Electronic Supplementary Information

UiO-66 Metal Organic Frameworks with High Contents of Flexible Adipic Acid co-Linker

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1. Experimental

1.1 Materials and methods

All materials were purchased from commercial vendors and used as received. $ZrCl_4$, adipic acid and terephthalic acid and K_3PO_4 were purchased from Sigma Aldrich. $ZrOCl_2 \cdot 8H_2O$ was purchased from Merck. 3-Methyladipic acid, acetic acid and formic acid were purchased from TCI. Concentrated hydrochloric acid was purchased from Honeywell. Anhydrous *N*,*N*-Dimethylformamide (DMF) was purchased from Acros.

Powder XRD data were collected using a Bruker D8-Advance X-ray powder diffractometer with Cu Kα radiation, at a resolution of 0.02° and a scan rate of 0.1-0.5 s/point.

Thermogravimetric analyses (TGA) data was collected using a TA Instrument Q500. Samples were heated at a rate of 5 °C/min to 600 °C under air.

Liquid state ^1H NMR on digested MOF samples were done using a JEOL 500 MHz spectrometer. Samples were digested in a saturated solution of K_3PO_4 dissolved in D_2O. The relaxation delay was increased to 30 seconds to ensure accurate integration.

Solid state NMR was done using a JEOL JNM-ECZ600R/M3 spectrometer with a MAS spin rate of 20 kHZ.

Sorption measurements were performed using a BELSORP-max Absorption Measurement Instrument equipped with cryogenic temperature controller.

Scanning electron Microscopy (SEM) analysis was performed with a JEOL JSM 5600 scanning electron microscope (tungsten source), equipped with an Oxford Link ISIS with an accelerating voltage of 10 to 15 kV. Prior to SEM analysis, samples were sputtered with gold using a JEOL JFC-1200 Fine Coater.

Infrared spectroscopy was performed on Perkin Elmer Spectrum 2000.

1.2 Synthesis of mixed adipate-terephthalate UiO-66

A 50 ml screw cap glass bottle was charged with terephthalic acid, adipic acid (see Table S1 for amounts) and DMF (20 mL). The mixture was agitated by ultrasonication until the terephthalic acid and adipic acid were fully dissolved, then concentrated hydrochloric acid (35 wt%, 100 μL) was added, followed by $ZrCl_4$ (233 mg, 1 mmol). The mixture was again agitated by ultrasonication until homogenous. The mixture was placed in a preheated oven at 130 °C for 24 hours. The white powder formed was collected by suction filtration, rinsed with DMF (about 5 mL) and then with ethanol (about 20 ml). The collected solids were then resuspended in water (20 mL) and heated to 80 °C for 2 hours to replace the DMF within the pores with water. The solids were then collected again by filtration, rinsed with water, and dried in an oven at 60 °C for 1 hour. Material composition in Table S1 was determined by digesting about 10 mg of sample in a solution of about 10 mg of K_3PO_4 in D_2O.

Table S1. Linker amounts employed in the synthesis of mixed linker UiO-66-*x*

Experiment	Terephthalic acid used		Adipic acid used		Mole percentage of adipate w.r.t terephthalate in MOF
	mg	mmol	mg	mmol	mol%
1	166	1	146	1	0
2	149	0.9	160	1.1	5
3	132	0.8	175	1.2	14
4	116	0.7	190	1.3	19
5	100	0.6	204	1.4	28
6	83	0.5	219	1.5	35
7	66	0.4	234	1.6	40
8	50	0.3	248	1.7	51
9	33	0.2	262	1.8	69
10	17	0.1	277	1.9	87

1.3 Synthesis of mixed 3-methlyadipate-terephthalate UiO-66

To investigate the generality of our method, we extended our study to another linear aliphatic acid, 3-methyladipate. Crystalline MOFs with Zr and 3-methyladipate have previously been reported,[1] and we chose this ligand to study if our method can be applied to other aliphatic acids, as well as to understand how the functional groups on the aliphatic ligand may affect the loading and properties on the obtained materials. The methods for the synthesis of the MOFs containing 3-methyladipate are the same as those for the MOFs containing adipate, as outlined below.

A 50 ml screw cap glass bottle was charged with terephthalic acid, 3-methyladipic acid (see Table S2 for amounts) and DMF (20 mL). The mixture was agitated by ultrasonication until the terephthalic acid and adipic acid were fully dissolved, then concentrated hydrochloric acid (35 wt%, 100 μL) was added, followed by $ZrCl_4$ (233 mg, 1 mmol). The mixture was again agitated by ultrasonication until homogenous. The mixture was placed in a preheated oven at 130 °C for 24 hours. The white powder formed was collected by suction filtration, rinsed with DMF (about 5 mL) and then with ethanol (about 20 ml). The collected solids were then resuspended in water (20 mL) and heated to 80 °C for 2 hours to replace the DMF within the pores with water. The solids were then collected again by filtration, rinsed with water, and dried in an oven at 60 °C for 1 hour. Material composition in Table S2 was determined by digesting about 10 mg of sample in a solution of about 10 mg of K_3PO_4 in D_2O.

Table S2. Linker amounts employed in the synthesis of mixed linker UiO-66-3Me-*x*

Experiment	Terephthalic acid used		3-Methyladipic acid used		Mole percentage of 3-methyladipate w.r.t terephthalate in MOF
	mg	mmol	mg	mmol	mol%
1	166	1	160	1	11
2	132	0.8	192	1.2	16
3	100	0.6	224	1.4	31

1.4 Thermolysis of adipic acid in UiO-66-*x*

Samples of mixed linker UiO-66-*x* (about 150 mg) were placed in a programmable furnace and the temperature was ramped from room temperature to 300 °C at 10 °C/min. The temperature was then held at 300 °C for 5 minutes, after which the samples were removed from the furnace and allowed to cool to room temperature under ambient conditions.

Table S3. Mole fraction of adipate (*x*) in UiO-66-*x*, measured by both liquid ^{1}H NMR (x_{NMR}) of digested samples and TGA (x_{TGA}), TGA mass loss of adipate and terephthalate as a weight % of ZrO_2 and corresponding ratio of terephthalate, adipate and defects in each sample as calculated by the method described by Shearer and coworkers.[2]

Experiment	x_{NMR}	x_{TGA}	Weight loss of terephthalate (wt% ZrO_2)	Number of terephthalates per Zr_6 node	Weight loss of adipate (wt% ZrO_2)	Number of adipates per Zr_6 node	Number of defects per Zr_6 node
1	0	0	110	5.5	0	0.0	0.5
2	5	6	108	5.4	6	0.3	0.3
3	14	16	96	4.8	16	0.9	0.3
4	19	20	90	4.5	20	1.1	0.4
5	28	27	75	3.7	25	1.4	0.8
6	35	31	69	3.4	27	1.5	1.0
7	40	36	60	3.0	30	1.7	1.3
8	51	46	45	2.2	34	1.9	1.8

Table S4. Mole fraction of 3-methyladipate (*x*) in UiO-66-3Me-*x*, measured by both liquid ^{1}H NMR (x_{NMR}) of digested samples and TGA (x_{TGA}), TGA mass loss of 3-methyladipate and terephthalate as a weight % of ZrO_2 and corresponding ratio of terephthalate, 3-methyladipate and defects in each sample as calculated as above.

Experiment	x_{NMR}	x_{TGA}	Weight loss of terephthalate (wt% ZrO_2)	Number of terephthalates per Zr_6 node	Weight loss of 3-methyladipate (wt% ZrO_2)	Number of 3-methyladipate per Zr_6 node	Number of defects per Zr_6 node
1	11	11	100	5.0	12	0.6	0.4
2	16	19	89	4.4	20	1.0	0.5
3	31	31	68	3.4	30	1.6	1.0

2. Scanning electron microscopy

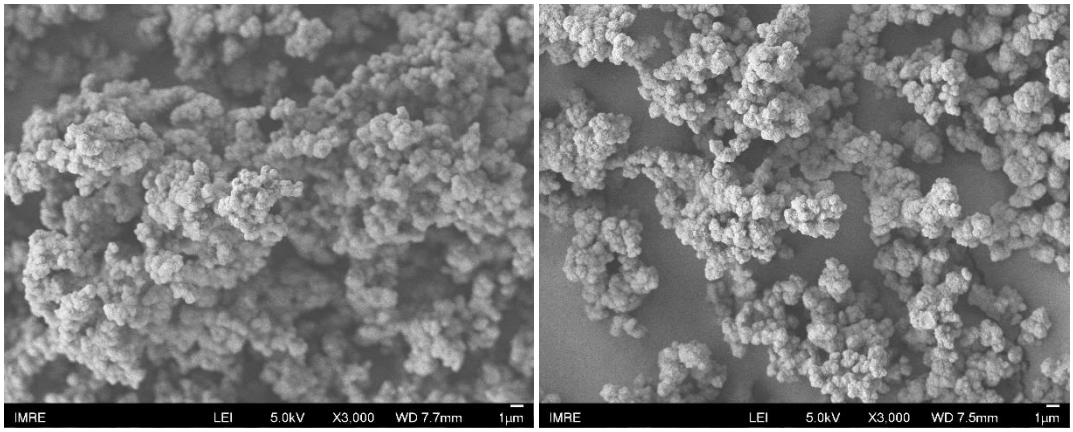

Figure S1: SEM images of **UiO-66-0** (left) and **UiO-66-0-th** (right)

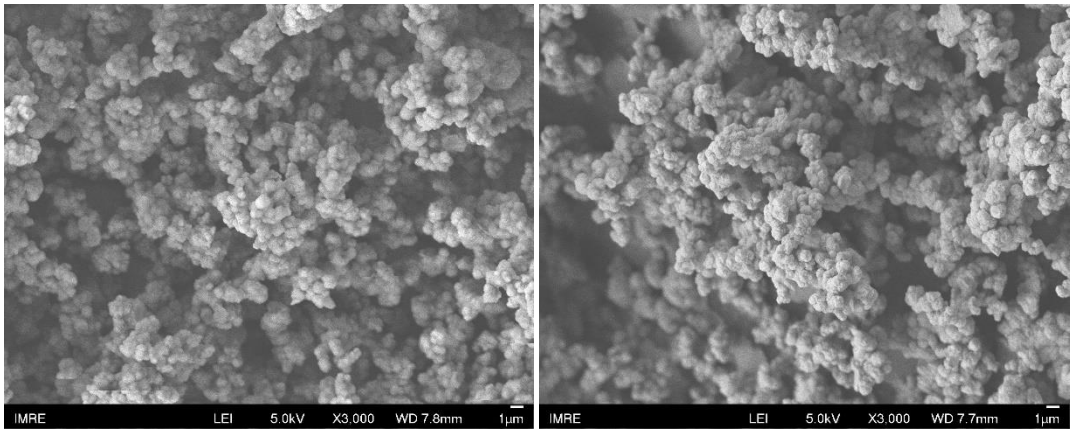

Figure S2: SEM images of **UiO-66-5** (left) and **UiO-66-5-th** (right)

