Angewandte Chemie
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Supporting Information

# Porous Solids Arising from Synergistic and Competing Modes of Assembly: Combining Coordination Chemistry and Covalent Bond Formation**

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ange_201411735_sm_miscellaneous_information.pdf

**Supporting Information**

Contents

## 1. Synthesis of materials

*Preparation of $H_3$-ATB*:
2,4,6-Tribromoaniline (1.80 g, 5.61 mmol), 4-(methoxycarbonyl)phenylboronic acid (5.63 g, 31.3 mmol), $K_2CO_3$ (1.16 g, 8.42 mmol), 170 mL 1,4-dioxane, and 10 mL $H_2O$ were added to a pressure vessel equipped with a magnetic stir bar. The resulting mixture was sparged with $N_2$ gas for 30 min. $Pd(PPh_3)_4$ (0.901 g, 0.842 mmol) was added into the mixture, the vessel was sealed, and the mixture was heated to 110 °C for 48 hr. After cooling the reaction mixture to room temperature the solvent was removed under reduced pressure. The residue was dissolved in 200 mL $CH_2Cl_2$ and washed with $H_2O$ (3×200 mL) followed by brine (300 mL). The organic layer was dried over anhydrous $Na_2SO_4$. The crude product was subjected to column chromatography (hexanes/ethyl acetate) to yield a light yellow solid (2.25 g, yield 83.2 %). $^1$H NMR (500 MHz, $CDCl_3$) δ 8.18 (*d*, 4H, *J* = 8.32 Hz), 8.06 (*d*, 2H, *J* = 8.32 Hz), 7.69-7.62 (*m*, 6H), 7.46 (*s*, 2H), 3.96 (*s*, 6H), 3.93 (*s*, 3H). HRMS (EI) calcd for $C_{30}H_{25}NO_6$ (m/z): 495.1682; found: 495.1680. The solid (2.00 g, 4.03 mmol), KOH (2.6 g, 40.0 mmol), 1,4-dioxane (80 mL), and $H_2O$ (20 mL) were added into a pressure vessel. The resultant suspension was heated to 110 °C for 12 hr. After cooling to room temperature the reaction mixture was filtered and solvent was removed under reduced pressure. The residue was dissolved in $H_2O$ (150 mL) and the solution was acidified with concentrated HCl *via* drop-wise addition until pH of the solution was 1. The target compound was collected by filtration, washed thoroughly with $H_2O$, and dried under vacuum to afford $H_3$-ATB (yield 1.65 g, 90.1%). $^1$H NMR (500 MHz, DMSO-$d_6$): δ 12.97 (*br*, 3H), 8.06 (*d*, 4H, *J* = 8.32 Hz), 7.94 (*d*, 2H, *J* = 8.51 Hz), 7.81 (*d*, 2H, *J* = 8.51 Hz), 7.70 (*d*, 4H, *J* = 8.32 Hz), 7.48 (*s*, 2H), 4.70 (*br*, 2H). $^{13}$C NMR (125 MHz, DMSO-$d_6$): 167.27, 167.18, 143.97, 143.70, 141.99, 129.99, 129.93, 129.63, 129.41, 128.54, 128.36, 127.78, 126.77, 125.72. HRMS (EI) calcd for $C_{27}H_{19}NO_6$ (m/z): 453.1212; found: 453.1230.

*Synthesis of MOF-177-$NH_2$*:
$H_3$-ATB (25.0 mg, 0.055 mmol) and $Zn(NO_3)_2 \cdot 6H_2O$ (43.2 mg, 0.145 mmol) were dissolved in 5.7 mL of anhydrous *N*,*N*-dimethylformamide. The mixture was sonicated for 15 min and the solution was clarified by filtration through a glass wool plug. The reaction mixture was heated to 85 °C. After 20 hr, colorless block-shaped crystals of a single phase were obtained. After cooling to room temperature the product was isolated by decanting the mother liquor and washing with fresh DMF (3×15 mL). The yield of the reaction determined from the weight of the solvent-free material (26.0 mg) is 40.1% based on $H_3$-ATB.

*Synthesis of UMCM-306*:
$H_3$-ATB (25.0 mg, 0.055 mmol), terepthalaldehyde (11.0 mg, 0.0822 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (43.2 mg, 0.145 mmol) were dissolved in 5.7 mL of anhydrous *N*,*N*-dimethylformamide. The mixture was sonicated for 15 min and the solution was clarified by filtration through a glass wool plug. The reaction mixture was heated to 85 °C. After 24 hr, yellow colored rod-shaped crystals of a single phase were obtained. After cooling to room temperature, the product was isolated by decanting the mother liquor and washing with fresh DMF (3×15 mL).The yield of the reaction determined from the weight of the solvent-free material (20.5 mg) is 36.5% based on $H_3$-ATB.

