	6197(4)	7823(5)	84(3)
O(2)	7558(8)	5712(4)	7541(5)	83(3)
O(3)	5368(9)	7545(4)	8718(4)	80(3)
O(4)	4657(8)	7780(3)	7493(4)	68(3)
O(5)	11281(7)	4136(3)	7923(5)	62(3)
O(6)	11519(8)	4342(4)	6949(5)	75(3)
O(7)	9261(9)	4538(4)	6182(5)	77(3)
O(8)	7851(8)	4983(4)	6471(5)	80(3)
O(9)	5178(11)	3377(5)	4819(6)	103(4)
O(10)	15525(9)	6754(4)	6352(5)	99(4)
O(11)	11403(8)	5349(4)	6470(5)	84(4)
O(12)	10894(8)	6060(4)	6938(5)	87(3)
O(13)	11190(8)	5076(4)	8729(5)	87(3)
O(14)	11375(11)	5819(5)	8232(8)	118(5)
O(15)	15478(10)	5873(4)	10254(5)	95(4)
O(16)	14397(11)	6835(4)	10350(6)	98(4)
O(17)	7637(8)	4544(4)	7779(5)	76(3)
O(18)	9118(8)	4372(4)	8463(5)	81(3)
O(19)	9772(7)	5104(3)	7450(5)	75(3)
Zn(1)	10220(1)	5797(1)	7619(1)	71(1)
Zn(2)	8228(1)	5091(1)	7317(1)	66(1)
Zn(3)	10400(1)	4857(1)	6732(1)	68(1)
Zn(4)	10326(1)	4672(1)	8133(1)	70(1)
C(44)	1387(17)	4059(7)	5108(8)	148(9)

Table **S9**. Bond lengths [Å] and angles [°] for Compound **1**.

C(1)-O(1)	1.225(15)
C(1)-O(2)	1.283(17)
C(1)-C(2)	1.50(2)
C(2)-C(3)	1.363(19)
C(2)-C(7)	1.44(2)
C(3)-C(4)	1.354(18)
C(3)-H(3)	0.9300
C(4)-C(5)	1.335(18)
C(4)-H(4)	0.9300
C(5)-C(6)	1.379(18)
C(5)-O(3)	1.411(16)
C(6)-C(7)	1.390(19)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.274(18)
C(8)-O(3)	1.383(16)
C(8)-C(13)	1.424(19)
C(9)-C(10)	1.391(18)
C(9)-O(4)	1.398(16)
C(10)-C(11)	1.389(18)
C(10)-H(10)	0.9300
C(11)-C(12)	1.337(19)
C(11)-C(14)	1.506(18)
C(12)-C(13)	1.340(19)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(14)-C(16)	1.44(2)
C(14)-C(15)	1.49(2)
C(14)-C(17)	1.51(2)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600

C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(23)	1.352(18)
C(18)-O(4)	1.394(15)
C(18)-C(19)	1.424(19)
C(19)-C(20)	1.368(17)
C(19)-H(19)	0.9300
C(20)-C(21)	1.389(18)
C(20)-H(20)	0.9300
C(21)-C(22)	1.391(18)
C(21)-C(48)#1	1.521(19)
C(22)-C(23)	1.381(18)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-O(10)	1.347(16)
C(24)-C(29)	1.39(2)
C(24)-C(25)	1.47(2)
C(25)-C(26)	1.38(2)
C(25)-H(25)	0.9300
C(26)-C(27)	1.42(2)
C(26)-H(26)	0.9300
C(27)-C(28)	1.38(2)
C(27)-C(30)	1.50(2)
C(28)-C(29)	1.395(19)
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
C(30)-O(11)	1.222(18)
C(30)-O(12)	1.296(17)
C(31)-O(8)	1.204(17)
C(31)-O(7)	1.302(18)
C(31)-C(32)	1.473(19)
C(32)-C(37)	1.348(19)
C(32)-C(33)	1.50(2)
C(33)-C(34)	1.34(2)

C(33)-H(33)	0.9300
C(34)-C(35)	1.42(2)
C(34)-H(34)	0.9300
C(35)-O(9)	1.347(19)
C(35)-C(36)	1.43(2)
C(36)-C(37)	1.43(2)
C(36)-H(36)	0.9300
C(37)-H(37)	0.9300
C(38)-C(43)	1.32(2)
C(38)-O(9)	1.39(3)
C(38)-C(39)	1.42(3)
C(39)-C(40)	1.46(3)
C(39)-H(39)	0.9300
C(40)-C(41)	1.37(3)
C(40)-C(44)	1.64(3)
C(41)-C(42)	1.36(3)
C(41)-H(41)	0.9300
C(42)-C(43)	1.39(2)
C(42)-H(42)	0.9300
C(43)-O(10)#2	1.374(19)
C(45)-C(44)	1.551(10)
C(45)-H(45A)	0.9600
C(45)-H(45B)	0.9600
C(45)-H(45C)	0.9600
C(46)-C(44)	1.534(10)
C(46)-H(46A)	0.9600
C(46)-H(46B)	0.9600
C(46)-H(46C)	0.9600
C(47)-C(44)	1.547(10)
C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600
C(47)-H(47C)	0.9600
C(48)-O(6)	1.20(2)
C(48)-O(5)	1.30(2)
C(48)-C(21)#3	1.521(19)
C(49)-O(18)	1.252(17)

C(49)-O(17)	1.318(16)
C(49)-C(50)	1.44(2)
C(50)-C(55)#4	1.319(19)
C(50)-C(51)#4	1.40(2)
C(51)-C(52)	1.37(2)
C(51)-C(50)#4	1.40(2)
C(51)-H(51)	0.9300
C(52)-C(53)	1.38(3)
C(52)-H(52)	0.9300
C(53)-C(54)	1.38(3)
C(53)-O(16)	1.405(19)
C(54)-C(55)	1.35(2)
C(54)-H(54)	0.9300
C(55)-C(50)#4	1.319(19)
C(55)-H(55)	0.9300
C(56)-O(16)	1.322(19)
C(56)-C(61)	1.34(2)
C(56)-C(57)	1.42(2)
C(57)-C(58)	1.15(2)
C(57)-H(57)	0.9300
C(58)-C(59)	1.43(3)
C(58)-H(58)	0.9300
C(59)-C(60)	1.48(3)
C(59)-C(62)	1.50(2)
C(60)-C(61)	1.36(2)
C(60)-H(60)	0.9300
C(61)-O(15)	1.50(2)
C(62)-C(63)	1.547(10)
C(62)-C(64)	1.548(10)
C(62)-C(65)	1.554(10)
C(63)-H(63A)	0.9600
C(63)-H(63B)	0.9600
C(63)-H(63C)	0.9600
C(64)-H(64A)	0.9600
C(64)-H(64B)	0.9600
C(64)-H(64C)	0.9600

C(65)-H(65A)	0.9600
C(65)-H(65B)	0.9600
C(65)-H(65C)	0.9600
C(66)-C(67)	1.36(2)
C(66)-C(71)	1.37(2)
C(66)-O(15)	1.440(19)
C(67)-C(68)	1.35(2)
C(67)-H(67)	0.9300
C(68)-C(69)	1.41(2)
C(68)-H(68)	0.9300
C(69)-C(70)	1.37(2)
C(69)-C(72)	1.48(2)
C(70)-C(71)	1.35(2)
C(70)-H(70)	0.9300
C(71)-H(71)	0.9300
C(72)-O(14)	1.23(2)
C(72)-O(13)	1.34(2)
O(1)-Zn(1)	1.910(10)
O(2)-Zn(2)	1.924(10)
O(5)-Zn(4)	1.928(9)
O(6)-Zn(3)	1.954(12)
O(7)-Zn(3)	1.939(12)
O(8)-Zn(2)	1.899(12)
O(10)-C(43)#2	1.374(19)
O(11)-Zn(3)	1.925(11)
O(12)-Zn(1)	1.929(11)
O(13)-Zn(4)	1.919(12)
O(14)-Zn(1)	1.851(15)
O(17)-Zn(2)	1.957(10)
O(18)-Zn(4)	1.904(10)
O(19)-Zn(2)	1.889(9)
O(19)-Zn(1)	1.933(9)
O(19)-Zn(4)	1.952(10)
O(19)-Zn(3)	1.956(10)
Zn(1)-Zn(2)	3.090(3)
Zn(3)-Zn(4)	3.149(3)