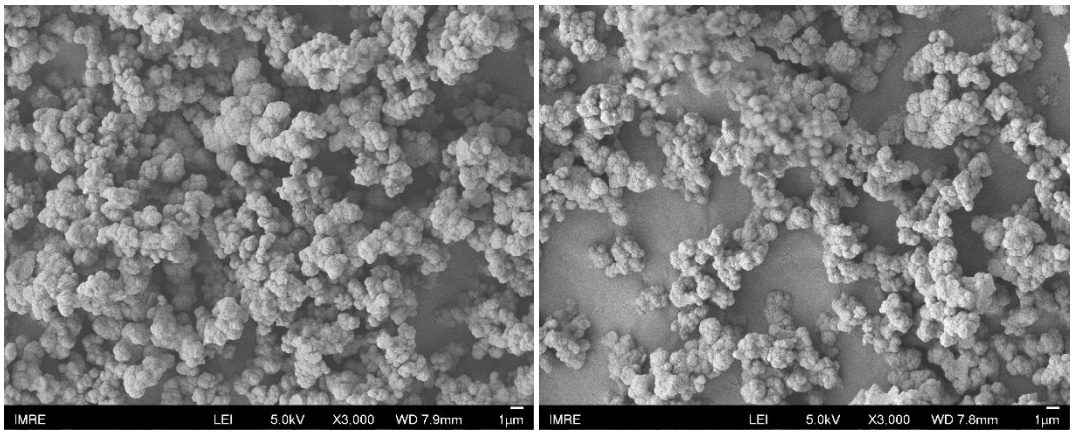

Figure S3: SEM images of **UiO-66-14** (left) and **UiO-66-14-th** (right)

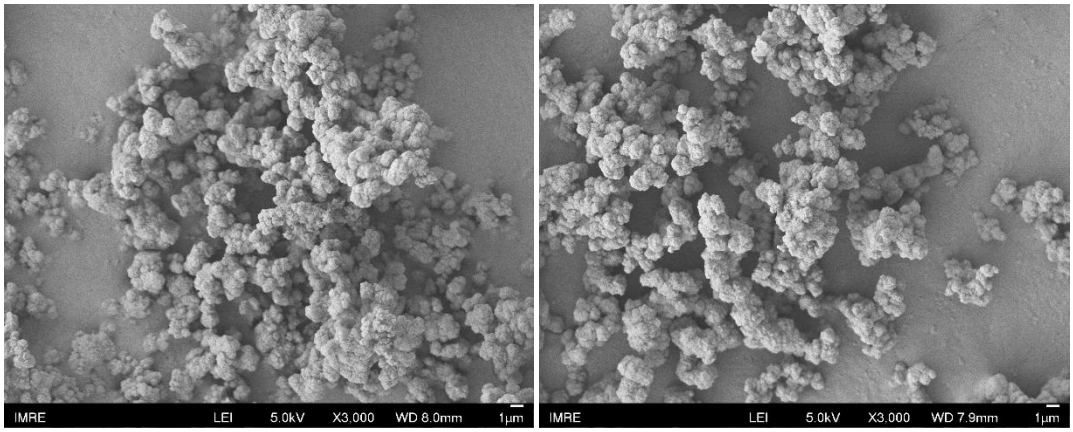

Figure S4: SEM images of **UiO-66-19** (left) and **UiO-66-19-th** (right)

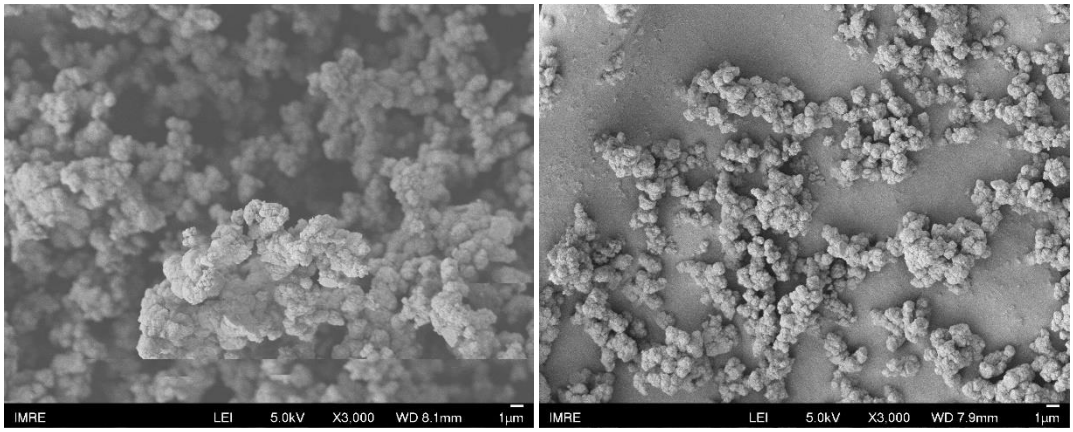

Figure S5: SEM images of **UiO-66-28** (left) and **UiO-66-28-th** (right)

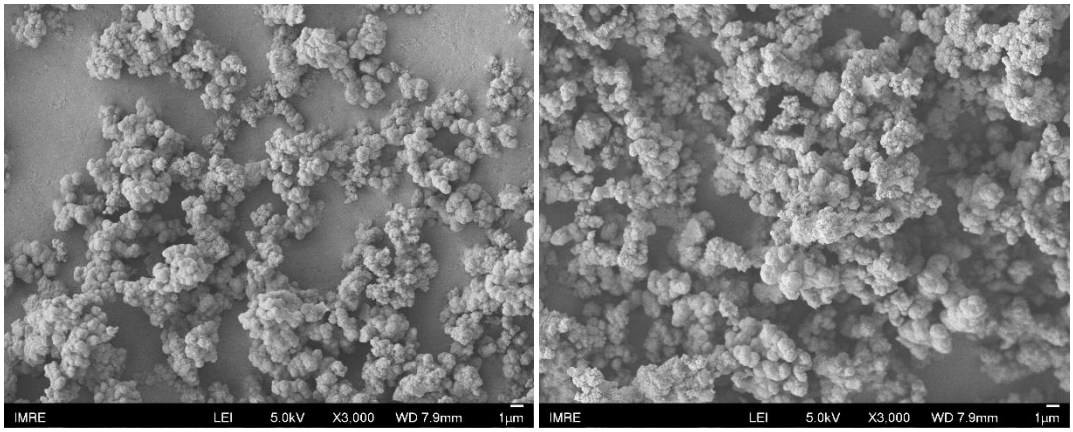

Figure S6: SEM images of **UiO-66-35** (left) and **UiO-66-35-th** (right)

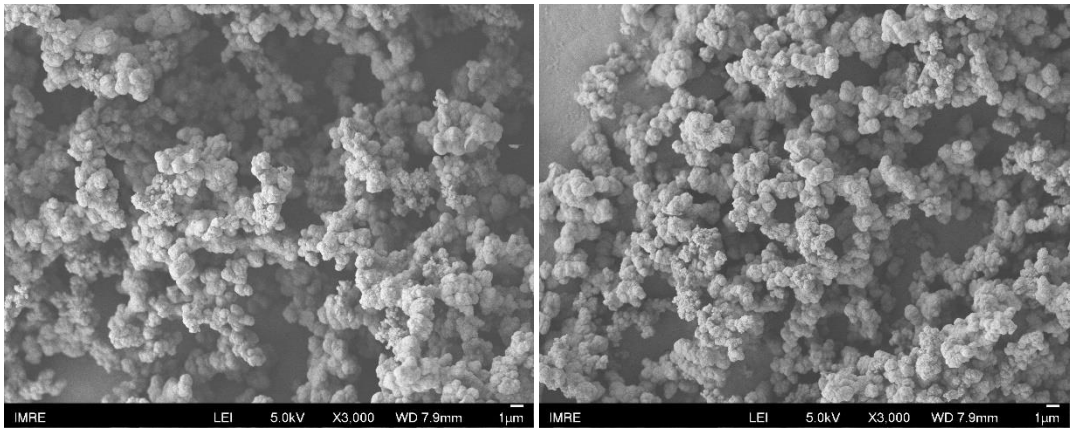

Figure S7: SEM images of **UiO-66-40** (left) and **UiO-66-40-th** (right)

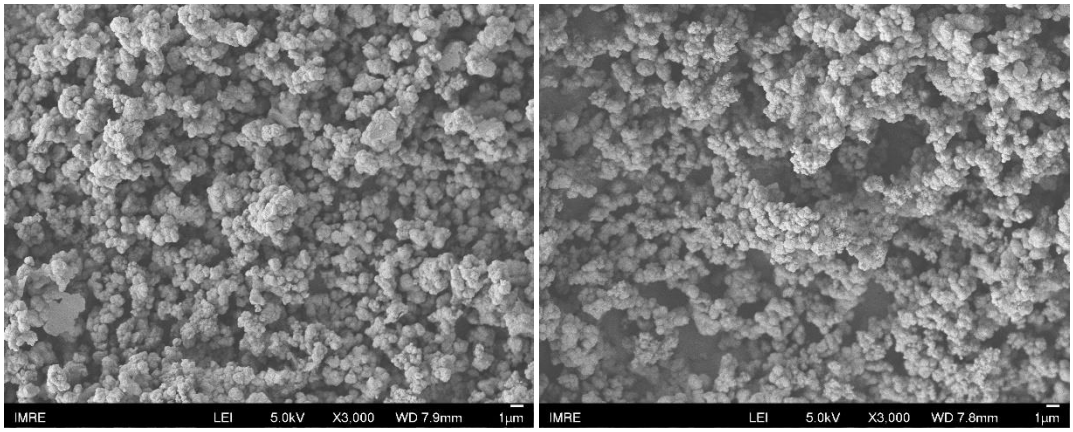

Figure S8: SEM images of **UiO-66-51** (left) and **UiO-66-51-th** (right)

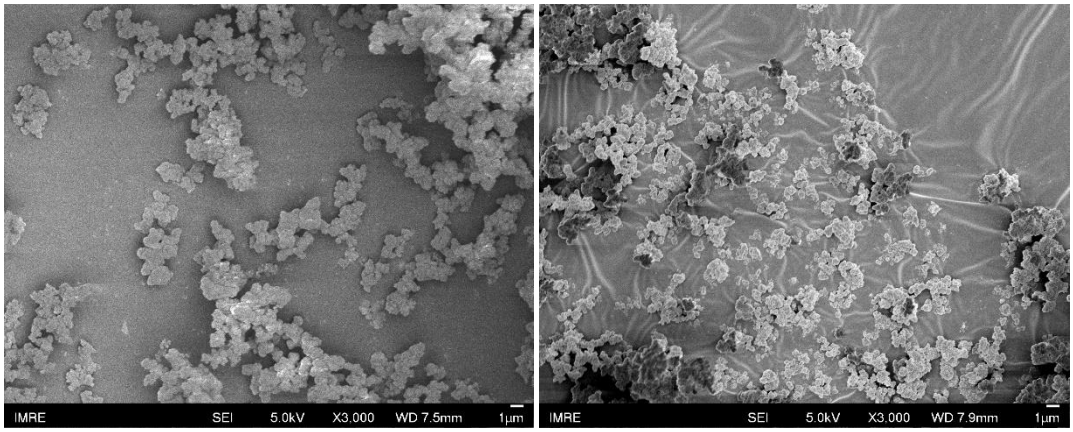

Figure S9: SEM images of **UiO-66-69** (left) and **UiO-66-87** (right)