*Synthesis of UMCM-307*:
$H_3$-ATB (44.0 mg, 0.097 mmol), anthracene-9,10-dialdehyde (11.4 mg, 0.0492 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (84.5 mg, 0.284 mmol) were dissolved in 14.0 mL of anhydrous *N*,*N*-dimethylformamide. The mixture was sonicated for 15 min and the solution was clarified by filtration through a glass wool plug. The reaction mixture was heated to 85 °C. After 40 hr, orange colored rod-shaped crystals of a single phase were obtained. After cooling to room temperature, the product was isolated by decanting the mother liquor and washing with fresh DMF (3×15 mL).The yield of the reaction determined from the weight of the solvent-free material (36.8 mg) is 35.8% based on $H_3$-ATB.

*Synthesis of UMCM-308*:
$H_3$-ATB (6.25 mg, 0.014 mmol), 1,4-diacetylbenzene (21.0 mg, 0.133 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (11.0 mg, 0.037 mmol) were dissolved in 1.25 mL of anhydrous *N*,*N*-dimethylformamide. The mixture was sonicated for 30 min and the solution was clarified by filtration through a glass wool plug. The reaction mixture was heated to 85 °C. After 20 hr, colorless rod-shaped crystals were obtained contaminated by ~5% MOF-177-$NH_2$. After cooling to room temperature, the product was isolated by decanting the mother liquor and washing with fresh DMF (3×3 mL).The yield of the reaction determined from the weight of the solvent-free material (5.4 mg) is 33% based on $H_3$-ATB.

## 2. PXRD patterns of MOF-177-$NH_2$, UMCM-306, -307, and -308

Samples for powder X-ray diffraction were soaked in mineral oil before collection of data. Data were collected on Rigaku R-Axis Spider diffractometer with an image plate detector and CuKα radiation operating in transmission mode. The powder samples were rotated on the goniometer in φ and oscillated in ω to minimize preferred orientation.

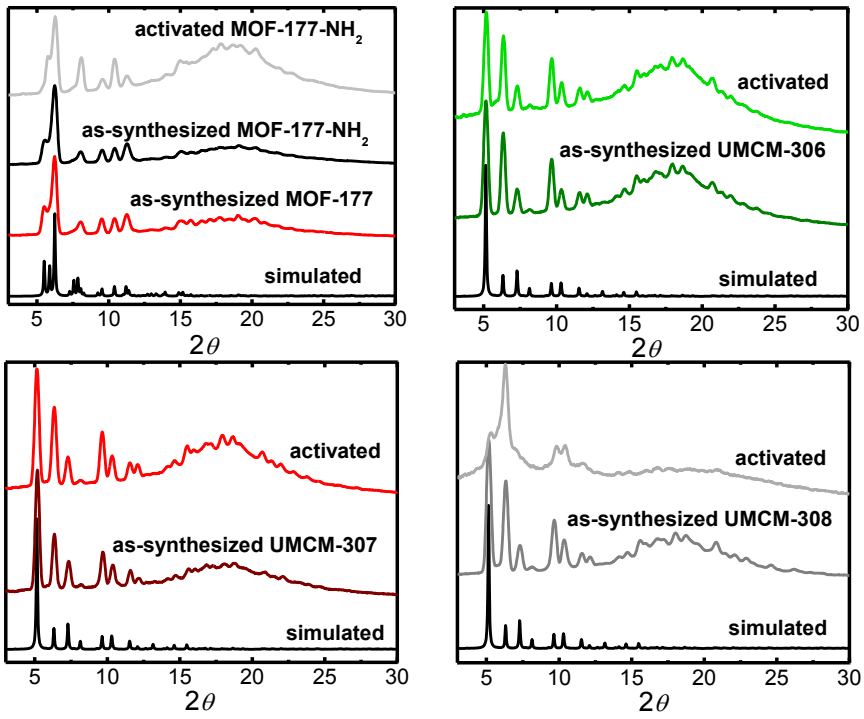



Figure 1: Comparison of simulated and as-synthesized PXRD patterns of materials

## 3. Single crystal X-ray diffraction for UMCM-306

Crystals of UMCM-306 exchanged in $CH_2Cl_2$ were coated in Paratone N oil. A clear yellow rod-shaped crystal (0.12 mm × 0.02 mm × 0.02 mm) was mounted on a cryoloop. X-ray diffraction data were collected on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and Micromax-007HF Cu-target micro-focus rotating anode ($\lambda$ = 1.54187 Å) operated at 1.2 kW power (crystal-to-detector distance was 42.00 mm) at 233K. A total of 1767 images were collected with an oscillation width of 1.0° in ω. The exposure time was 30 sec for the low angle images, 120 sec for high angle images. The integration of the data yielded a total of 126420 reflections to a maximum 2θ value of 113.84° of which 3614 were independent and 2675 were greater than 2σ(I). Decay of the crystal during data collection was negligible. The structure was solved by direct methods and refined against all data in the the space group *P* $4_2$/*m n m* with Z = 2 for the formula $C_{50}H_{26}N_2O_{13}Zn_4$