O(1)-C(1)-O(2)	126.1(14)
O(1)-C(1)-C(2)	117.8(17)
O(2)-C(1)-C(2)	116.0(14)
C(3)-C(2)-C(7)	123.5(14)
C(3)-C(2)-C(1)	119.6(16)
C(7)-C(2)-C(1)	116.9(16)
C(4)-C(3)-C(2)	119.5(14)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(5)-C(4)-C(3)	118.2(14)
C(5)-C(4)-H(4)	120.9
C(3)-C(4)-H(4)	120.9
C(4)-C(5)-C(6)	125.3(14)
C(4)-C(5)-O(3)	116.2(14)
C(6)-C(5)-O(3)	118.4(14)
C(5)-C(6)-C(7)	118.9(15)
C(5)-C(6)-H(6)	120.5
C(7)-C(6)-H(6)	120.5
C(6)-C(7)-C(2)	114.5(15)
C(6)-C(7)-H(7)	122.8
C(2)-C(7)-H(7)	122.8
C(9)-C(8)-O(3)	123.7(15)
C(9)-C(8)-C(13)	119.9(15)
O(3)-C(8)-C(13)	116.4(15)
C(8)-C(9)-C(10)	121.5(15)
C(8)-C(9)-O(4)	123.8(14)
C(10)-C(9)-O(4)	114.6(15)
C(9)-C(10)-C(11)	120.0(17)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	116.6(15)
C(12)-C(11)-C(14)	122.9(14)
C(10)-C(11)-C(14)	120.4(16)
C(11)-C(12)-C(13)	124.0(17)
C(11)-C(12)-H(12)	118.0

C(13)-C(12)-H(12)	118.0
C(12)-C(13)-C(8)	117.7(15)
C(12)-C(13)-H(13)	121.1
C(8)-C(13)-H(13)	121.1
C(16)-C(14)-C(15)	107.4(15)
C(16)-C(14)-C(11)	115.2(15)
C(15)-C(14)-C(11)	112.3(12)
C(16)-C(14)-C(17)	102.8(17)
C(15)-C(14)-C(17)	107.3(19)
C(11)-C(14)-C(17)	111.1(13)
C(23)-C(18)-O(4)	123.9(15)
C(23)-C(18)-C(19)	120.7(14)
O(4)-C(18)-C(19)	115.3(14)
C(20)-C(19)-C(18)	119.2(14)
C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(19)-C(20)-C(21)	119.7(14)
C(19)-C(20)-H(20)	120.2
C(21)-C(20)-H(20)	120.2
C(20)-C(21)-C(22)	120.2(13)
C(20)-C(21)-C(48)#1	121.9(15)
C(22)-C(21)-C(48)#1	117.7(15)
C(23)-C(22)-C(21)	119.9(15)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(18)-C(23)-C(22)	119.9(15)
C(18)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
O(10)-C(24)-C(29)	127.0(17)
O(10)-C(24)-C(25)	111.7(16)
C(29)-C(24)-C(25)	120.8(15)
C(26)-C(25)-C(24)	113.7(16)
C(26)-C(25)-H(25)	123.2
C(24)-C(25)-H(25)	123.2
C(25)-C(26)-C(27)	124.8(17)
C(25)-C(26)-H(26)	117.6

C(27)-C(26)-H(26)	117.6
C(28)-C(27)-C(26)	119.8(16)
C(28)-C(27)-C(30)	116.9(15)
C(26)-C(27)-C(30)	123.2(16)
C(27)-C(28)-C(29)	117.7(15)
C(27)-C(28)-H(28)	121.2
C(29)-C(28)-H(28)	121.2
C(28)-C(29)-C(24)	122.6(16)
C(28)-C(29)-H(29)	118.7
C(24)-C(29)-H(29)	118.7
O(11)-C(30)-O(12)	128.1(15)
O(11)-C(30)-C(27)	118.6(15)
O(12)-C(30)-C(27)	113.0(17)
O(8)-C(31)-O(7)	127.6(14)
O(8)-C(31)-C(32)	119.1(17)
O(7)-C(31)-C(32)	113.2(16)
C(37)-C(32)-C(31)	127.0(17)
C(37)-C(32)-C(33)	117.0(15)
C(31)-C(32)-C(33)	116.0(16)
C(34)-C(33)-C(32)	120.6(17)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(33)-C(34)-C(35)	122(2)
C(33)-C(34)-H(34)	119.0
C(35)-C(34)-H(34)	119.0
O(9)-C(35)-C(34)	129.7(19)
O(9)-C(35)-C(36)	112(2)
C(34)-C(35)-C(36)	118.2(17)
C(37)-C(36)-C(35)	119.1(16)
C(37)-C(36)-H(36)	120.5
C(35)-C(36)-H(36)	120.5
C(32)-C(37)-C(36)	122.9(17)
C(32)-C(37)-H(37)	118.6
C(36)-C(37)-H(37)	118.6
C(43)-C(38)-O(9)	114(2)
C(43)-C(38)-C(39)	120(3)

O(9)-C(38)-C(39)	126(2)
C(38)-C(39)-C(40)	114(2)
C(38)-C(39)-H(39)	122.9
C(40)-C(39)-H(39)	122.9
C(41)-C(40)-C(39)	129(2)
C(41)-C(40)-C(44)	115(2)
C(39)-C(40)-C(44)	115.0(19)
C(42)-C(41)-C(40)	107(2)
C(42)-C(41)-H(41)	126.7
C(40)-C(41)-H(41)	126.7
C(41)-C(42)-C(43)	131(2)
C(41)-C(42)-H(42)	114.5
C(43)-C(42)-H(42)	114.5
C(38)-C(43)-O(10)#2	124(2)
C(38)-C(43)-C(42)	118(2)
O(10)#2-C(43)-C(42)	117(2)
O(6)-C(48)-O(5)	130.8(15)
O(6)-C(48)-C(21)#3	116.3(17)
O(5)-C(48)-C(21)#3	112.7(17)
O(18)-C(49)-O(17)	124.8(17)
O(18)-C(49)-C(50)	121.5(16)
O(17)-C(49)-C(50)	113.6(16)
C(55)#4-C(50)-C(51)#4	117.9(17)
C(55)#4-C(50)-C(49)	124.9(19)
C(51)#4-C(50)-C(49)	117.1(17)
C(52)-C(51)-C(50)#4	122.6(18)
C(52)-C(51)-H(51)	118.7
C(50)#4-C(51)-H(51)	118.7
C(51)-C(52)-C(53)	113.7(19)
C(51)-C(52)-H(52)	123.1
C(53)-C(52)-H(52)	123.1
C(52)-C(53)-C(54)	126.3(17)
C(52)-C(53)-O(16)	110(2)
C(54)-C(53)-O(16)	124(2)
C(55)-C(54)-C(53)	114.6(19)
C(55)-C(54)-H(54)	122.7

C(53)-C(54)-H(54)	122.7
C(50)#4-C(55)-C(54)	124.7(19)
C(50)#4-C(55)-H(55)	117.7
C(54)-C(55)-H(55)	117.7
O(16)-C(56)-C(61)	125.5(19)
O(16)-C(56)-C(57)	125(2)
C(61)-C(56)-C(57)	108(2)
C(58)-C(57)-C(56)	134(3)
C(58)-C(57)-H(57)	113.1
C(56)-C(57)-H(57)	113.1
C(57)-C(58)-C(59)	118(3)
C(57)-C(58)-H(58)	120.8
C(59)-C(58)-H(58)	120.8
C(58)-C(59)-C(60)	115.9(18)
C(58)-C(59)-C(62)	121(2)
C(60)-C(59)-C(62)	122.6(19)
C(61)-C(60)-C(59)	115(2)
C(61)-C(60)-H(60)	122.5
C(59)-C(60)-H(60)	122.5
C(56)-C(61)-C(60)	128(2)
C(56)-C(61)-O(15)	121.0(15)
C(60)-C(61)-O(15)	111(2)
C(59)-C(62)-C(63)	112.3(16)
C(59)-C(62)-C(64)	108.9(16)
C(63)-C(62)-C(64)	103.2(17)
C(59)-C(62)-C(65)	109.8(17)
C(63)-C(62)-C(65)	109(2)
C(64)-C(62)-C(65)	113.0(18)
C(67)-C(66)-C(71)	123.4(18)
C(67)-C(66)-O(15)	117(2)
C(71)-C(66)-O(15)	119.5(18)
C(68)-C(67)-C(66)	117.7(18)
C(68)-C(67)-H(67)	121.2
C(66)-C(67)-H(67)	121.2
C(67)-C(68)-C(69)	120.7(17)
C(67)-C(68)-H(68)	119.6