3. Powder X-ray Diffraction

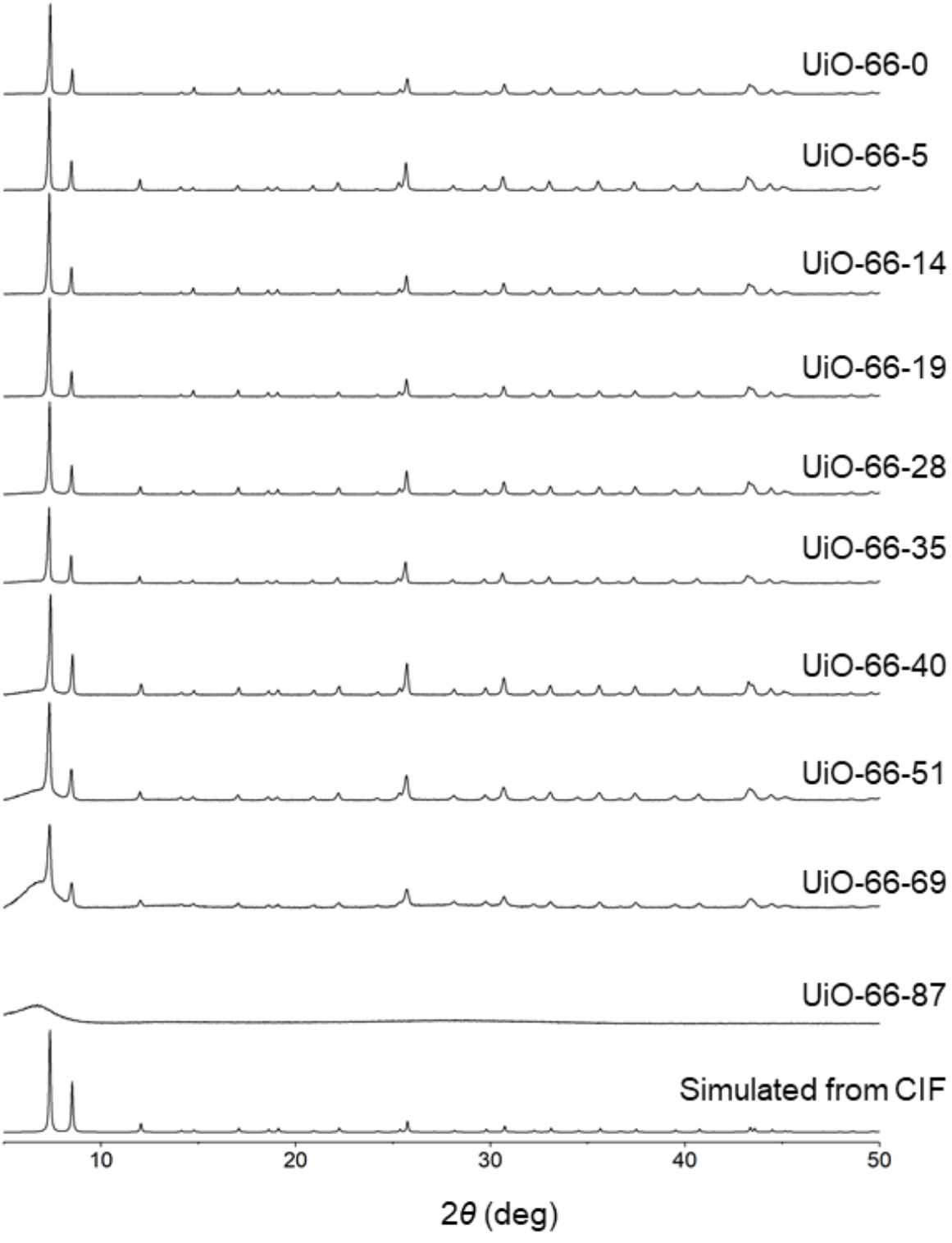

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Figure S10: Powder X-ray diffraction patterns of UiO-66-*x* samples (before thermolysis)

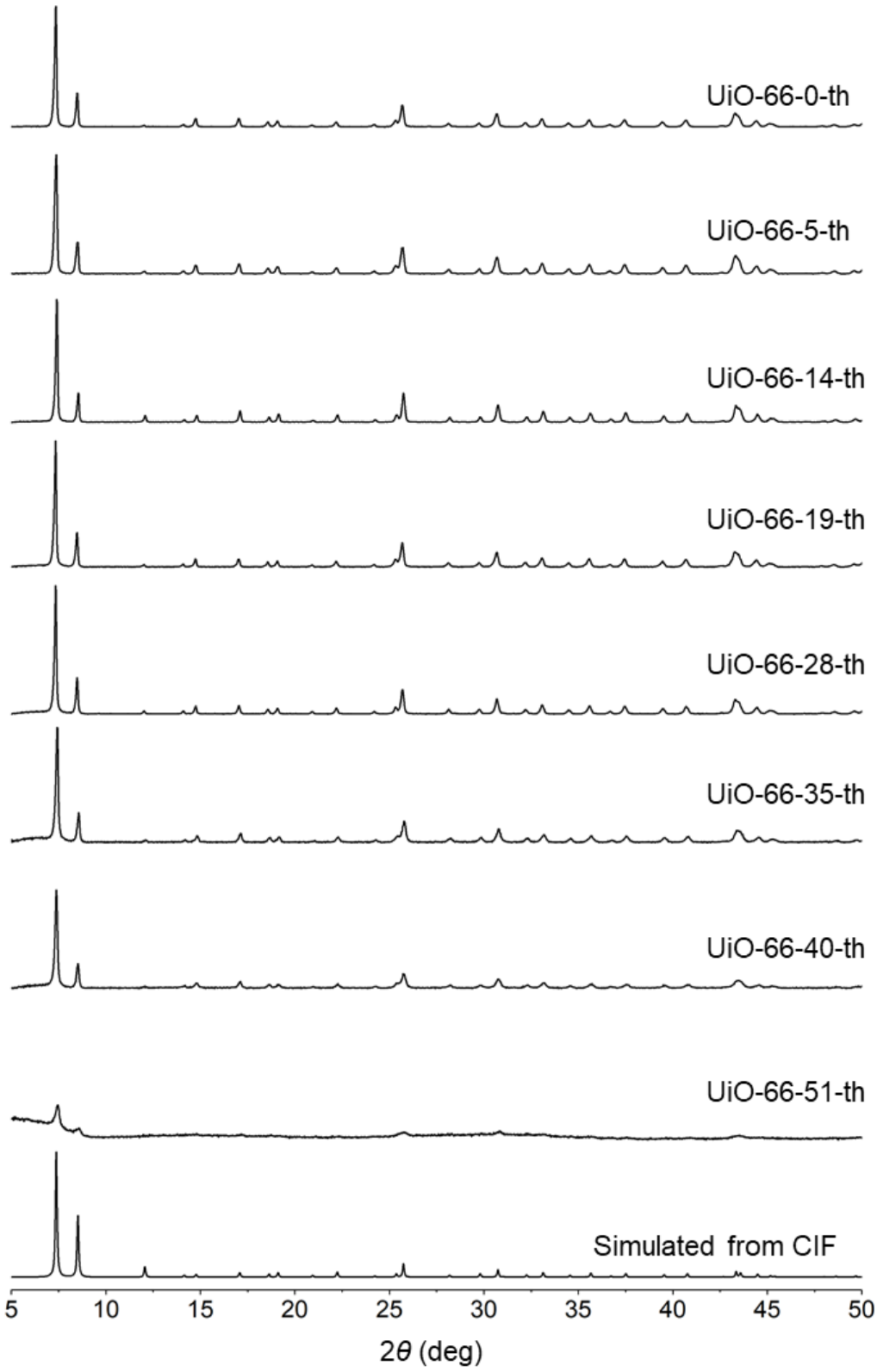

Figure S11: Powder X-ray diffraction patterns of UiO-66-*x*-th samples (after thermolysis)

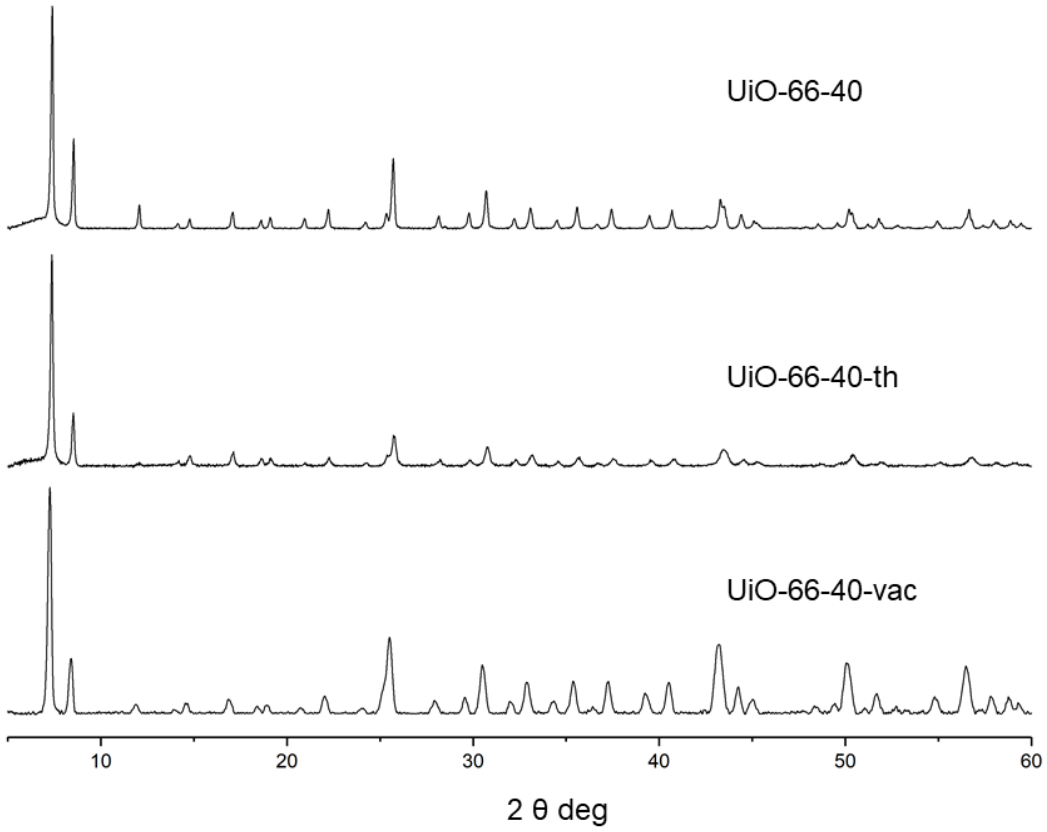

Figure S12: Comparison of XRD patterns of UiO-66-40, as synthesized, after thermolysis and after evacuation.

Table S5: List of selected peaks, full width at half maximum (FWHM) and crystallite size calculated by the Scherrer equation.