using SHELXL-97 in the Crystal Structure (v. 4.0) software package.[1] All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed at calculated positions (C-H = 0.93 Å) using a riding model with isotropic thermal parameters 1.2 times that of the attached carbon atom. Full matrix least-squares refinement based on $F^2$ converged at R1 = 0.1647 and wR2 = 0.4256 [based on I > 2sigma(I)], R1 = 0.1808 and wR2 = 0.4413 for all data. The SQUEEZE[2] subroutine of the PLATON program suite was used to address the disordered solvent/oil in the large cavity present in the structure. Additional refinement details are given in the CIF file.

**Table 1.** Crystal data and structure refinement for UMCM-306

| Compound | UMCM-306 |
|---|---|
| Empirical formula | $C_{50}H_{26}N_2O_{13}Zn_4$ |
| Formula Weight | 1124.21 |
| Temperature of run | 233K |
| Crystal dimensions | 0.12 × 0.02 × 0.02 $mm^3$ |
| Wavelength | 1.54187 Å |
| Crystal system | Tetragonal |
| Space group | *P* $4_2$/*m n m* |
| Unit cell parameters | a = 24.1097(7) Å b = 24.1097(7) Å c = 17.0615(12) Å 9917.5(8) $Å^3$<br>α = 90.00º β = 90.00º γ = 90.000(3)º |
| Z | 2 |
| Density (calculated) | 0.376 $g/cm^3$ |
| Absorption coefficient | 0.685 $mm^{-1}$ |
| F(000) | 1128 |
| Theta range for data collection | 2.60 to 56.90 |
| Index ranges | -26≤h≤26, -26≤k≤26, -18≤l≤17 |
| Reflections collected | 126420 |
| Independent reflections | 3614 [R(int) = 0.0812] |
| Completeness to highest theta | 100 % |
| Absorption correction | Multi-scan |
| Max. and min. transmission | 0.675 and 0.464 |
| Refinement method | Full-matrix least-squares on $F^2$ |

| | |
|---|---|
| Data/ Restraints/ parameter | 3614 / 0 / 151 |
| Goodness of fit on $F^2$ | 1.828 |
| Final R indices [I>2σ(I)][a,b] | R1 = 0.1647, wR2 = 0.4256 [a,b] |
| R indices (all data) [a,b] | R1 = 0.1808, wR2 = 0.4413 |

a) $wR2 = |\Sigma w(|Fo|^2 - |Fc|^2)|/\Sigma|w(Fo)^2|^{1/2}$ , $w = 1 / [\sigma^2(Fo^2) + (mP)^2 + nP]$ and $P = [\max(Fo^2,0) + 2Fc^2)] / 3$ ($m$ and $n$ are constants); $\sigma = [\Sigma[w(Fo^2 - Fc^2)^2]/(n - p)]^{1/2}$ b) $R1 = \Sigma||Fo| - |Fc|| /\Sigma|Fo|$

## 4. $^1$H NMR spectroscopic data of digested MOF-177-NH$_2$, UMCM-306, -307, and -308

Solvent free materials were digested in 35 wt% DCl in $D_2O$ diluted with DMSO-$d_6$ solution before performing $^1$H NMR spectroscopic experiments.