C(69)-C(68)-H(68)	119.6
C(70)-C(69)-C(68)	119.2(18)
C(70)-C(69)-C(72)	118.7(19)
C(68)-C(69)-C(72)	121.9(19)
C(71)-C(70)-C(69)	120.6(18)
C(71)-C(70)-H(70)	119.7
C(69)-C(70)-H(70)	119.7
C(70)-C(71)-C(66)	118.2(18)
C(70)-C(71)-H(71)	120.9
C(66)-C(71)-H(71)	120.9
O(14)-C(72)-O(13)	124(2)
O(14)-C(72)-C(69)	121.9(19)
O(13)-C(72)-C(69)	114(2)
C(1)-O(1)-Zn(1)	131.3(11)
C(1)-O(2)-Zn(2)	127.4(9)
C(8)-O(3)-C(5)	120.7(12)
C(18)-O(4)-C(9)	122.0(11)
C(48)-O(5)-Zn(4)	124.7(10)
C(48)-O(6)-Zn(3)	129.2(11)
C(31)-O(7)-Zn(3)	122.0(9)
C(31)-O(8)-Zn(2)	125.0(10)
C(35)-O(9)-C(38)	119.0(17)
C(24)-O(10)-C(43)#2	117.5(13)
C(30)-O(11)-Zn(3)	127.5(11)
C(30)-O(12)-Zn(1)	122.1(10)
C(72)-O(13)-Zn(4)	127.3(13)
C(72)-O(14)-Zn(1)	131.7(14)
C(66)-O(15)-C(61)	121.4(13)
C(56)-O(16)-C(53)	119.7(17)
C(49)-O(17)-Zn(2)	126.5(10)
C(49)-O(18)-Zn(4)	133.3(12)
Zn(2)-O(19)-Zn(1)	107.9(5)
Zn(2)-O(19)-Zn(4)	111.5(4)
Zn(1)-O(19)-Zn(4)	109.6(5)
Zn(2)-O(19)-Zn(3)	110.6(5)
Zn(1)-O(19)-Zn(3)	110.0(4)

Zn(4)-O(19)-Zn(3)	107.4(4)
O(14)-Zn(1)-O(1)	111.1(6)
O(14)-Zn(1)-O(12)	101.4(6)
O(1)-Zn(1)-O(12)	113.5(5)
O(14)-Zn(1)-O(19)	110.4(5)
O(1)-Zn(1)-O(19)	110.8(4)
O(12)-Zn(1)-O(19)	109.1(4)
O(14)-Zn(1)-Zn(2)	134.5(5)
O(1)-Zn(1)-Zn(2)	76.5(3)
O(12)-Zn(1)-Zn(2)	116.7(3)
O(19)-Zn(1)-Zn(2)	35.6(3)
O(19)-Zn(2)-O(8)	106.5(4)
O(19)-Zn(2)-O(2)	113.4(4)
O(8)-Zn(2)-O(2)	108.5(5)
O(19)-Zn(2)-O(17)	111.1(4)
O(8)-Zn(2)-O(17)	109.9(5)
O(2)-Zn(2)-O(17)	107.3(4)
O(19)-Zn(2)-Zn(1)	36.6(3)
O(8)-Zn(2)-Zn(1)	113.7(3)
O(2)-Zn(2)-Zn(1)	77.5(3)
O(17)-Zn(2)-Zn(1)	131.7(3)
O(11)-Zn(3)-O(7)	123.1(5)
O(11)-Zn(3)-O(6)	94.8(4)
O(7)-Zn(3)-O(6)	106.9(4)
O(11)-Zn(3)-O(19)	110.2(5)
O(7)-Zn(3)-O(19)	109.3(4)
O(6)-Zn(3)-O(19)	111.4(5)
O(11)-Zn(3)-Zn(4)	119.5(4)
O(7)-Zn(3)-Zn(4)	116.8(3)
O(6)-Zn(3)-Zn(4)	75.5(3)
O(19)-Zn(3)-Zn(4)	36.3(3)
O(18)-Zn(4)-O(13)	111.3(5)
O(18)-Zn(4)-O(5)	108.2(4)
O(13)-Zn(4)-O(5)	105.5(4)
O(18)-Zn(4)-O(19)	108.7(4)
O(13)-Zn(4)-O(19)	109.0(4)

O(5)-Zn(4)-O(19)	114.2(4)
O(18)-Zn(4)-Zn(3)	123.6(4)
O(13)-Zn(4)-Zn(3)	121.0(3)
O(5)-Zn(4)-Zn(3)	77.8(3)
O(19)-Zn(4)-Zn(3)	36.4(3)
C(46)-C(44)-C(47)	108.6(17)
C(46)-C(44)-C(45)	115.7(19)
C(47)-C(44)-C(45)	111.5(16)
C(46)-C(44)-C(40)	105.1(18)
C(47)-C(44)-C(40)	102.9(16)
C(45)-C(44)-C(40)	112.1(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y+1/2,-z+3/2 #2 -x+2,-y+1,-z+1 #3 -x+2,y-1/2,-z+3/2

#4 -x+2,-y+1,-z+2

Table **S10**. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	43(10)	67(12)	93(13)	21(10)	19(9)	14(9)
C(2)	70(12)	85(13)	71(13)	22(10)	34(10)	15(10)
C(3)	35(8)	80(12)	84(13)	-31(10)	20(8)	-9(9)
C(4)	19(8)	89(12)	89(13)	-12(9)	-6(8)	-20(8)
C(5)	84(12)	47(10)	58(11)	-3(8)	15(9)	7(9)
C(6)	73(11)	80(12)	60(12)	1(10)	27(9)	-7(10)
C(7)	75(12)	70(11)	90(13)	-7(9)	44(10)	2(9)
C(8)	67(12)	53(9)	38(11)	-24(8)	-8(10)	12(8)
C(9)	30(8)	118(13)	38(11)	-41(10)	12(8)	-21(8)
C(10)	49(10)	42(9)	130(15)	-18(9)	11(10)	-18(7)
C(11)	25(8)	53(9)	94(13)	-30(9)	27(9)	-19(7)
C(12)	66(11)	112(15)	82(15)	25(11)	-2(10)	25(11)
C(13)	94(12)	84(12)	40(11)	-4(8)	8(10)	26(10)
C(14)	46(10)	64(11)	82(12)	-9(9)	-1(9)	-9(8)
C(15)	53(11)	126(17)	210(20)	-49(17)	-7(13)	9(11)
C(16)	47(11)	300(30)	160(20)	-140(20)	26(13)	-43(15)
C(17)	30(11)	190(20)	460(50)	170(30)	58(18)	45(13)
C(18)	47(10)	61(11)	57(12)	9(9)	-12(9)	11(8)
C(19)	50(9)	54(10)	80(12)	-2(8)	-4(9)	7(8)
C(20)	20(7)	67(10)	81(12)	0(9)	-12(7)	-10(7)
C(21)	21(7)	64(10)	72(11)	-3(9)	3(8)	-3(7)
C(22)	32(8)	86(12)	75(12)	7(9)	-10(8)	7(8)
C(23)	61(10)	101(13)	14(8)	-8(8)	5(7)	5(9)
C(24)	76(12)	86(14)	83(13)	-1(10)	22(10)	-29(11)
C(25)	104(15)	86(13)	135(18)	-12(12)	62(13)	17(12)
C(26)	90(14)	123(18)	114(17)	-16(13)	62(12)	-12(13)
C(27)	95(14)	64(12)	60(12)	3(9)	19(10)	-4(10)
C(28)	50(10)	90(13)	131(16)	-33(11)	39(10)	-18(10)
C(29)	93(14)	92(15)	83(14)	-15(11)	39(10)	-2(11)