2 θ (deg)	FWHM (deg)			Crystallite size (nm)		
	UiO-66-40	UiO-66-40-th	UiO-66-40-vac	UiO-66-40	UiO-66-40-th	UiO-66-40-vac
7.4	0.14	0.17	0.23	56	47	35
8.5	0.14	0.16	0.23	59	49	35
25.7	0.17	0.19	0.29	47	42	28
29.8	0.16	0.25	0.42	52	32	19
30.7	0.18	0.26	0.33	45	32	25
33.1	0.18	0.25	0.20	45	33	41
35.6	0.18	0.24	0.32	47	35	26
37.5	0.19	0.24	0.31	45	35	27
40.7	0.19	0.25	0.31	45	34	27

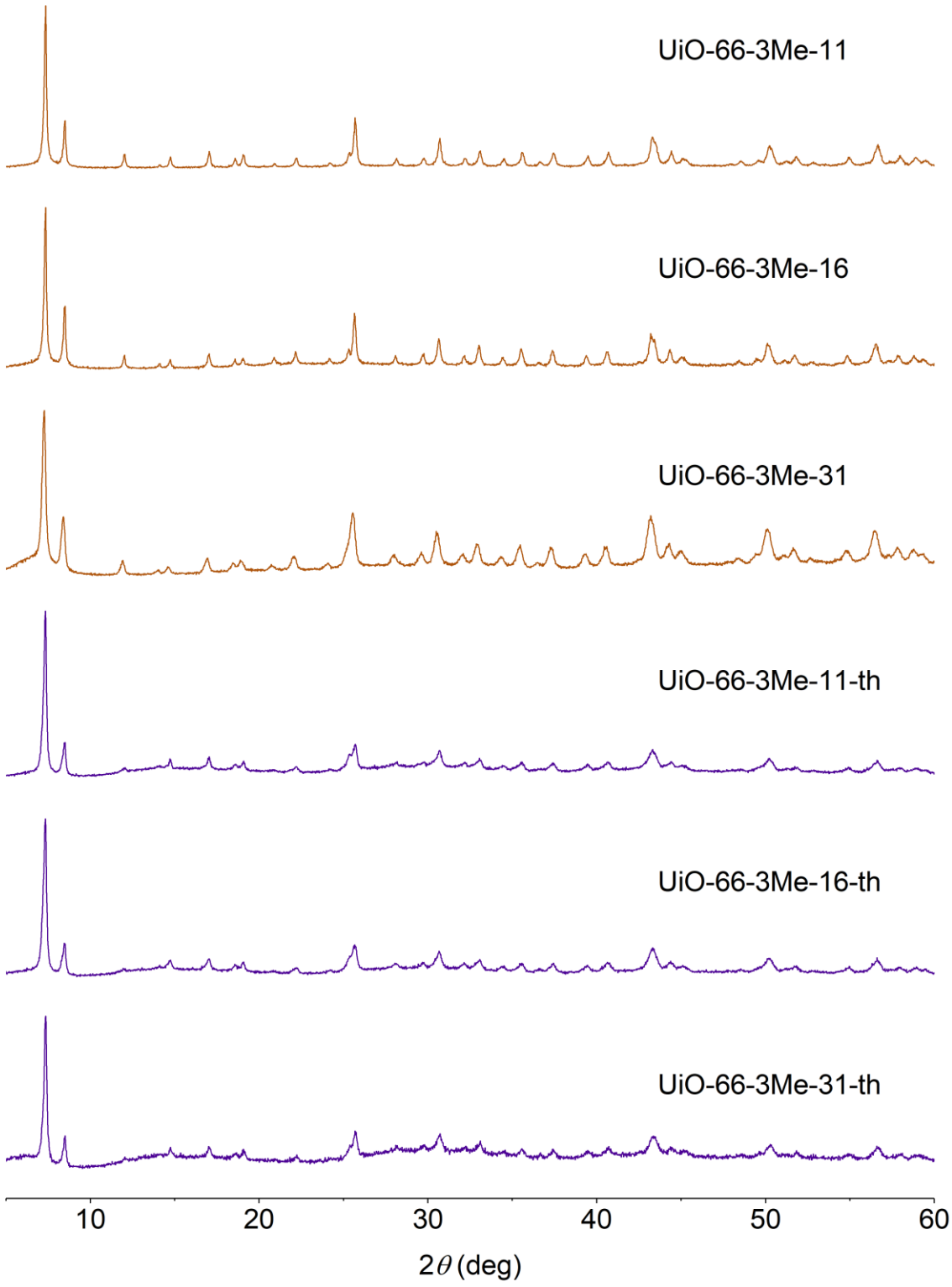

Figure S13: Powder X-ray diffraction patterns of mixed ligand MOFs containing 3-methyladipate and terephthalate before thermolysis, UiO-66-3Me-*x* (highlighted in orange) and after thermolysis, UiO-66-3Me-*x*-th (highlighted in purple).

4. NMR of Digested UiO-66 samples

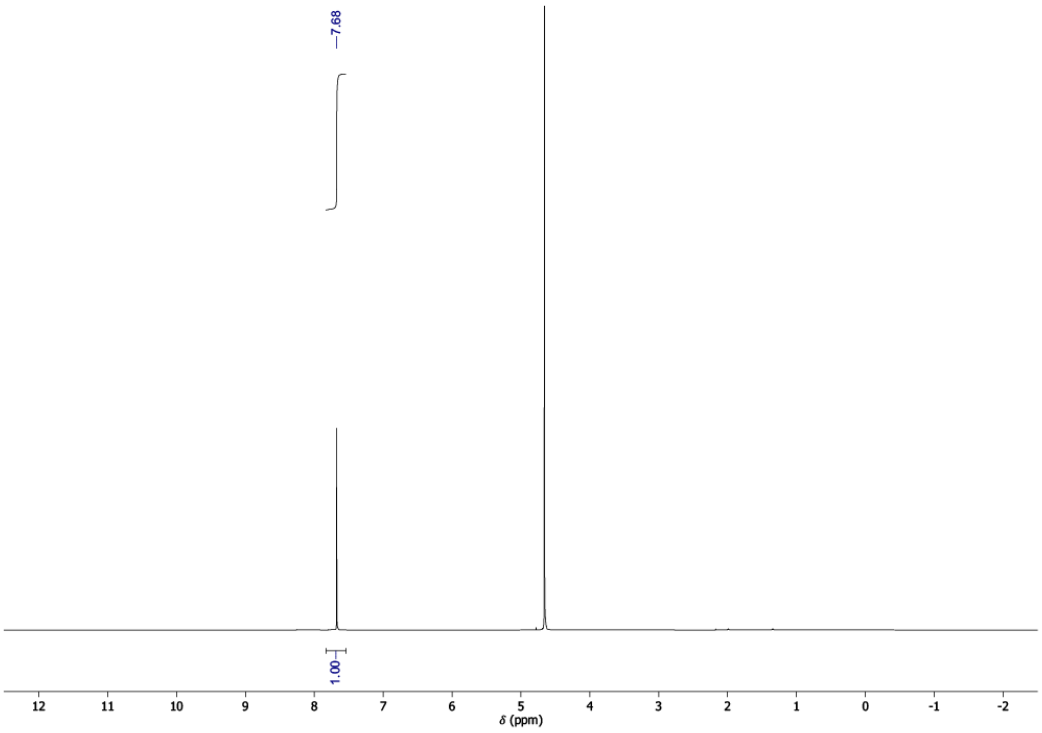

Figure S14. ^{1}H NMR spectrum of UiO-66-0 digested in K_3PO_4 in D_2O.

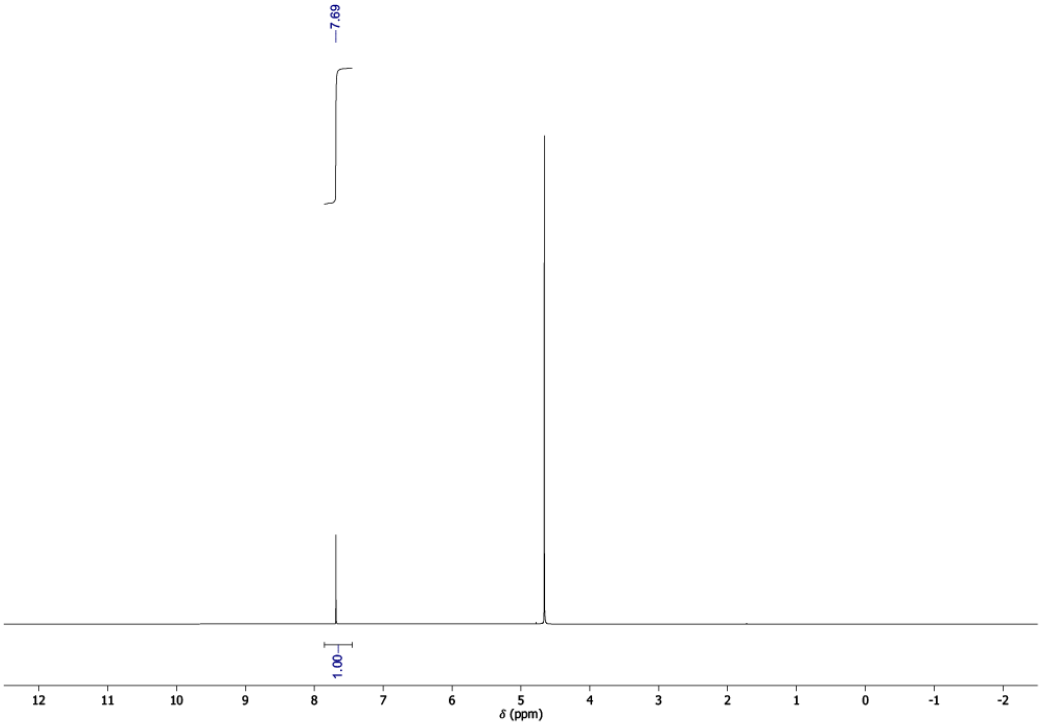

Figure S15. ^{1}H NMR spectrum of UiO-66-0-th digested in K_3PO_4 in D_2O.

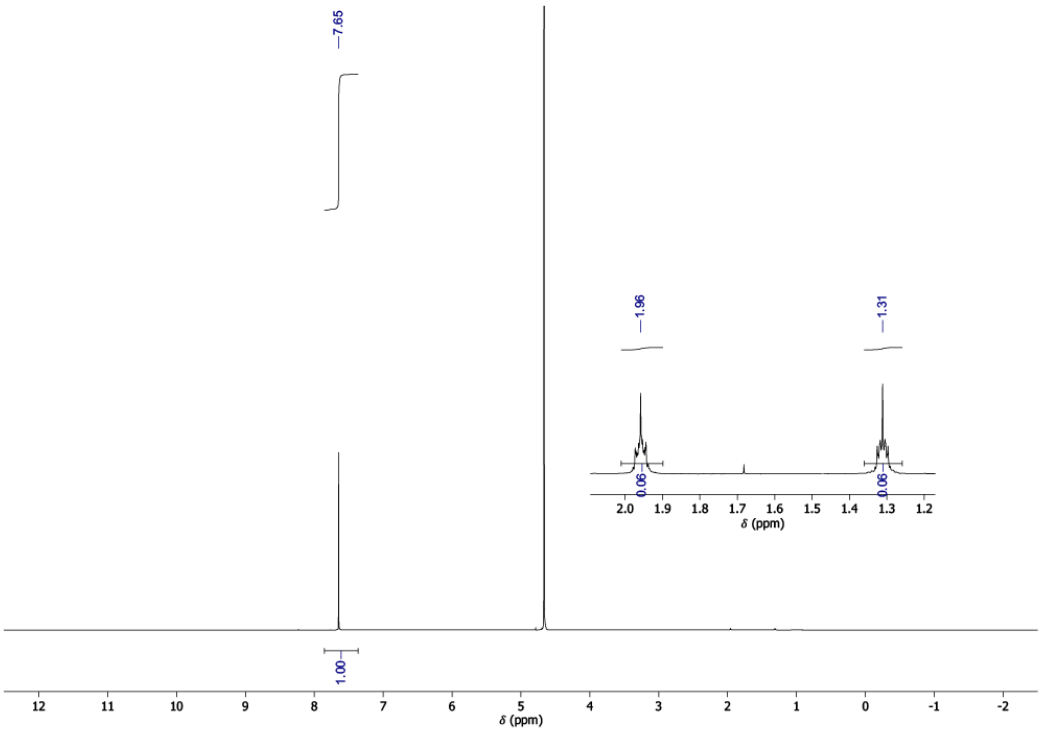

Figure S16. ^{1}H NMR spectrum of UiO-66-5 digested in K_3PO_4 in D_2O.