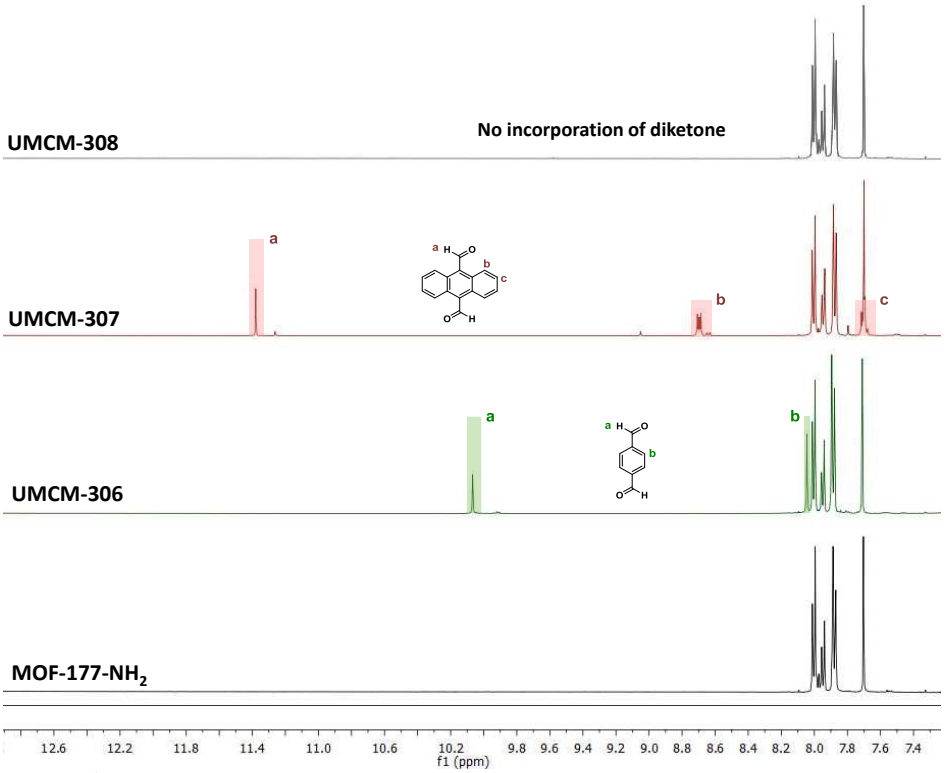



Figure 2. $^1$H NMR spectra of digested MOF-177-NH$_2$, UMCM-306, -307, and -308

## 5. Raman spectroscopic data of MOF-177-NH$_2$, UMCM-306, and -308

Raman spectroscopic experiments were performed using a Renishaw inVia Raman Microscope equipped RenCam CCD detector, 633 nm laser, 1800 lines/nm grating, and 50 μm slit. Spectra were collected in extended scan mode in the range of 4000-100 cm$^{-1}$ and then analyzed using Wire 3.4 software package. Calibration was performed for all experiments using a silicon standard.

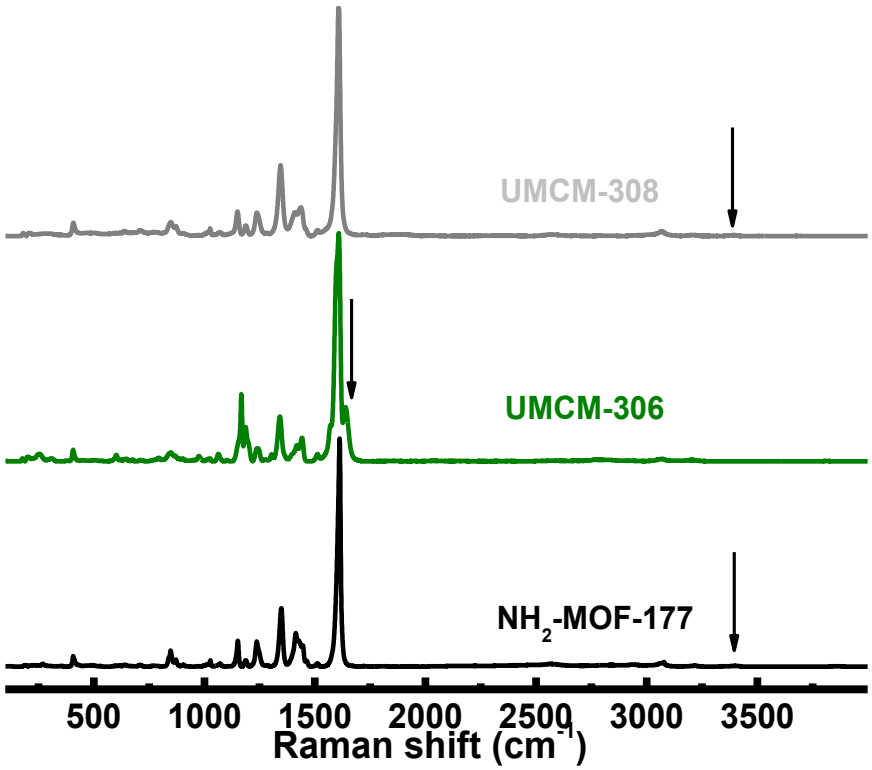



Figure 3. Full Raman spectra of materials showing presence of imine C=N stretching at 1634 $cm^{-1}$ in UMCM-306 and $NH_2$ stretching in MOF-177-$NH_2$ and UMCM-308 at ~3400 $cm^{-1}$.