C(30)	31(9)	113(15)	65(12)	21(11)	25(8)	16(10)
C(31)	93(14)	63(11)	23(10)	-2(8)	-18(9)	-17(11)
C(32)	85(13)	62(11)	44(10)	1(9)	21(9)	-8(9)
C(33)	87(13)	92(13)	75(13)	-10(10)	45(10)	-4(12)
C(34)	121(17)	150(20)	110(18)	-74(15)	69(14)	-92(16)
C(35)	74(13)	121(17)	46(12)	4(11)	-12(10)	-35(13)
C(36)	170(20)	54(11)	35(11)	-14(8)	23(12)	-13(13)
C(37)	110(14)	77(13)	61(12)	-7(10)	18(10)	-6(11)
C(38)	160(20)	170(20)	65(15)	-71(14)	55(16)	-106(17)
C(39)	94(15)	290(30)	89(16)	-129(17)	13(13)	-12(16)
C(40)	90(12)	205(14)	131(15)	-46(13)	16(11)	-32(11)
C(41)	96(11)	204(14)	141(15)	-58(12)	21(11)	-26(11)
C(42)	89(11)	203(15)	152(15)	-50(13)	20(11)	-25(12)
C(43)	34(9)	129(16)	140(20)	-28(14)	44(12)	-26(10)
C(45)	160(20)	155(19)	150(20)	-20(15)	68(16)	-41(16)
C(46)	111(19)	290(40)	220(30)	110(30)	-80(20)	10(20)
C(47)	170(20)	148(19)	123(19)	52(15)	87(16)	22(16)
C(48)	26(9)	53(11)	119(18)	-32(11)	17(11)	-20(8)
C(49)	72(13)	86(13)	58(12)	6(10)	-8(11)	13(11)
C(50)	41(10)	95(14)	120(17)	-8(12)	40(11)	-2(10)
C(51)	62(13)	105(16)	180(20)	50(15)	6(14)	49(12)
C(52)	83(15)	106(16)	180(20)	78(15)	59(16)	13(13)
C(53)	130(20)	81(13)	110(19)	13(13)	85(17)	-29(13)
C(54)	114(16)	117(17)	75(15)	-30(13)	30(13)	-67(14)
C(55)	97(14)	89(12)	64(12)	-7(9)	8(10)	-65(11)
C(56)	61(13)	127(17)	74(14)	11(11)	-40(10)	-1(13)
C(57)	160(20)	170(20)	109(18)	7(15)	-13(18)	-110(20)
C(58)	53(13)	200(20)	180(30)	21(19)	-32(15)	-40(13)
C(59)	63(9)	160(14)	110(11)	88(11)	14(9)	-3(9)
C(60)	61(8)	164(12)	121(10)	88(10)	12(8)	10(9)
C(61)	43(8)	153(13)	114(11)	86(10)	13(9)	4(10)
C(62)	96(12)	200(20)	118(17)	70(16)	-17(13)	-33(13)
C(63)	112(18)	250(30)	210(30)	120(20)	38(18)	-7(18)
C(64)	90(15)	310(30)	92(18)	-34(18)	6(13)	-36(18)
C(65)	128(19)	320(40)	120(20)	-70(20)	15(15)	130(20)
C(66)	71(13)	77(14)	98(17)	-32(12)	-5(12)	-3(11)

C(67)	82(13)	40(10)	116(16)	-7(10)	15(12)	6(10)
C(68)	68(12)	64(12)	113(16)	-38(12)	15(11)	-31(10)
C(69)	113(16)	62(12)	79(15)	-1(11)	13(13)	-1(12)
C(70)	85(13)	89(13)	84(14)	21(11)	4(11)	-18(11)
C(71)	72(13)	114(16)	88(16)	1(13)	-1(12)	-22(12)
C(72)	68(14)	120(20)	102(19)	-63(15)	31(13)	-45(14)
O(1)	55(7)	72(7)	128(10)	-6(6)	29(7)	-14(6)
O(2)	52(7)	62(7)	133(10)	-26(7)	7(6)	-8(6)
O(3)	84(8)	95(8)	60(7)	0(6)	7(6)	24(7)
O(4)	57(7)	75(7)	71(8)	-19(6)	3(6)	-7(6)
O(5)	39(6)	64(6)	87(8)	-4(6)	21(5)	10(5)
O(6)	63(7)	86(9)	79(9)	20(7)	25(6)	-2(6)
O(7)	91(8)	70(7)	76(8)	-3(6)	32(7)	24(6)
O(8)	89(8)	54(7)	98(10)	-18(6)	19(7)	10(6)
O(9)	98(10)	115(10)	96(10)	-37(8)	16(8)	-70(9)
O(10)	75(8)	122(9)	109(10)	-14(7)	49(7)	-50(7)
O(11)	79(8)	54(7)	123(10)	4(7)	24(7)	1(6)
O(12)	63(7)	75(7)	131(10)	0(7)	47(7)	-20(6)
O(13)	66(7)	96(9)	101(9)	-1(7)	24(6)	-15(7)
O(14)	105(11)	103(11)	141(14)	6(9)	-3(10)	-11(9)
O(15)	100(9)	81(9)	107(10)	28(7)	25(8)	36(8)
O(16)	86(9)	93(9)	116(11)	-17(8)	10(8)	2(7)
O(17)	56(7)	78(7)	98(9)	-3(7)	25(6)	-10(6)
O(18)	40(6)	80(7)	125(10)	1(7)	9(6)	1(6)
O(19)	62(6)	71(7)	98(8)	1(6)	29(6)	-6(5)
Zn(1)	49(1)	67(1)	99(2)	-3(1)	21(1)	-7(1)
Zn(2)	53(1)	63(1)	84(2)	-4(1)	21(1)	-5(1)
Zn(3)	51(1)	63(1)	90(2)	4(1)	13(1)	-1(1)
Zn(4)	52(1)	69(1)	89(2)	-4(1)	16(1)	-7(1)
C(44)	200(30)	125(18)	130(20)	-10(14)	67(18)	-44(16)

Table **S11**. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Compound **1⊃PX'**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6750(20)	9374(6)	3302(11)	110(6)
C(2)	7591(13)	9274(5)	3785(6)	122(6)
C(3)	7225(12)	9081(6)	4213(8)	255(12)
C(4)	7995(17)	8953(6)	4633(6)	256(13)
C(5)	9130(16)	9019(5)	4626(6)	160(7)
C(6)	9495(11)	9212(5)	4199(7)	136(7)
C(7)	8726(15)	9340(4)	3778(6)	94(6)
C(8)	10650(11)	9088(6)	5266(6)	154(6)
C(9)	11454(16)	8804(4)	5166(6)	166(6)
C(10)	12581(14)	8894(5)	5299(6)	156(5)
C(11)	12905(12)	9268(6)	5533(6)	129(5)
C(12)	12102(18)	9552(4)	5634(5)	128(7)
C(13)	10974(15)	9462(5)	5500(6)	128(7)
C(14)	9200(20)	9643(10)	5729(11)	164(9)
C(15)	9280(40)	9449(12)	6185(14)	320(30)
C(16)	8480(30)	9506(10)	6548(9)	240(20)
C(17)	7764(18)	9820(6)	6438(9)	85(5)
C(18)	7749(15)	10015(6)	5972(8)	95(6)
C(19)	8450(20)	9915(9)	5617(9)	160(9)
C(20)	14200(20)	9301(9)	5604(11)	139(6)
C(21)	14593(18)	9366(11)	5104(10)	216(16)
C(22)	14350(20)	9718(10)	5885(11)	196(9)
C(23)	14780(20)	9094(16)	5981(16)	350(30)
C(24)	6897(16)	11168(7)	7791(10)	66(5)
C(25)	7570(19)	11538(6)	7811(8)	64(5)
C(26)	8290(16)	11634(5)	8231(8)	61(5)
C(27)	8958(15)	11985(6)	8260(8)	89(5)
C(28)	8845(17)	12256(7)	7853(9)	100(5)

C(29)	8070(19)	12181(7)	7427(9)	116(7)
C(30)	7423(16)	11813(7)	7403(9)	96(6)
C(31)	10000(30)	12772(7)	8296(11)	111(6)
C(32)	11170(30)	12713(7)	8393(14)	150(9)
C(33)	11740(20)	12862(8)	8896(17)	147(11)
C(34)	11130(30)	13053(8)	9242(13)	155(11)
C(35)	9990(20)	13083(6)	9160(10)	129(6)
C(36)	9470(20)	12938(6)	8671(10)	119(5)
C(37)	12980(30)	12841(11)	9005(16)	207(10)
C(38)	13260(30)	12353(12)	9076(14)	259(16)
C(39)	13400(20)	13036(10)	9516(13)	221(11)
C(40)	13580(20)	13023(9)	8596(13)	211(11)
C(41)	2205(18)	8278(8)	6689(8)	101(5)
C(42)	3297(18)	8226(6)	6867(8)	106(6)
C(43)	3868(15)	8563(7)	7122(7)	98(5)
C(44)	3385(19)	8930(7)	7202(8)	89(6)
C(45)	2260(20)	8957(6)	7023(8)	104(7)
C(46)	1643(17)	8626(9)	6793(9)	115(7)
C(47)	3950(20)	9307(8)	7421(7)	84(6)
C(48)	7245(13)	9841(8)	8771(10)	70(6)
C(49)	8064(17)	9660(7)	9217(9)	91(5)
C(50)	8678(14)	9328(6)	9105(8)	96(5)
C(51)	9483(16)	9165(6)	9534(9)	105(6)
C(52)	9525(18)	9351(8)	9994(10)	107(6)
C(53)	8940(19)	9656(7)	10118(9)	114(6)
C(54)	8175(16)	9822(6)	9714(9)	102(6)
C(54A)	7040(14)	9916(8)	6845(9)	76(6)
C(55)	10774(15)	8882(5)	10413(6)	120(8)
C(56)	11924(16)	8930(4)	10535(6)	152(6)
C(57)	12622(11)	8589(6)	10547(5)	147(6)
C(58)	12170(14)	8201(5)	10436(6)	139(6)
C(59)	11021(15)	8154(4)	10314(6)	162(7)
C(60)	10323(11)	8494(6)	10302(5)	113(7)
C(61)	13180(20)	7906(8)	10476(10)	126(7)
C(62)	12750(50)	7472(10)	10335(17)	400(40)
C(63)	13660(20)	7895(13)	11010(10)	270(20)