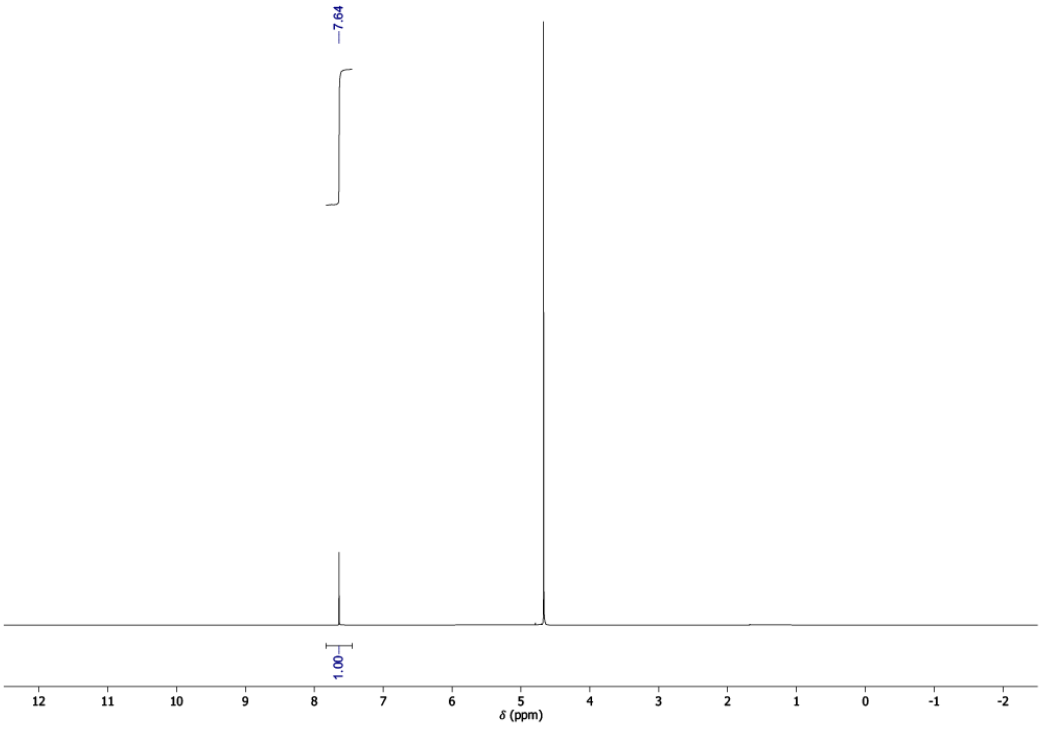

Figure S17. ^{1}H NMR spectrum of UiO-66-5-th digested in K_3PO_4 in D_2O.

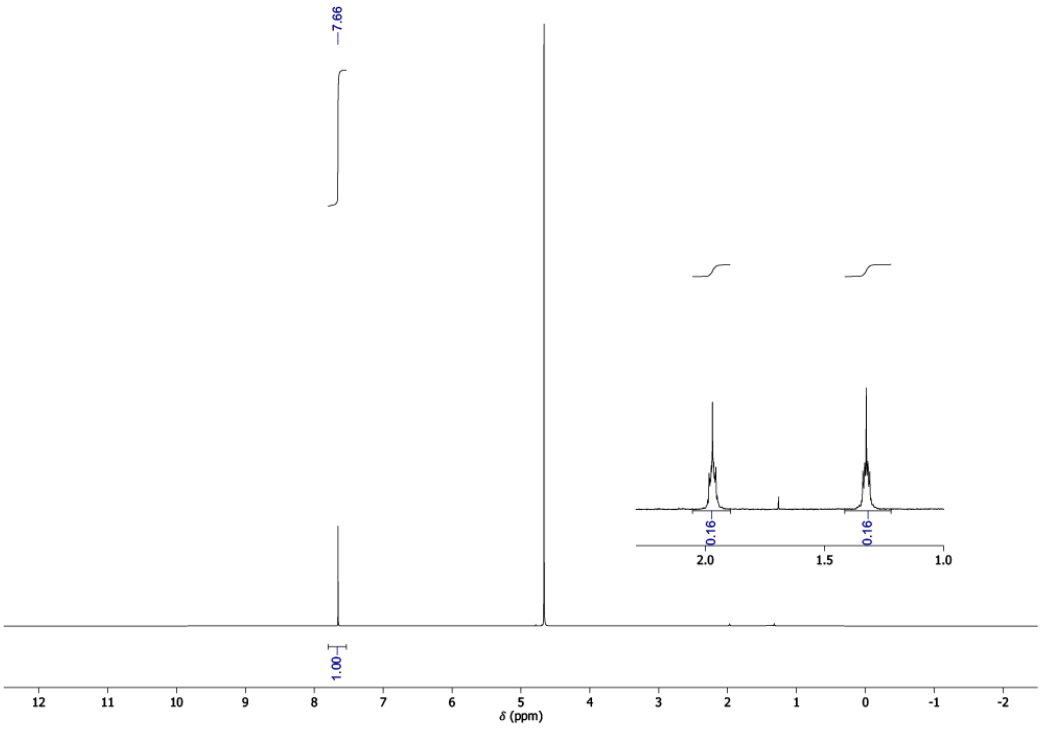

Figure S18. ^{1}H NMR spectrum of UiO-66-14 digested in K_3PO_4 in D_2O.

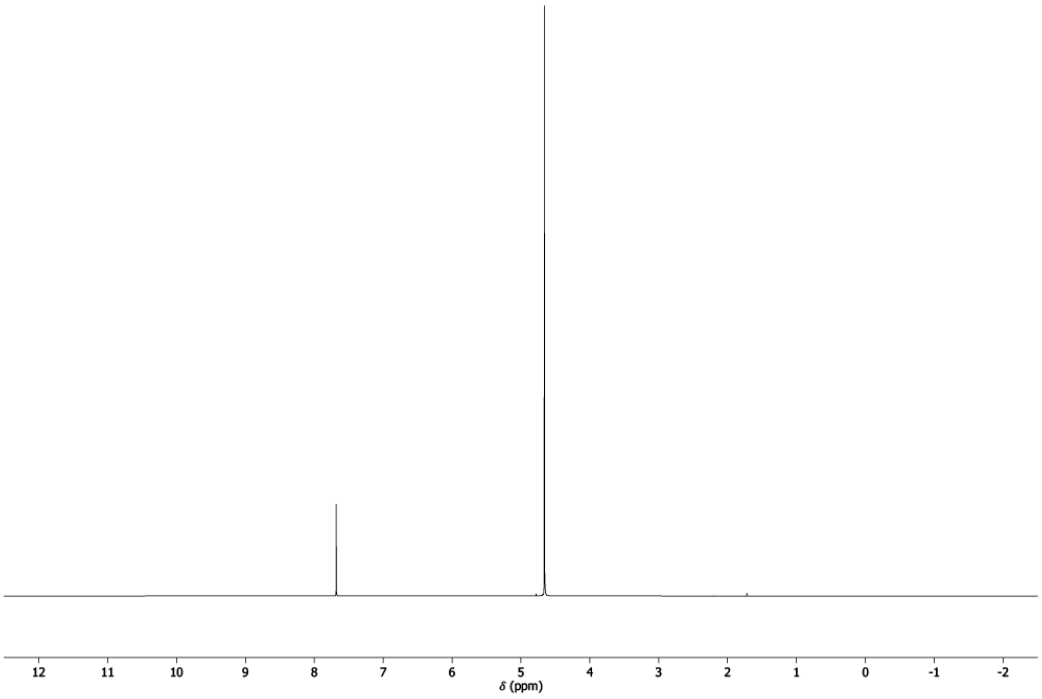

Figure S19. ^{1}H NMR spectrum of UiO-66-14-th digested in K_3PO_4 in D_2O.

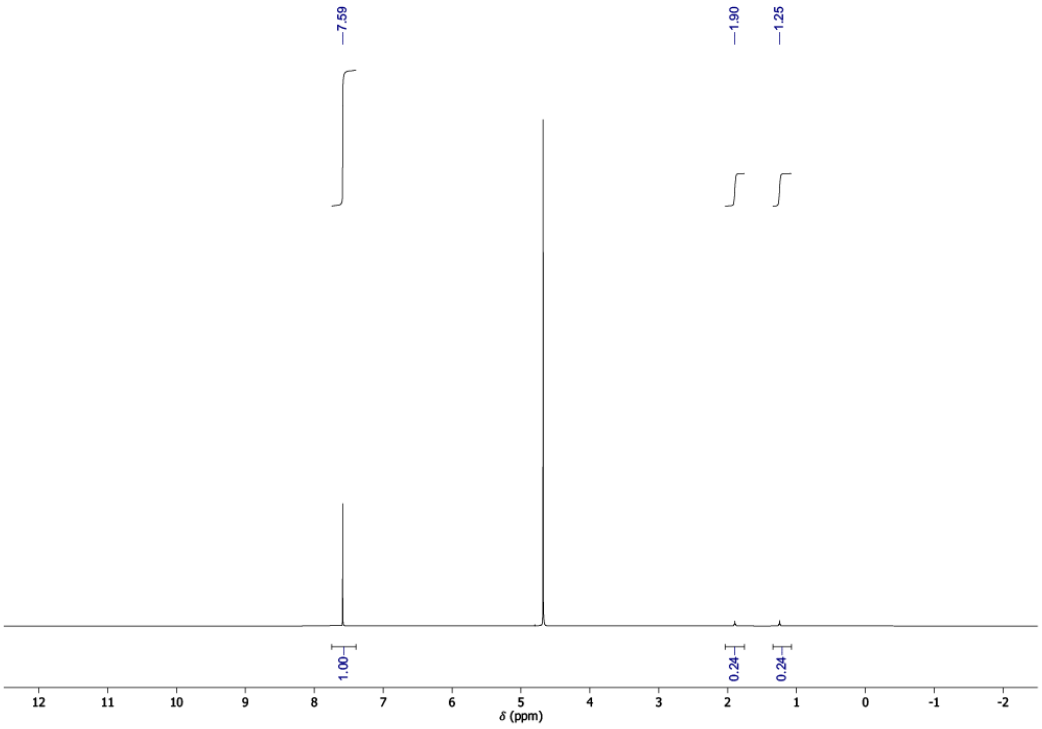

Figure S20. ^{1}H NMR spectrum of UiO-66-19 digested in K_3PO_4 in D_2O.