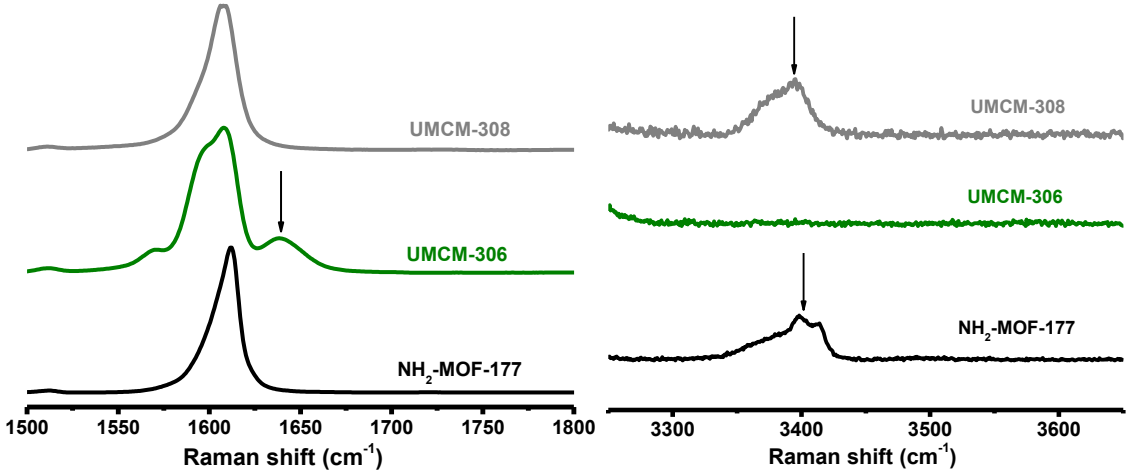
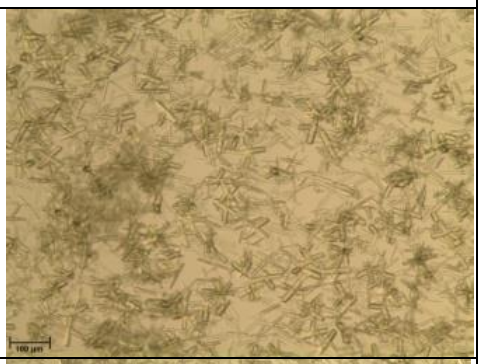
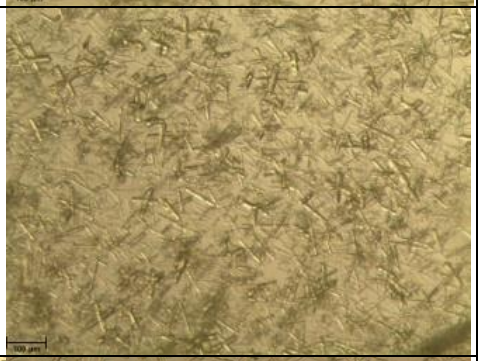
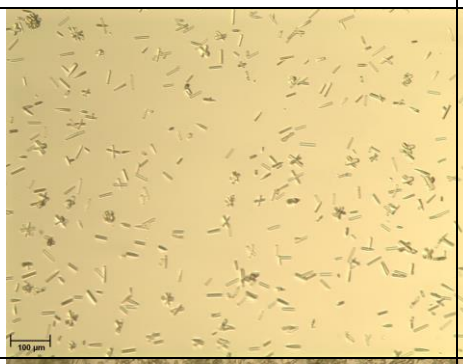
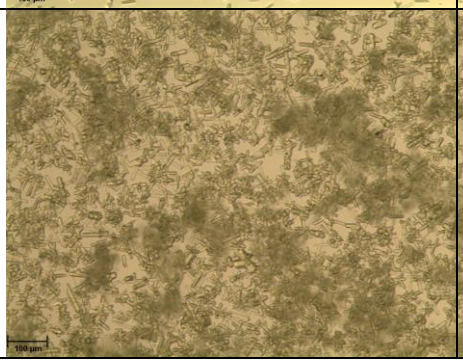
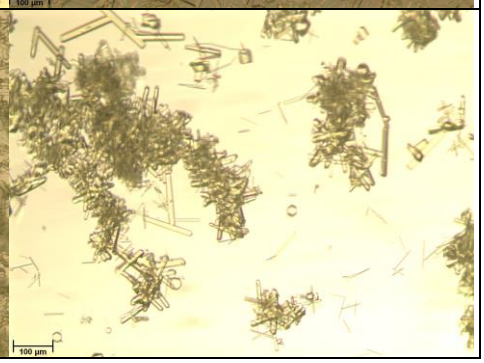
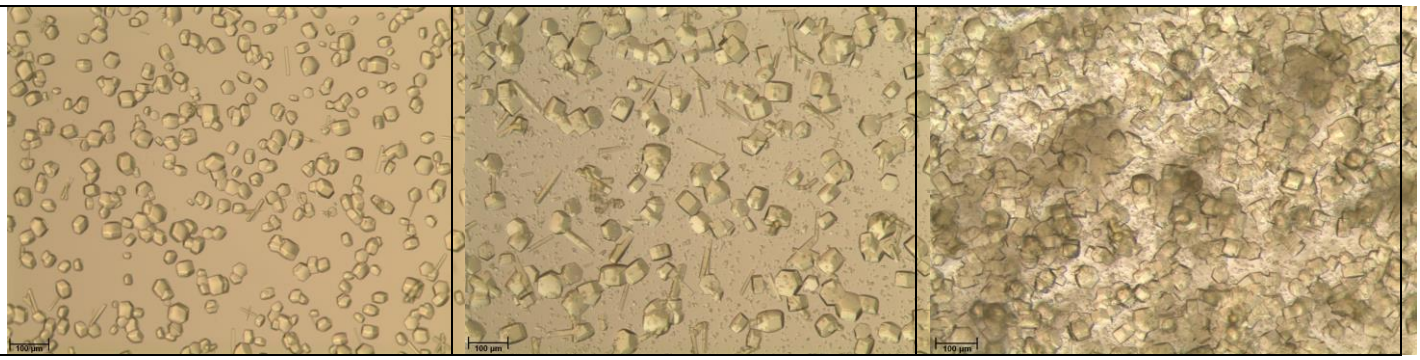