C(64)	13933(17)	8037(9)	10079(10)	188(12)
C(65)	8410(30)	8592(6)	10515(15)	97(7)
C(66)	8683(17)	8648(6)	11002(14)	86(6)
C(67)	7900(30)	8837(6)	11301(8)	83(6)
C(68)	6790(20)	8934(6)	11079(12)	74(6)
C(69)	6528(16)	8835(6)	10571(15)	82(5)
C(70)	7310(30)	8664(6)	10254(8)	95(6)
C(71)	3940(20)	10868(5)	8605(11)	74(7)
C(72S)	5050(30)	9404(18)	9339(17)	420(50)
C(73S)	3250(50)	9319(16)	9560(20)	550(60)
C(74S)	3560(30)	9727(11)	8784(15)	175(12)
C(75S)	-100(20)	10190(16)	8331(14)	350(40)
C(76S)	-780(20)	10514(10)	7636(15)	242(18)
C(77S)	1150(20)	10284(7)	7733(8)	105(7)
C(78S)	4760(30)	2481(13)	7450(20)	410(40)
C(79S)	3790(30)	2204(15)	7373(12)	250(20)
C(80S)	2770(40)	2398(8)	7229(11)	228(18)
C(81S)	1790(30)	2170(13)	7170(10)	223(15)
C(82S)	1830(30)	1748(12)	7254(12)	197(15)
C(83S)	700(30)	1462(10)	7242(13)	245(18)
C(84S)	2900(40)	1592(11)	7418(11)	250(30)
C(85S)	3940(50)	1782(15)	7480(30)	410(50)
N(1)	4020(30)	9543(9)	9284(13)	228(14)
N(2)	126(14)	10296(5)	7885(8)	106(5)
O(1)	5769(10)	9280(4)	3348(4)	96(4)
O(2)	7108(8)	9563(4)	2942(5)	75(3)
O(3)	9631(17)	8897(7)	5180(8)	213(8)
O(4)	9910(20)	9618(11)	5356(7)	350(20)
O(5)	6962(10)	9707(4)	7215(5)	93(5)
O(6)	6514(10)	10265(4)	6750(4)	79(3)
O(7)	6265(10)	11080(3)	7345(6)	81(4)
O(8)	6914(9)	10955(4)	8187(5)	70(4)
O(9)	9465(13)	12626(4)	7831(6)	133(5)
O(10)	8298(12)	12943(4)	8565(7)	142(6)
O(11)	5022(13)	9249(3)	7588(5)	90(4)
O(12)	3420(11)	9620(5)	7451(6)	111(5)

O(13)	7014(10)	9626(4)	8356(5)	75(4)
O(14)	6840(10)	10189(4)	8864(4)	75(4)
O(15)	10217(11)	9201(6)	10451(6)	159(7)
O(16)	9092(14)	8408(4)	10157(5)	128(5)
O(17)	3577(10)	10764(4)	8149(6)	83(4)
O(18)	4952(13)	10812(4)	8834(5)	86(4)
O(19)	1932(11)	10120(4)	7969(6)	127(5)
O(20)	4156(10)	9895(4)	8537(6)	119(5)
O(100)	5243(7)	10253(3)	7751(3)	57(3)
Zn(1)	5946(2)	9723(1)	7744(1)	81(1)
Zn(2)	5492(2)	10567(1)	7154(1)	78(1)
Zn(3)	5862(2)	10532(1)	8381(1)	78(1)
Zn(4)	3579(2)	10185(1)	7777(1)	88(1)

Table **S12**. Bond lengths [Å] and angles [°] for Compound **1⊃PX'**.

C(1)-O(2)	1.23(2)
C(1)-O(1)	1.25(2)
C(1)-C(2)	1.53(2)
C(2)-C(3)	1.3900
C(2)-C(7)	1.3900
C(3)-C(4)	1.3900
C(4)-C(5)	1.3900
C(5)-C(6)	1.3900
C(5)-O(3)	1.52(2)
C(6)-C(7)	1.3900
C(8)-O(3)	1.37(2)
C(8)-C(9)	1.3900
C(8)-C(13)	1.3900
C(8)-O(4)	1.97(3)
C(9)-C(10)	1.3900
C(10)-C(11)	1.3900
C(11)-C(12)	1.3900
C(11)-C(20)	1.55(3)
C(12)-C(13)	1.3900
C(13)-O(4)	1.38(2)
C(14)-C(19)	1.27(3)
C(14)-C(15)	1.33(3)
C(14)-O(4)	1.37(3)
C(15)-C(16)	1.45(4)
C(16)-C(17)	1.35(3)
C(17)-C(18)	1.35(2)
C(17)-C(54A)	1.49(3)
C(18)-C(19)	1.37(3)
C(20)-C(23)	1.30(3)
C(20)-C(21)	1.44(3)
C(20)-C(22)	1.54(3)
C(24)-O(8)	1.23(2)
C(24)-O(7)	1.32(2)
C(24)-C(25)	1.45(2)

C(25)-C(26)	1.33(2)
C(25)-C(30)	1.37(2)
C(26)-C(27)	1.39(2)
C(27)-C(28)	1.36(3)
C(28)-C(29)	1.36(2)
C(28)-O(9)	1.42(2)
C(29)-C(30)	1.43(2)
C(31)-C(36)	1.34(3)
C(31)-O(9)	1.37(2)
C(31)-C(32)	1.42(3)
C(32)-C(33)	1.46(4)
C(33)-C(34)	1.38(4)
C(33)-C(37)	1.49(4)
C(34)-C(35)	1.37(3)
C(35)-C(36)	1.41(3)
C(36)-O(10)	1.40(2)
C(37)-C(39)	1.48(4)
C(37)-C(40)	1.48(4)
C(37)-C(38)	1.63(4)
C(41)-C(46)	1.36(3)
C(41)-O(10)#1	1.37(2)
C(41)-C(42)	1.35(2)
C(42)-C(43)	1.41(2)
C(43)-C(44)	1.36(2)
C(44)-C(45)	1.37(2)
C(44)-C(47)	1.48(3)
C(45)-C(46)	1.40(2)
C(47)-O(12)	1.22(2)
C(47)-O(11)	1.32(2)
C(48)-O(14)	1.27(2)
C(48)-O(13)	1.27(2)
C(48)-C(49)	1.53(3)
C(49)-C(50)	1.36(2)
C(49)-C(54)	1.37(2)
C(50)-C(51)	1.47(2)
C(51)-C(52)	1.32(3)

C(52)-C(53)	1.28(3)
C(52)-O(15)	1.43(2)
C(53)-C(54)	1.40(2)
C(54A)-O(5)	1.18(2)
C(54A)-O(6)	1.31(2)
C(55)-O(15)	1.249(19)
C(55)-C(56)	1.3900
C(55)-C(60)	1.3900
C(56)-C(57)	1.3900
C(57)-C(58)	1.3900
C(58)-C(59)	1.3900
C(58)-C(61)	1.55(2)
C(59)-C(60)	1.3900
C(60)-O(16)	1.508(18)
C(61)-C(63)	1.42(3)
C(61)-C(64)	1.51(3)
C(61)-C(62)	1.53(4)
C(65)-C(66)	1.26(2)
C(65)-C(70)	1.43(3)
C(65)-O(16)	1.44(2)
C(66)-C(67)	1.44(2)
C(67)-C(68)	1.42(3)
C(68)-C(69)	1.34(2)
C(68)-C(71)#2	1.43(3)
C(69)-C(70)	1.44(2)
C(71)-O(17)	1.24(2)
C(71)-O(18)	1.29(2)
C(71)-C(68)#2	1.43(3)
C(72S)-N(1)	1.31(3)
C(73S)-N(1)	1.45(4)
C(74S)-O(20)	1.16(3)
C(74S)-N(1)	1.46(4)
C(75S)-N(2)	1.26(3)
C(76S)-N(2)	1.38(3)
C(77S)-O(19)	1.18(2)
C(77S)-N(2)	1.34(3)