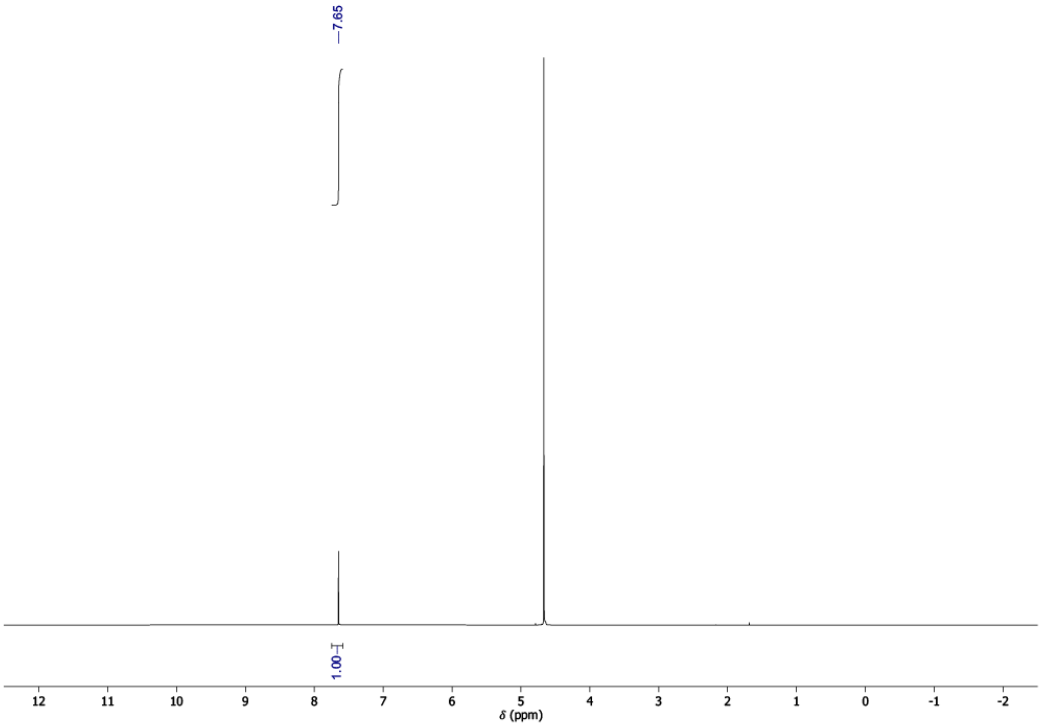

Figure S21. ^{1}H NMR spectrum of UiO-66-19-th digested in K_3PO_4 in D_2O.

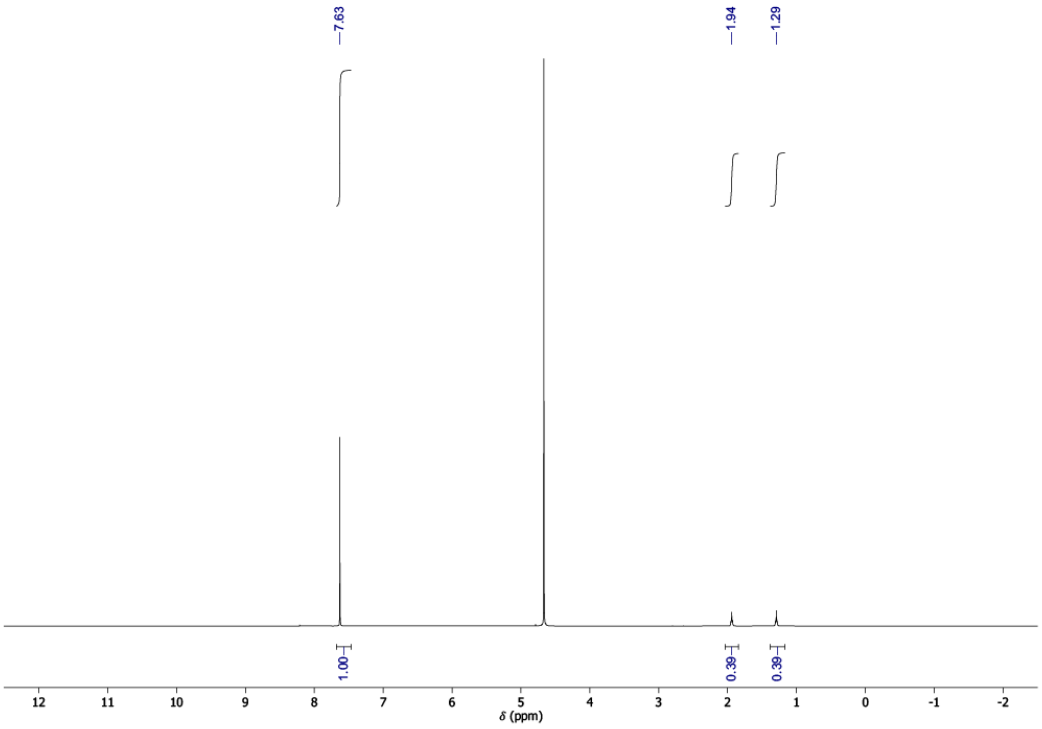

Figure S22. ^{1}H NMR spectrum of UiO-66-28 digested in K_3PO_4 in D_2O.

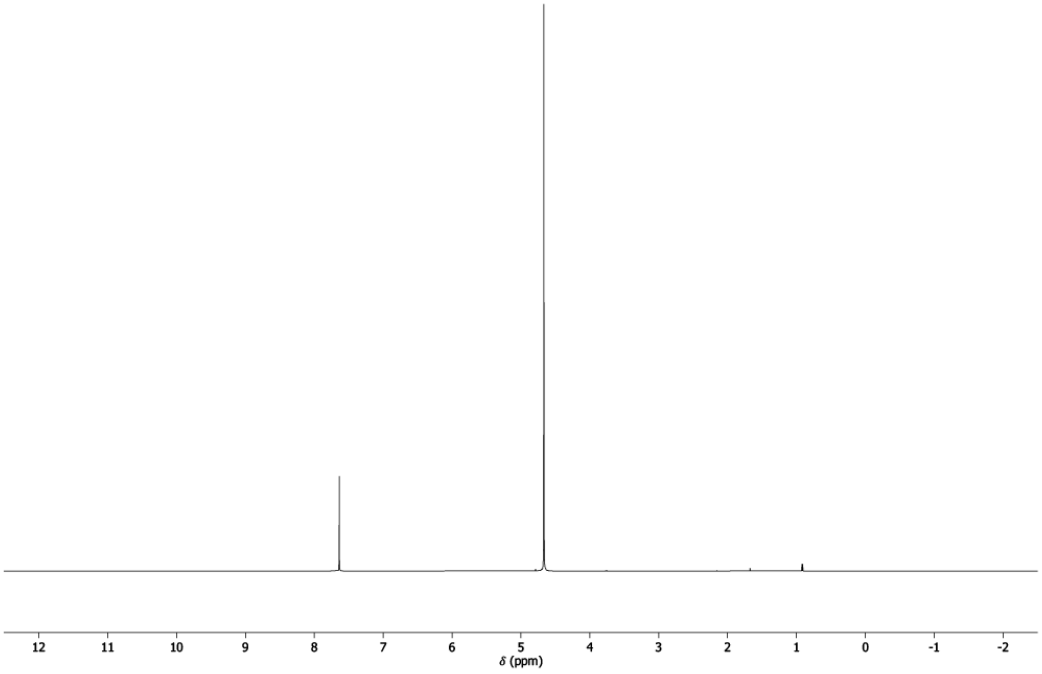

Figure S23. ^{1}H NMR spectrum of UiO-66-28-th digested in K_3PO_4 in D_2O.

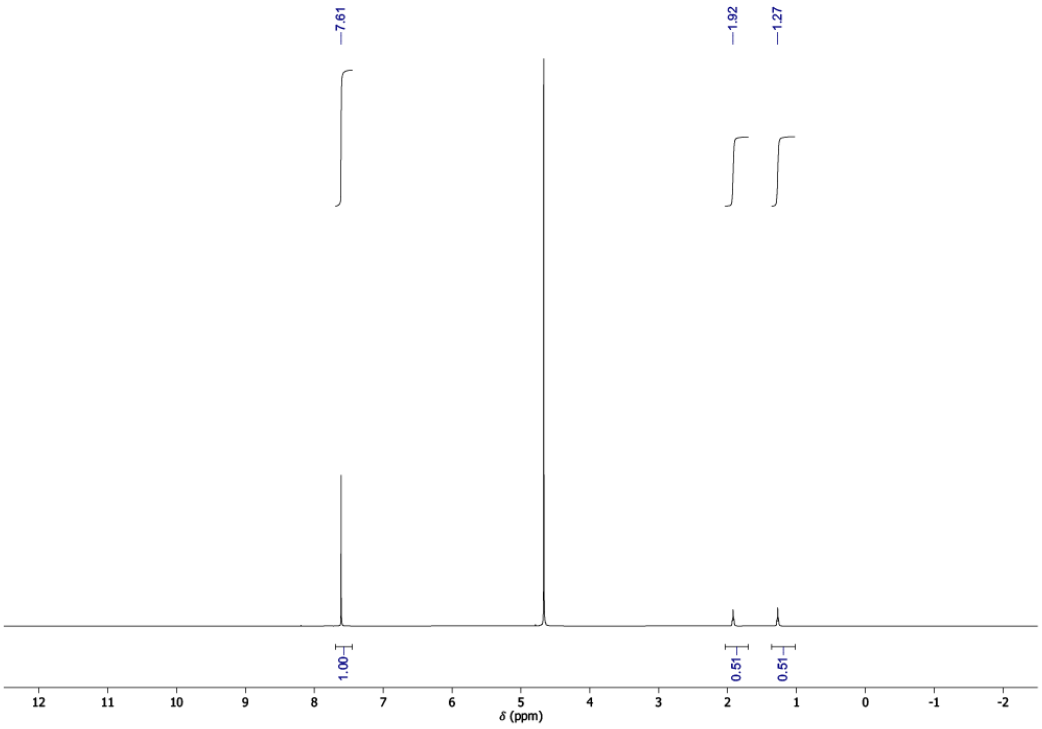

Figure S24. ^{1}H NMR spectrum of UiO-66-35 digested in K_3PO_4 in D_2O.