Figure 4. Partial Raman spectra of materials showing presence of imine C=N stretching at 1634 $cm^{-1}$ in UMCM-306 and $NH_2$ stretching in MOF-177-$NH_2$ and UMCM-308 at ~3400 $cm^{-1}$.

### 6. Microscopic images after aging experiments

Five different vials containing $Zn(NO_3)_2 \cdot 6H_2O$ (14.5 mg, 0.048 mmol) and DMF (1.5 mL) were preheated (aged) at 85 °C for 1, 2, 4, 8, 16 hours. $H_3$-ATB (8.33 mg, 0.018 mmol) and terepthalaldehyde (3.67 mg, 0.027 mmol) dissolved in 0.5 mL fresh DMF were added in each pre-heated vial through septum lid using a syringe. The reaction mixtures were again heated to 85 °C and analyzed after 6, 10, and 22 hr *via* optical microscopy. The images were taken with a Spot Insight Color camera fixed to a Leica DMIL microscope. All scale bars indicate a dimension of 100 µm.

| | After 6 hr in oven | After 10 hr in oven | After 22 hr in oven |
|---|---|---|---|
| **1 hr aged** | **No crystals** | **No crystals** |  |
| **2 hr aged** | **No crystals** | **No crystals** |  |
| **4 hr aged** | **No crystals** |  |  |
| **8 hr aged** | **No crystals** |  |  |

| | |
|---|---|
| **16 hr aged** |  |

## 7. TGA traces of MOF-177-$NH_2$, UMCM-306, -307, and -308

Thermogravimetric analyses were performed on a TA Q50 equipment. Samples were activated before experiments. The temperature was ramped from 25 °C to 600 °C with a rate of 2 °C/ min under flow of $N_2$ gas.

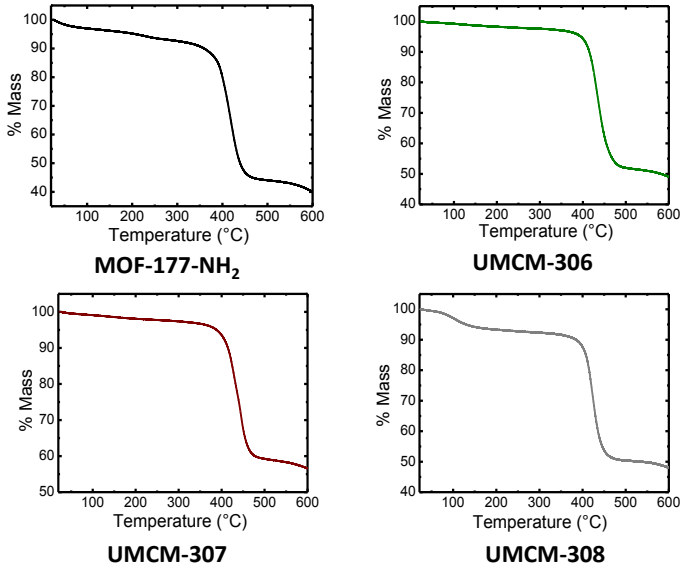



Figure 5. TGA traces of activated materials

## 8. Activation of materials and gas sorption measurements

All materials were exchanged in fresh DMF for 24 hr before flowing supercritical $CO_2$ activation.[3] $N_2$ adsorption/desorption isotherms were measured volumetrically at 77K in the range of $1.00 \times 10^{-5} \leq P/P_0 \leq 1.00$ with an Autosorb-1C outfitted with the micropore option by Quantachrome Instruments (Boyton Beach, Florida, U.S.A.) running version 1.2 ASwin software package. Ultra-high purity He (99.999%, for void volume determination) and $N_2$ (99.999%) were purchased from Cryogenic Gases and used as received.