C(78S)-C(79S)	1.47(4)
C(79S)-C(80S)	1.3900
C(79S)-C(85S)	1.41(6)
C(80S)-C(81S)	1.3900
C(81S)-C(82S)	1.3900
C(82S)-C(84S)	1.41(4)
C(82S)-C(83S)	1.65(4)
C(84S)-C(85S)	1.3900
O(1)-Zn(2)#3	1.923(11)
O(2)-Zn(4)#3	2.088(12)
O(5)-Zn(1)	1.953(13)
O(6)-Zn(2)	1.981(14)
O(7)-Zn(2)	1.944(13)
O(8)-Zn(3)	1.982(13)
O(10)-C(41)#4	1.37(2)
O(11)-Zn(1)	1.915(13)
O(12)-Zn(4)	2.021(16)
O(13)-Zn(1)	1.922(13)
O(14)-Zn(3)	1.947(13)
O(17)-Zn(4)	2.113(15)
O(18)-Zn(3)	1.935(14)
O(19)-Zn(4)	2.126(12)
O(20)-Zn(4)	2.198(13)
O(100)-Zn(2)	1.903(9)
O(100)-Zn(3)	1.918(9)
O(100)-Zn(1)	1.927(9)
O(100)-Zn(4)	2.032(9)
Zn(1)-Zn(3)	3.112(3)
Zn(1)-Zn(2)	3.152(3)
Zn(2)-O(1)#3	1.923(11)
Zn(2)-Zn(3)	3.129(3)
Zn(4)-O(2)#3	2.088(12)

O(2)-C(1)-O(1)	129(2)
O(2)-C(1)-C(2)	117(2)
O(1)-C(1)-C(2)	114(2)

C(3)-C(2)-C(7)	120.0
C(3)-C(2)-C(1)	119.6(17)
C(7)-C(2)-C(1)	120.1(17)
C(2)-C(3)-C(4)	120.0
C(5)-C(4)-C(3)	120.0
C(6)-C(5)-C(4)	120.0
C(6)-C(5)-O(3)	136.8(16)
C(4)-C(5)-O(3)	102.4(16)
C(7)-C(6)-C(5)	120.0
C(6)-C(7)-C(2)	120.0
O(3)-C(8)-C(9)	107.6(18)
O(3)-C(8)-C(13)	131.4(18)
C(9)-C(8)-C(13)	120.0
O(3)-C(8)-O(4)	90.3(15)
C(9)-C(8)-O(4)	160.6(13)
C(13)-C(8)-O(4)	44.6(12)
C(10)-C(9)-C(8)	120.0
C(11)-C(10)-C(9)	120.0
C(10)-C(11)-C(12)	120.0
C(10)-C(11)-C(20)	109.4(17)
C(12)-C(11)-C(20)	130.5(17)
C(11)-C(12)-C(13)	120.0
O(4)-C(13)-C(12)	146(2)
O(4)-C(13)-C(8)	91(2)
C(12)-C(13)-C(8)	120.0
C(19)-C(14)-C(15)	120(3)
C(19)-C(14)-O(4)	112(3)
C(15)-C(14)-O(4)	128(3)
C(14)-C(15)-C(16)	122(3)
C(17)-C(16)-C(15)	115(2)
C(18)-C(17)-C(16)	118(2)
C(18)-C(17)-C(54A)	126(2)
C(16)-C(17)-C(54A)	116(2)
C(17)-C(18)-C(19)	123(2)
C(14)-C(19)-C(18)	120(3)
C(23)-C(20)-C(21)	122(3)

C(23)-C(20)-C(22)	95(3)
C(21)-C(20)-C(22)	105(2)
C(23)-C(20)-C(11)	119(2)
C(21)-C(20)-C(11)	111(2)
C(22)-C(20)-C(11)	100(2)
O(8)-C(24)-O(7)	123(2)
O(8)-C(24)-C(25)	120(2)
O(7)-C(24)-C(25)	118(2)
C(26)-C(25)-C(30)	118.1(19)
C(26)-C(25)-C(24)	121.7(18)
C(30)-C(25)-C(24)	120(2)
C(25)-C(26)-C(27)	123.1(18)
C(28)-C(27)-C(26)	119.5(18)
C(29)-C(28)-C(27)	119(2)
C(29)-C(28)-O(9)	115(2)
C(27)-C(28)-O(9)	126(2)
C(28)-C(29)-C(30)	119.8(19)
C(25)-C(30)-C(29)	120(2)
C(36)-C(31)-O(9)	124(3)
C(36)-C(31)-C(32)	120(3)
O(9)-C(31)-C(32)	117(3)
C(31)-C(32)-C(33)	116(3)
C(34)-C(33)-C(32)	120(3)
C(34)-C(33)-C(37)	121(3)
C(32)-C(33)-C(37)	119(3)
C(35)-C(34)-C(33)	123(3)
C(34)-C(35)-C(36)	115(3)
C(31)-C(36)-O(10)	116(3)
C(31)-C(36)-C(35)	125(3)
O(10)-C(36)-C(35)	119(3)
C(39)-C(37)-C(40)	109(3)
C(39)-C(37)-C(33)	111(3)
C(40)-C(37)-C(33)	115(3)
C(39)-C(37)-C(38)	106(3)
C(40)-C(37)-C(38)	111(3)
C(33)-C(37)-C(38)	104(3)

C(46)-C(41)-O(10)#1	124(2)
C(46)-C(41)-C(42)	122(2)
O(10)#1-C(41)-C(42)	114(2)
C(41)-C(42)-C(43)	117(2)
C(44)-C(43)-C(42)	124.3(19)
C(43)-C(44)-C(45)	115(2)
C(43)-C(44)-C(47)	127(2)
C(45)-C(44)-C(47)	117(2)
C(44)-C(45)-C(46)	122.7(19)
C(41)-C(46)-C(45)	118.0(19)
O(12)-C(47)-O(11)	127(2)
O(12)-C(47)-C(44)	120(2)
O(11)-C(47)-C(44)	113(2)
O(14)-C(48)-O(13)	127.1(18)
O(14)-C(48)-C(49)	115(2)
O(13)-C(48)-C(49)	118(2)
C(50)-C(49)-C(54)	121(2)
C(50)-C(49)-C(48)	117(2)
C(54)-C(49)-C(48)	121(2)
C(49)-C(50)-C(51)	117(2)
C(52)-C(51)-C(50)	117(2)
C(53)-C(52)-C(51)	128(3)
C(53)-C(52)-O(15)	110(3)
C(51)-C(52)-O(15)	122(2)
C(52)-C(53)-C(54)	116(2)
C(49)-C(54)-C(53)	121(2)
O(5)-C(54A)-O(6)	124.0(19)
O(5)-C(54A)-C(17)	124(2)
O(6)-C(54A)-C(17)	112(2)
O(15)-C(55)-C(56)	114.9(17)
O(15)-C(55)-C(60)	124.9(16)
C(56)-C(55)-C(60)	120.0
C(57)-C(56)-C(55)	120.0
C(56)-C(57)-C(58)	120.0
C(59)-C(58)-C(57)	120.0
C(59)-C(58)-C(61)	134.5(15)