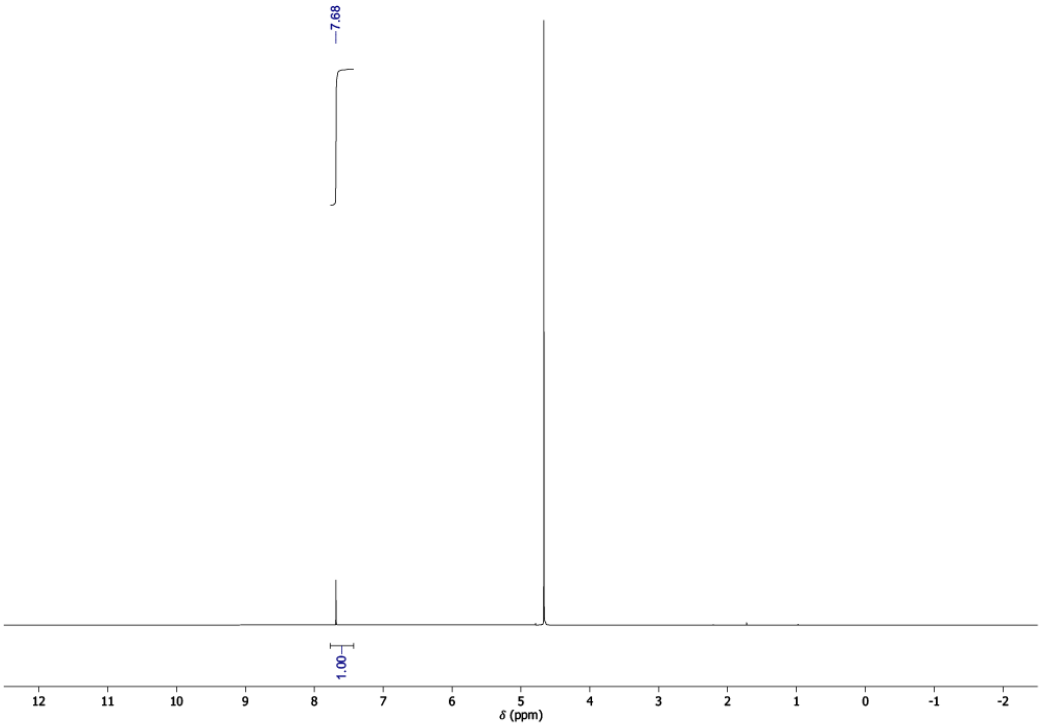

Figure S25. ^{1}H NMR spectrum of UiO-66-35-th digested in K_3PO_4 in D_2O.

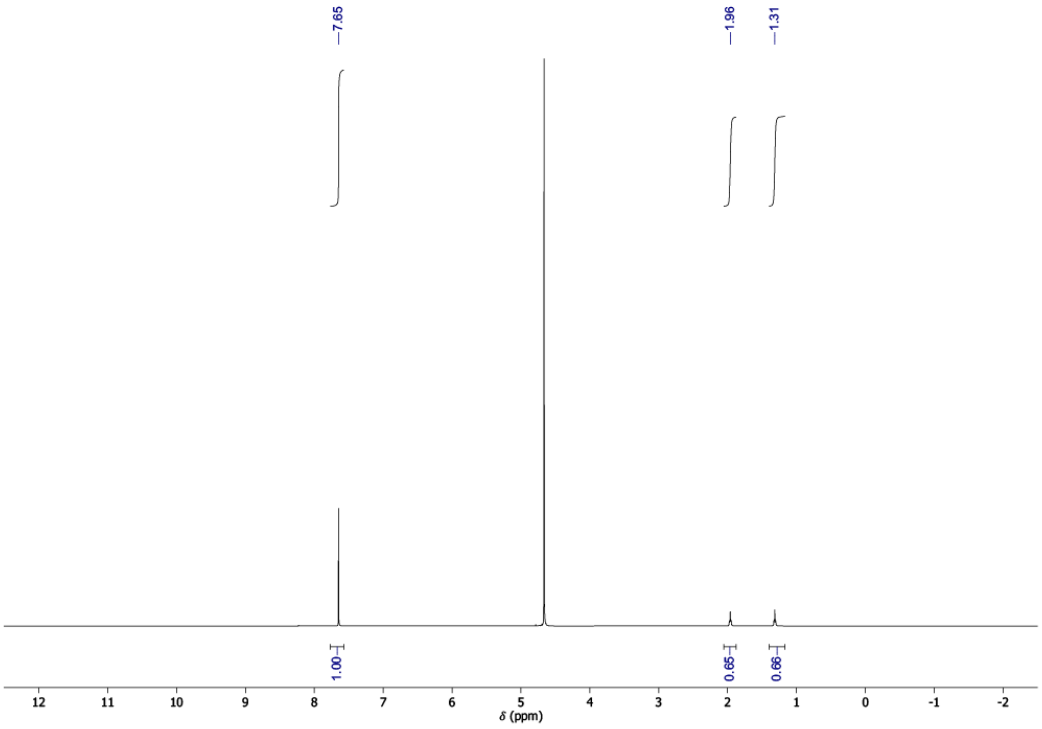

Figure S26. ^{1}H NMR spectrum of UiO-66-40 digested in K_3PO_4 in D_2O.

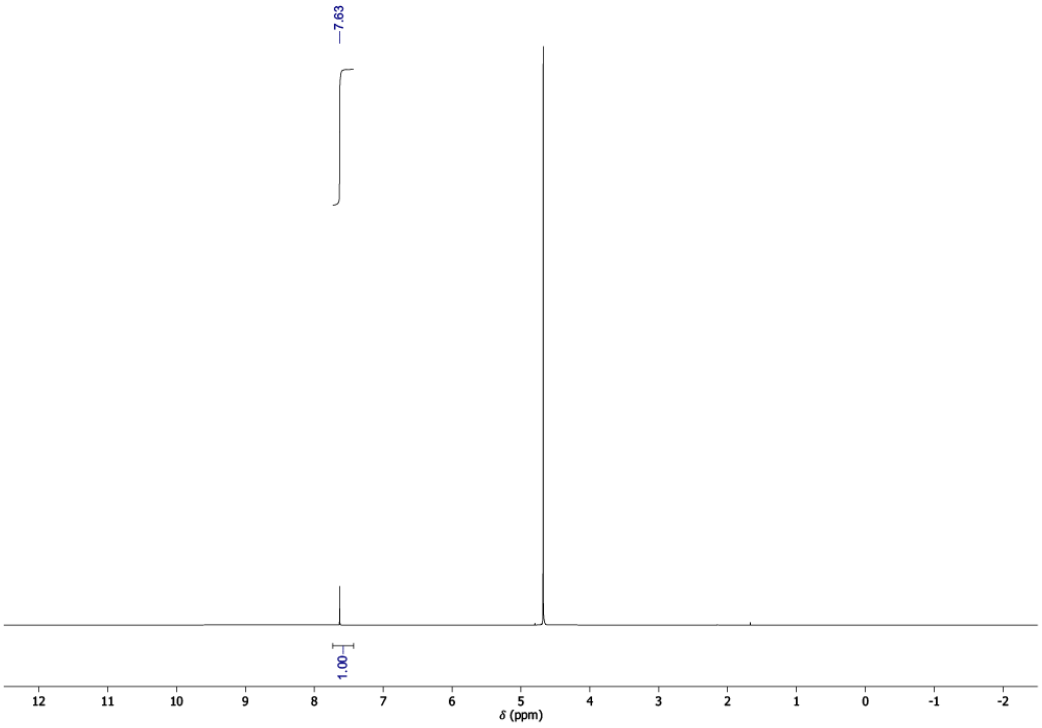

Figure S27. ^{1}H NMR spectrum of UiO-66-40-th digested in K_3PO_4 in D_2O.

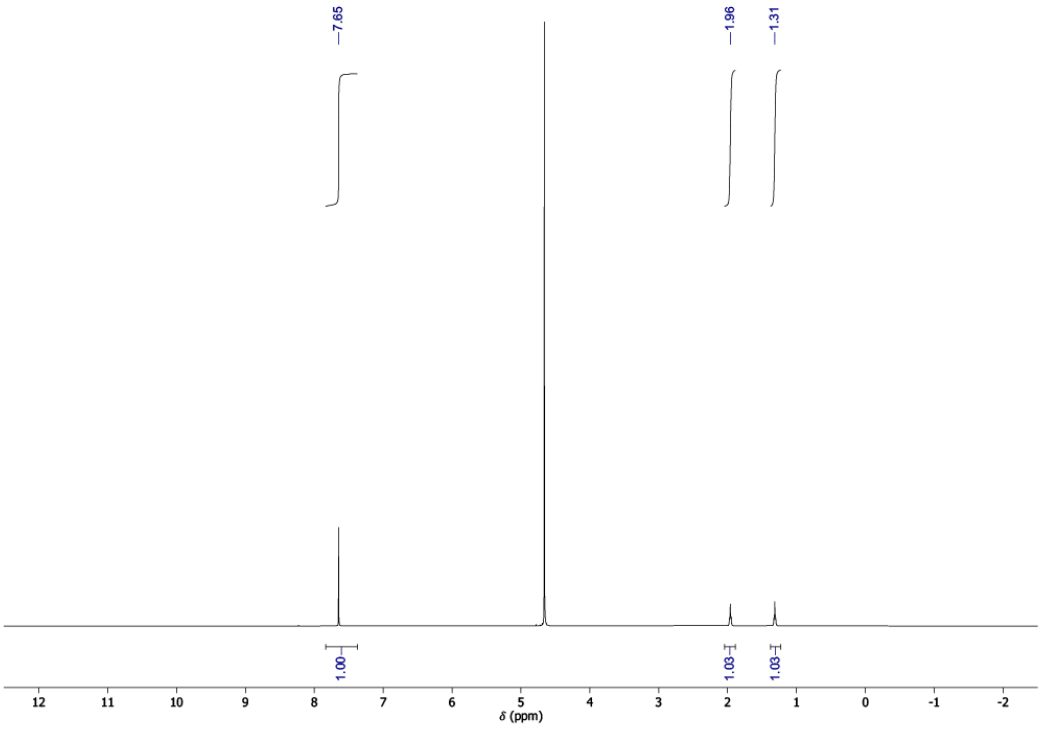

Figure S28. ^{1}H NMR spectrum of UiO-66-51 digested in K_3PO_4 in D_2O.

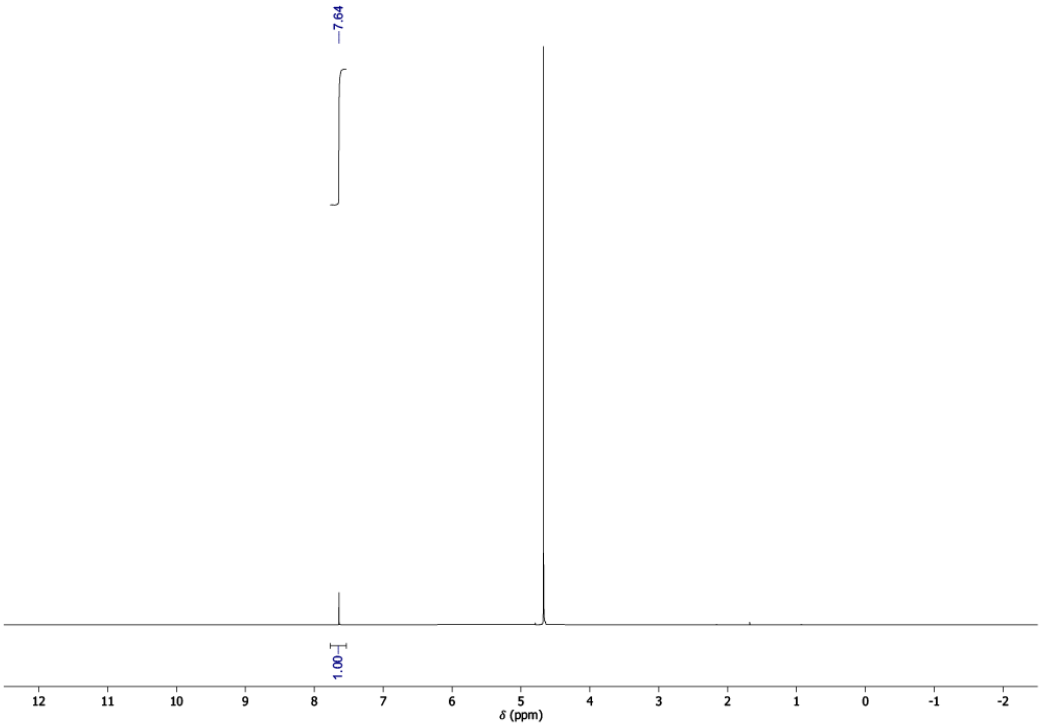

Figure S29. ^{1}H NMR spectrum of UiO-66-51-th digested in K_3PO_4 in D_2O.