[1] *G*. M. Sheldrick, *SHELXS '97 and SHELXL '97*. (University of Göttingen, Germany, 1997).

[2] a) A. L. Spek, *J. Appl. Cryst.* **2003**, *36*, 7-13 ; b) A.L.Spek, *Acta Cryst. D65*, **2009**, *v. 51012*, 148-155.

[3] B. Liu, A. G. Wong-Foy, A. J. Matzger, *Chem. Commun.* **2013**, *49*, 1419-1421.

# Datablock: UMCM-306

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Bond precision: C-C = 0.0140 A Wavelength=1.54187

Cell: a=24.1097(7) b=24.1097(7) c=17.0615(12)
alpha=90 beta=90 gamma=90

Temperature: 233 K

| | Calculated | Reported |
|---|---|---|
| Volume | 9917.5(9) | 9917.5(8) |
| Space group | P 42/m n m | P 42/m n m |
| Hall group | -P 4n 2n | -P 4n 2n |
| Moiety formula | C12.18 H6.70 N0.50 O3.25 Zn, 0.175(C2) | C50 H26 N2 O13 Zn4 |
| Sum formula | C12.53 H6.70 N0.50 O3.25 Zn | C50 H26 N2 O13 Zn4 |
| Mr | 281.57 | 1124.21 |
| Dx,g cm-3 | 0.377 | 0.376 |
| Z | 8 | 2 |
| Mu (mm-1) | 0.685 | 0.685 |
| F000 | 1130.8 | 1128.0 |
| F000' | 1121.41 | |
| h,k,lmax | 26,26,18 | 26,26,18 |
| Nref | 3614 | 3614 |
| Tmin,Tmax | 0.984,0.986 | 0.464,0.675 |
| Tmin' | 0.921 | |

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 56.920

R(reflections)= 0.1647( 2675) wR2(reflections)= 0.4413( 3614)

S = 1.828 Npar= 151

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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

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## Alert level A

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.315
Additional refinement cycles may be required.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5434

PLAT080_ALERT_2_A Maximum Shift/Error ..... 0.31

PLAT222_ALERT_3_A Large Non-Solvent H Uiso(max)/Uiso(min) .. 10.0
Ratio

PLAT234_ALERT_4_A Large Hirshfeld Difference C4 -- C5 .. 0.36
Ang.

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure !
Info

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## Alert level B

RFACG01_ALERT_3_B The value of the R factor is > 0.15

R factor given 0.165
RFACR01_ALERT_3_B The value of the weighted R factor is > 0.35
Weighted R factor given 0.441
PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 ..... 0.3772
Check
PLAT082_ALERT_2_B High R1 Value ..... 0.16
Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.44
Report
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) Range 10.0
Ratio
PLAT234_ALERT_4_B Large Hirshfeld Difference N1 -- C16 .. 0.29
Ang.
PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for ..... O1
Check
PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for ..... C7
Check

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## Alert level C

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Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 0.52
Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please
Check
PLAT147_ALERT_1_C su on Symmetry Constrained Cell Angle(s) ..... Please
Check
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**And 3 other PLAT161 Alerts**
More ...
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**And 3 other PLAT162 Alerts**
More ...
PLAT163_ALERT_4_C Missing or Zero su (esd) on z-coordinate for ... C10
**And 3 other PLAT163 Alerts**
More ...
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Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C2 .. 0.22
Ang.
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PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C3
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PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0140
Ang.