C(57)-C(58)-C(61)	105.5(16)
C(58)-C(59)-C(60)	120.0
C(59)-C(60)-C(55)	120.0
C(59)-C(60)-O(16)	115.7(13)
C(55)-C(60)-O(16)	124.3(13)
C(63)-C(61)-C(64)	117(2)
C(63)-C(61)-C(58)	107(2)
C(64)-C(61)-C(58)	108.7(19)
C(63)-C(61)-C(62)	107(3)
C(64)-C(61)-C(62)	108(2)
C(58)-C(61)-C(62)	108(3)
C(66)-C(65)-C(70)	123(2)
C(66)-C(65)-O(16)	127(3)
C(70)-C(65)-O(16)	110(3)
C(65)-C(66)-C(67)	120(2)
C(68)-C(67)-C(66)	122(2)
C(69)-C(68)-C(67)	115(2)
C(69)-C(68)-C(71)#2	125(3)
C(67)-C(68)-C(71)#2	120(3)
C(68)-C(69)-C(70)	124(2)
C(65)-C(70)-C(69)	116.0(19)
O(17)-C(71)-O(18)	126(2)
O(17)-C(71)-C(68)#2	119(2)
O(18)-C(71)-C(68)#2	115(2)
O(20)-C(74S)-N(1)	119(3)
O(19)-C(77S)-N(2)	125(2)
C(80S)-C(79S)-C(85S)	126(2)
C(80S)-C(79S)-C(78S)	115(4)
C(85S)-C(79S)-C(78S)	119(4)
C(81S)-C(80S)-C(79S)	120.0
C(80S)-C(81S)-C(82S)	120.0
C(84S)-C(82S)-C(81S)	114(2)
C(84S)-C(82S)-C(83S)	122(4)
C(81S)-C(82S)-C(83S)	123(3)
C(85S)-C(84S)-C(82S)	131(4)
C(84S)-C(85S)-C(79S)	109(5)

C(72S)-N(1)-C(74S)	119(3)
C(72S)-N(1)-C(73S)	116(3)
C(74S)-N(1)-C(73S)	117(4)
C(75S)-N(2)-C(77S)	125(2)
C(75S)-N(2)-C(76S)	108(2)
C(77S)-N(2)-C(76S)	125(2)
C(1)-O(1)-Zn(2)#3	123.4(14)
C(1)-O(2)-Zn(4)#3	136.2(13)
C(8)-O(3)-C(5)	105.5(16)
C(14)-O(4)-C(13)	118.6(18)
C(14)-O(4)-C(8)	118(2)
C(13)-O(4)-C(8)	44.9(10)
C(54A)-O(5)-Zn(1)	132.1(13)
C(54A)-O(6)-Zn(2)	131.0(12)
C(24)-O(7)-Zn(2)	127.4(13)
C(24)-O(8)-Zn(3)	131.5(13)
C(31)-O(9)-C(28)	116.6(17)
C(41)#4-O(10)-C(36)	118.0(16)
C(47)-O(11)-Zn(1)	118.1(12)
C(47)-O(12)-Zn(4)	140.3(14)
C(48)-O(13)-Zn(1)	129.9(12)
C(48)-O(14)-Zn(3)	127.3(13)
C(55)-O(15)-C(52)	119(2)
C(65)-O(16)-C(60)	113.1(19)
C(71)-O(17)-Zn(4)	130.4(12)
C(71)-O(18)-Zn(3)	111.7(14)
C(77S)-O(19)-Zn(4)	123.1(16)
C(74S)-O(20)-Zn(4)	123(2)
Zn(2)-O(100)-Zn(3)	110.0(4)
Zn(2)-O(100)-Zn(1)	110.8(4)
Zn(3)-O(100)-Zn(1)	108.1(4)
Zn(2)-O(100)-Zn(4)	110.5(4)
Zn(3)-O(100)-Zn(4)	107.4(4)
Zn(1)-O(100)-Zn(4)	110.0(4)
O(11)-Zn(1)-O(13)	110.3(6)
O(11)-Zn(1)-O(100)	118.6(5)

O(13)-Zn(1)-O(100)	112.8(5)
O(11)-Zn(1)-O(5)	103.7(5)
O(13)-Zn(1)-O(5)	98.7(5)
O(100)-Zn(1)-O(5)	110.6(5)
O(11)-Zn(1)-Zn(3)	137.1(4)
O(13)-Zn(1)-Zn(3)	76.9(4)
O(100)-Zn(1)-Zn(3)	35.8(3)
O(5)-Zn(1)-Zn(3)	117.3(4)
O(11)-Zn(1)-Zn(2)	122.9(4)
O(13)-Zn(1)-Zn(2)	126.3(4)
O(100)-Zn(1)-Zn(2)	34.4(3)
O(5)-Zn(1)-Zn(2)	76.9(4)
Zn(3)-Zn(1)-Zn(2)	59.92(6)
O(100)-Zn(2)-O(1)#3	118.9(5)
O(100)-Zn(2)-O(7)	112.4(5)
O(1)#3-Zn(2)-O(7)	104.9(5)
O(100)-Zn(2)-O(6)	109.6(5)
O(1)#3-Zn(2)-O(6)	105.6(5)
O(7)-Zn(2)-O(6)	104.3(5)
O(100)-Zn(2)-Zn(3)	35.2(3)
O(1)#3-Zn(2)-Zn(3)	132.7(4)
O(7)-Zn(2)-Zn(3)	77.2(4)
O(6)-Zn(2)-Zn(3)	119.8(4)
O(100)-Zn(2)-Zn(1)	34.9(3)
O(1)#3-Zn(2)-Zn(1)	128.2(4)
O(7)-Zn(2)-Zn(1)	125.6(4)
O(6)-Zn(2)-Zn(1)	74.8(4)
Zn(3)-Zn(2)-Zn(1)	59.41(6)
O(100)-Zn(3)-O(18)	122.9(5)
O(100)-Zn(3)-O(14)	113.6(5)
O(18)-Zn(3)-O(14)	103.4(6)
O(100)-Zn(3)-O(8)	107.8(4)
O(18)-Zn(3)-O(8)	105.1(5)
O(14)-Zn(3)-O(8)	101.8(5)
O(100)-Zn(3)-Zn(1)	36.0(3)
O(18)-Zn(3)-Zn(1)	141.1(4)

O(14)-Zn(3)-Zn(1)	77.9(4)
O(8)-Zn(3)-Zn(1)	112.8(3)
O(100)-Zn(3)-Zn(2)	34.9(3)
O(18)-Zn(3)-Zn(2)	125.1(4)
O(14)-Zn(3)-Zn(2)	131.0(4)
O(8)-Zn(3)-Zn(2)	74.3(4)
Zn(1)-Zn(3)-Zn(2)	60.67(6)
O(100)-Zn(4)-O(12)	97.2(5)
O(100)-Zn(4)-O(2)#3	101.8(4)
O(12)-Zn(4)-O(2)#3	89.2(5)
O(100)-Zn(4)-O(17)	88.8(4)
O(12)-Zn(4)-O(17)	173.7(5)
O(2)#3-Zn(4)-O(17)	91.5(5)
O(100)-Zn(4)-O(19)	168.5(5)
O(12)-Zn(4)-O(19)	88.1(6)
O(2)#3-Zn(4)-O(19)	88.5(5)
O(17)-Zn(4)-O(19)	85.7(5)
O(100)-Zn(4)-O(20)	83.1(4)
O(12)-Zn(4)-O(20)	88.7(5)
O(2)#3-Zn(4)-O(20)	174.9(5)
O(17)-Zn(4)-O(20)	90.0(5)
O(19)-Zn(4)-O(20)	86.7(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+3/2 #2 -x+1,-y+2,-z+2 #3 -x+1,-y+2,-z+1

#4 -x+1,y+1/2,-z+3/2

Table **S13**. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound **1⊃PX'**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	67(17)	85(13)	168(19)	63(12)	-24(13)	-15(11)
C(2)	79(17)	97(12)	181(19)	69(12)	-20(12)	-24(11)
C(3)	231(17)	260(17)	262(18)	67(14)	-7(14)	-23(14)
C(4)	241(15)	260(15)	259(16)	45(10)	10(10)	-17(10)
C(5)	141(10)	173(11)	157(11)	1(9)	-7(9)	-23(9)
C(6)	111(12)	172(13)	124(12)	-14(11)	8(11)	-26(11)
C(7)	74(15)	112(15)	95(15)	-3(12)	6(13)	20(13)
C(8)	154(6)	154(6)	154(6)	0(1)	21(1)	0(1)
C(9)	165(9)	170(8)	161(8)	-15(7)	18(7)	-7(7)
C(10)	156(6)	157(6)	156(6)	0(1)	22(1)	0(1)
C(11)	120(9)	142(9)	128(9)	8(8)	31(9)	-7(9)
C(12)	118(19)	127(18)	139(18)	-5(15)	12(15)	-30(16)
C(13)	128(7)	128(7)	128(7)	0(1)	18(2)	0(1)
C(14)	150(20)	270(30)	86(14)	-2(18)	51(17)	107(16)
C(15)	440(60)	410(60)	130(30)	110(30)	100(30)	350(50)
C(16)	340(40)	330(40)	78(17)	80(20)	100(20)	270(40)
C(17)	85(6)	85(6)	84(6)	0(1)	12(1)	0(1)
C(18)	85(14)	106(15)	95(15)	12(13)	16(13)	0(12)
C(19)	140(20)	260(30)	84(13)	-4(17)	46(16)	95(16)
C(20)	115(11)	163(12)	143(12)	19(11)	29(12)	-4(12)
C(21)	85(17)	410(50)	160(20)	60(30)	50(17)	-20(20)
C(22)	134(16)	250(20)	205(19)	5(18)	18(16)	-20(18)
C(23)	120(20)	580(80)	370(50)	330(60)	60(30)	90(40)
C(24)	43(13)	70(20)	90(20)	-14(16)	20(15)	-15(14)
C(25)	83(15)	52(15)	59(15)	7(14)	17(13)	-18(14)
C(26)	60(12)	56(14)	63(14)	-6(11)	-6(12)	-15(11)
C(27)	71(10)	89(16)	98(16)	3(10)	-23(12)	1(12)
C(28)	79(11)	102(18)	110(16)	0(11)	-22(13)	1(12)
C(29)	127(18)	114(19)	106(17)	53(14)	13(15)	-17(16)

C(30)	100(10)	93(10)	94(10)	-1(9)	14(8)	-20(9)
C(31)	106(9)	94(9)	127(10)	6(8)	-9(8)	-12(8)
C(32)	130(30)	79(17)	240(30)	23(19)	30(20)	-16(17)
C(33)	80(20)	76(19)	270(40)	-40(20)	-40(30)	-6(15)
C(34)	110(30)	110(20)	220(30)	0(20)	-80(20)	3(18)
C(35)	129(13)	92(11)	154(14)	4(11)	-26(12)	-6(11)
C(36)	114(11)	91(10)	140(12)	5(9)	-26(10)	-9(9)
C(37)	132(19)	210(20)	260(30)	30(20)	-33(19)	-28(17)
C(38)	249(18)	251(18)	273(18)	7(11)	22(10)	2(11)
C(39)	140(20)	240(20)	260(30)	20(20)	-50(20)	-20(19)
C(40)	130(19)	220(20)	270(30)	40(20)	4(19)	-41(18)
C(41)	78(13)	57(12)	157(15)	-10(11)	-28(13)	-3(17)
C(42)	80(12)	65(11)	161(15)	-10(11)	-27(13)	-1(15)
C(43)	52(13)	87(18)	149(13)	25(13)	-5(10)	23(11)
C(44)	41(14)	80(19)	142(13)	30(14)	-8(10)	22(12)
C(45)	120(20)	40(16)	149(18)	-11(13)	2(15)	13(15)
C(46)	88(17)	69(17)	180(20)	-15(15)	-15(15)	15(18)
C(47)	90(20)	60(19)	99(15)	1(13)	-7(14)	-20(20)
C(48)	24(12)	77(19)	102(19)	60(18)	-13(14)	-13(12)
C(49)	65(13)	120(16)	91(12)	45(14)	25(11)	10(11)
C(50)	67(13)	131(16)	94(11)	45(13)	23(10)	26(10)
C(51)	91(10)	112(10)	115(10)	14(9)	25(9)	20(8)
C(52)	95(10)	115(10)	106(9)	26(9)	-3(8)	-14(8)
C(53)	111(12)	120(13)	104(11)	27(11)	-13(11)	-27(11)
C(54)	94(16)	106(16)	96(17)	31(14)	-21(14)	0(12)
C(54A)	42(13)	90(19)	89(19)	-5(16)	-11(14)	28(13)
C(55)	99(11)	135(12)	129(11)	3(9)	30(9)	10(9)
C(56)	156(14)	175(15)	133(11)	37(12)	44(12)	22(12)
C(57)	152(11)	166(12)	133(9)	28(11)	53(9)	21(10)
C(58)	138(9)	158(10)	128(8)	12(9)	44(8)	0(8)
C(59)	162(7)	162(7)	161(7)	0(1)	22(1)	0(1)
C(60)	126(11)	103(10)	110(10)	-6(8)	19(9)	33(9)
C(61)	128(11)	122(11)	125(11)	-11(9)	11(9)	10(9)
C(62)	770(110)	140(30)	360(60)	60(30)	310(70)	160(50)
C(63)	140(20)	540(70)	120(20)	10(30)	8(18)	160(30)
C(64)	96(17)	300(40)	180(20)	40(20)	38(17)	70(20)

C(65)	130(30)	87(15)	90(20)	10(15)	50(20)	22(14)
C(66)	95(18)	93(15)	73(18)	24(13)	24(18)	27(14)
C(67)	120(20)	61(13)	75(15)	-4(12)	40(20)	-8(13)
C(68)	80(30)	88(15)	50(20)	10(15)	-2(18)	-17(16)
C(69)	80(16)	76(14)	90(20)	11(13)	30(20)	19(13)
C(70)	120(20)	72(14)	94(17)	-11(13)	10(20)	-7(13)
C(71)	100(20)	56(13)	80(20)	3(14)	80(20)	17(14)
C(72S)	120(30)	780(110)	380(60)	460(70)	70(30)	30(40)
C(73S)	640(100)	490(80)	640(100)	430(80)	580(90)	380(70)
C(75S)	110(20)	730(110)	230(40)	260(50)	50(30)	110(40)
C(76S)	72(19)	280(40)	360(50)	80(30)	-30(20)	40(20)
C(78S)	190(40)	360(60)	630(100)	-20(60)	-120(50)	-130(40)
C(79S)	180(40)	400(80)	150(30)	-40(40)	-50(30)	50(50)
C(80S)	170(40)	210(40)	290(40)	20(30)	-10(30)	-70(40)
C(81S)	220(50)	200(40)	240(40)	10(30)	10(30)	90(40)
C(82S)	280(50)	110(30)	210(30)	0(20)	40(30)	50(30)
C(83S)	350(50)	170(30)	240(40)	-20(20)	100(30)	-90(30)
C(84S)	440(70)	200(40)	150(30)	80(30)	140(40)	200(50)
C(85S)	370(80)	220(50)	710(140)	80(60)	270(90)	-10(50)
N(1)	200(30)	260(30)	250(30)	130(20)	150(30)	90(20)
N(2)	61(14)	149(15)	109(14)	17(11)	16(12)	-1(11)
O(1)	55(9)	112(10)	110(9)	49(7)	-23(8)	-19(8)
O(2)	41(7)	79(8)	102(9)	-2(7)	-5(7)	1(6)
O(3)	196(11)	222(11)	211(11)	50(9)	-13(9)	-34(9)
O(4)	300(30)	650(60)	93(13)	60(20)	45(16)	340(40)
O(5)	98(10)	108(11)	76(9)	39(8)	24(8)	37(8)
O(6)	64(8)	110(10)	62(8)	4(7)	7(6)	-4(8)
O(7)	75(9)	75(9)	90(9)	14(7)	3(8)	-22(7)
O(8)	62(8)	74(9)	74(9)	10(7)	8(7)	-20(6)
O(9)	151(13)	74(10)	167(14)	28(9)	-2(11)	-52(9)
O(10)	100(13)	69(10)	242(17)	28(10)	-31(11)	-11(9)
O(11)	66(9)	64(9)	135(10)	6(7)	-9(8)	5(8)
O(12)	75(10)	54(10)	194(15)	-6(9)	-15(9)	4(8)
O(13)	58(8)	88(10)	77(9)	13(8)	-4(7)	10(7)
O(14)	78(9)	61(8)	82(9)	17(7)	-9(7)	9(7)
O(15)	94(11)	213(17)	165(14)	107(14)	-1(10)	5(11)

O(16)	185(15)	102(10)	109(11)	7(9)	66(11)	9(10)
O(17)	97(10)	84(9)	70(9)	-1(8)	24(9)	28(7)
O(18)	65(9)	95(10)	103(11)	8(7)	25(9)	13(8)
O(19)	66(9)	139(12)	182(13)	100(11)	40(9)	15(8)
O(20)	68(8)	107(10)	183(13)	66(10)	18(9)	12(7)
O(100)	32(6)	64(7)	75(7)	15(5)	6(5)	4(5)
Zn(1)	61(2)	80(2)	100(2)	16(1)	5(1)	5(1)
Zn(2)	58(2)	85(2)	90(2)	11(1)	0(1)	-3(1)
Zn(3)	60(2)	84(2)	90(2)	12(1)	11(1)	0(1)
Zn(4)	52(2)	84(2)	128(2)	14(1)	16(1)	0(1)

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