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Atom count from _chemical_formula_sum:C50 H26 N2 O13 Zn4

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            Atom count from the _atom_site data:  C50.1 H26.8 N2 O13 Zn4
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CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
            From the CIF: _cell_formula_units_Z    2
            From the CIF: _chemical_formula_sum  C50 H26 N2 O13 Zn4
            TEST: Compare cell contents of formula and atom_site data

            atom    Z*formula  cif sites diff
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            H          52.00     53.60   -1.60
            N           4.00      4.00    0.00
            O          26.00     26.00    0.00
            Zn          8.00      8.00    0.00
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Info
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Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please
Check
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Ratio
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su
And 3 other PLAT230 Alerts
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su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn2    --  O1      ..       11.1
su
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Note
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Ang.
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Info
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Note
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   6 ALERT level A = Most likely a serious problem - resolve or explain
   9 ALERT level B = A potentially serious problem, consider carefully
  23 ALERT level C = Check. Ensure it is not caused by an omission or
oversight
  32 ALERT level G = General information/check it is not something unexpected
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   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  31 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   8 ALERT type 3 Indicator that the structure quality may be low
  19 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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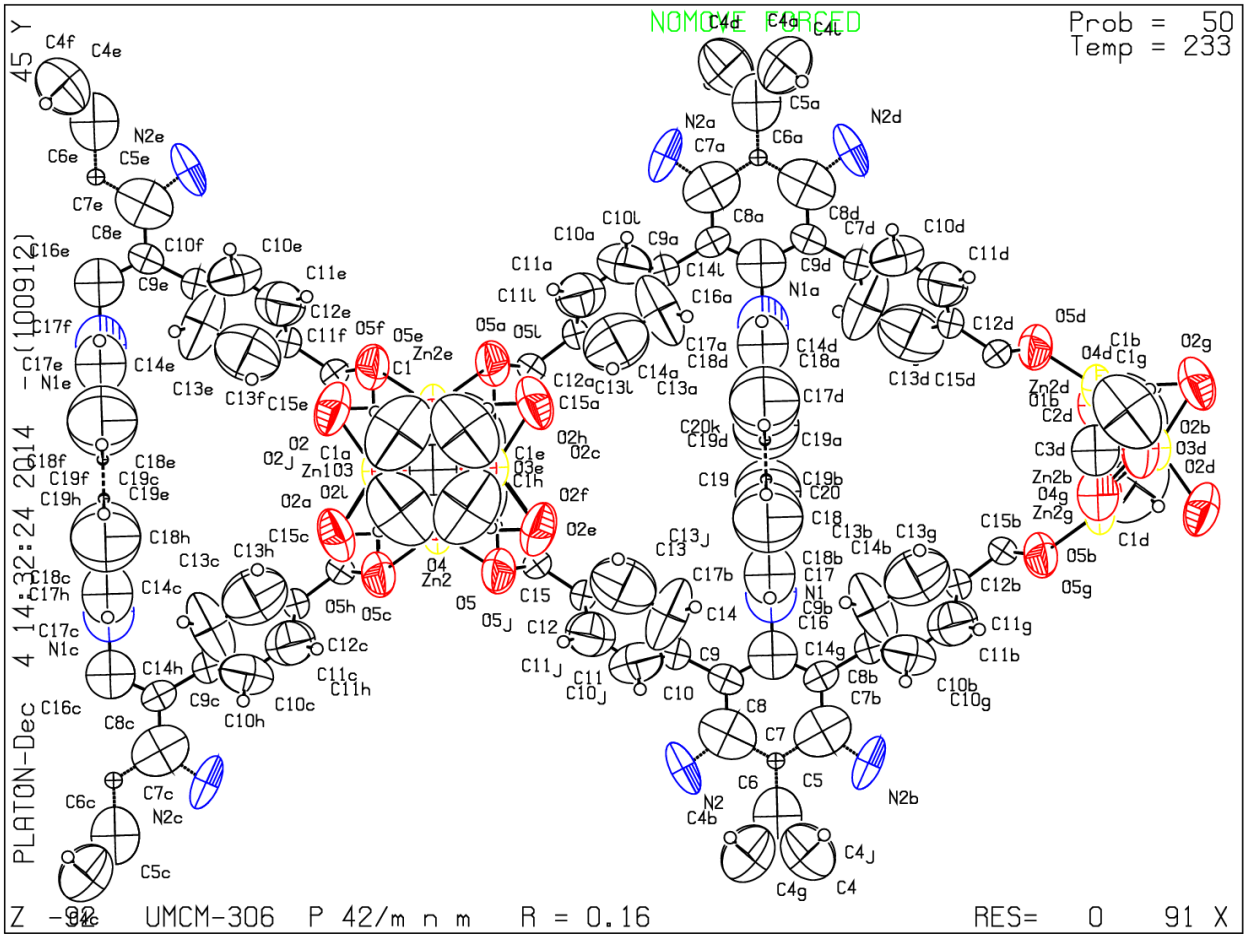
**PLATON version of 20/08/2014; check.def file version of 18/08/2014**

# **Datablock UMCM-306** - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 233
45 Y
PLATON-Dec 4 14:32:24 2014 (100912)
Z -92 UMCM-306 P 42/m n m R = 0.16
RES= 0 91 X