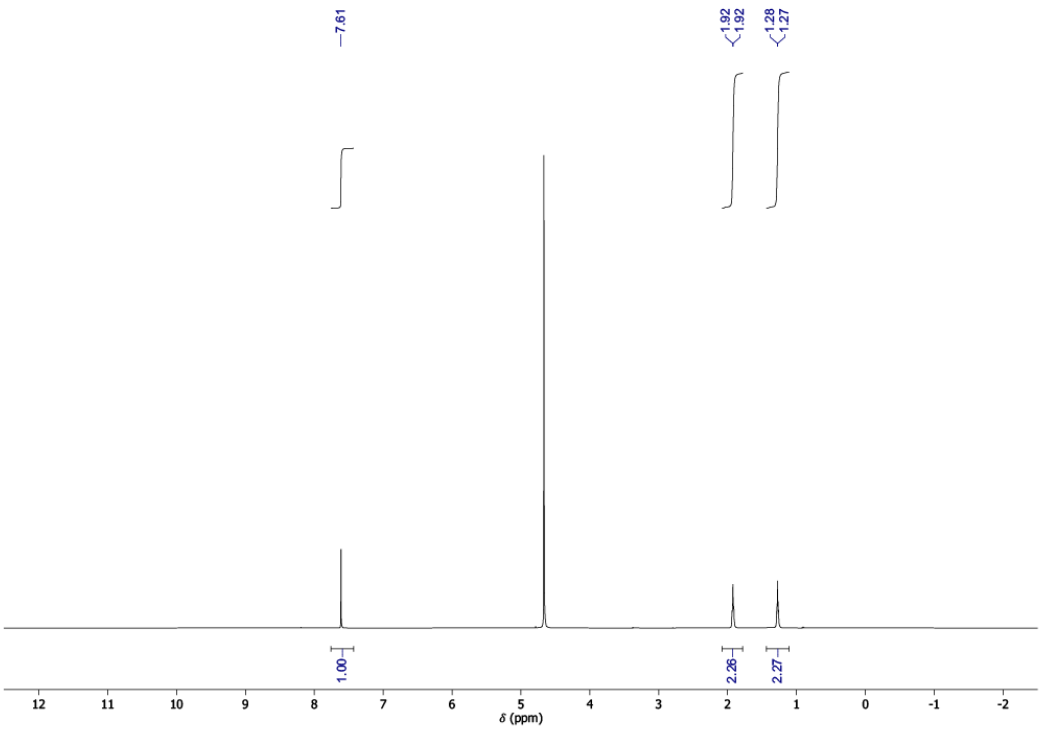

Figure S30. ^{1}H NMR spectrum of UiO-66-69 digested in K_3PO_4 in D_2O.

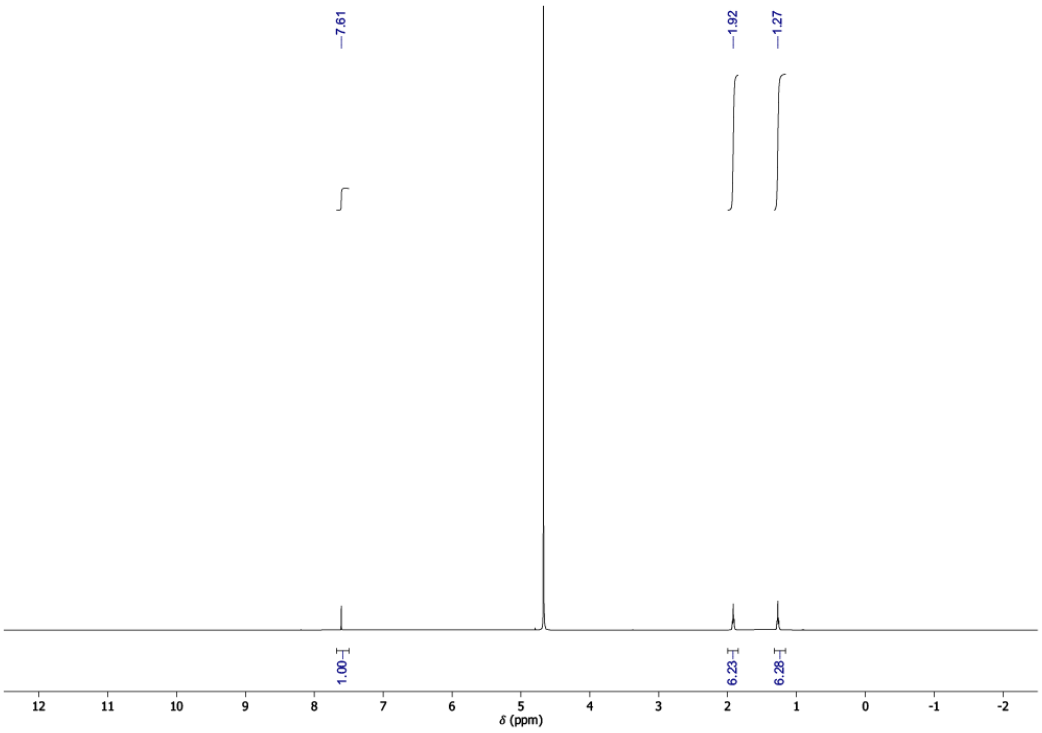

Figure S31. ^{1}H NMR spectrum of UiO-66-87 digested in K_3PO_4 in D_2O.

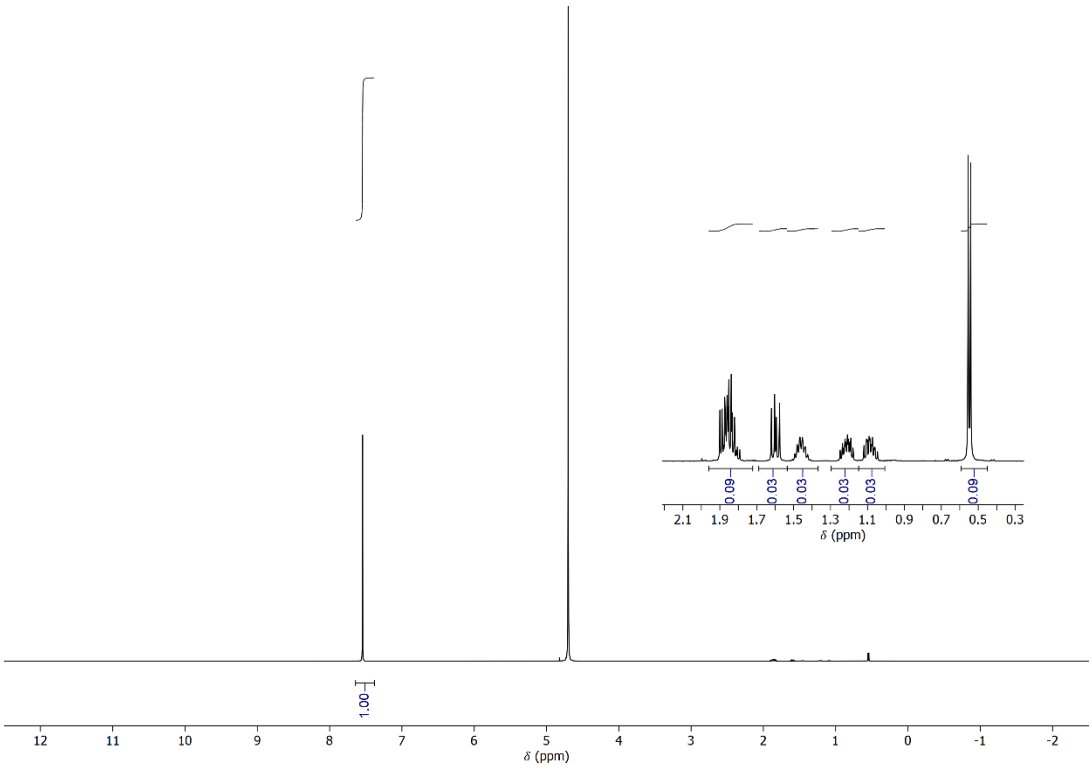

Figure S32. ^{1}H NMR spectrum of UiO-66-3Me-11 digested in K_3PO_4 in D_2O.

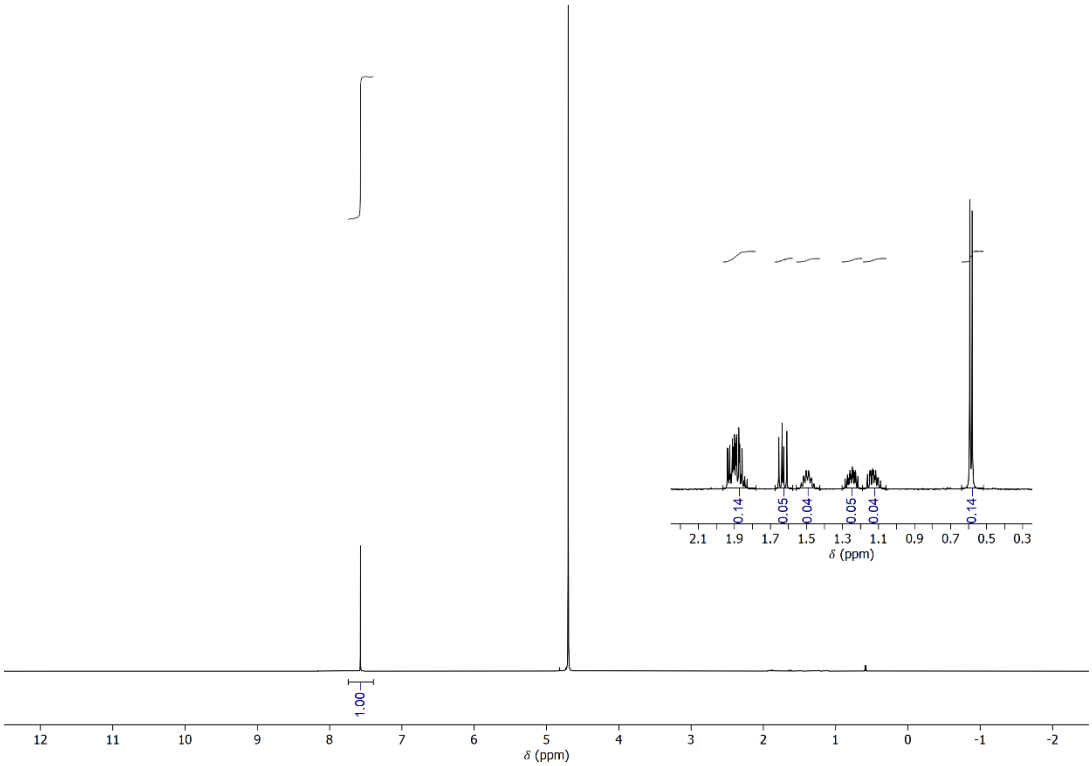

Figure S33. ^{1}H NMR spectrum of UiO-66-3Me-16 digested in K_3PO_4 in D_2O.

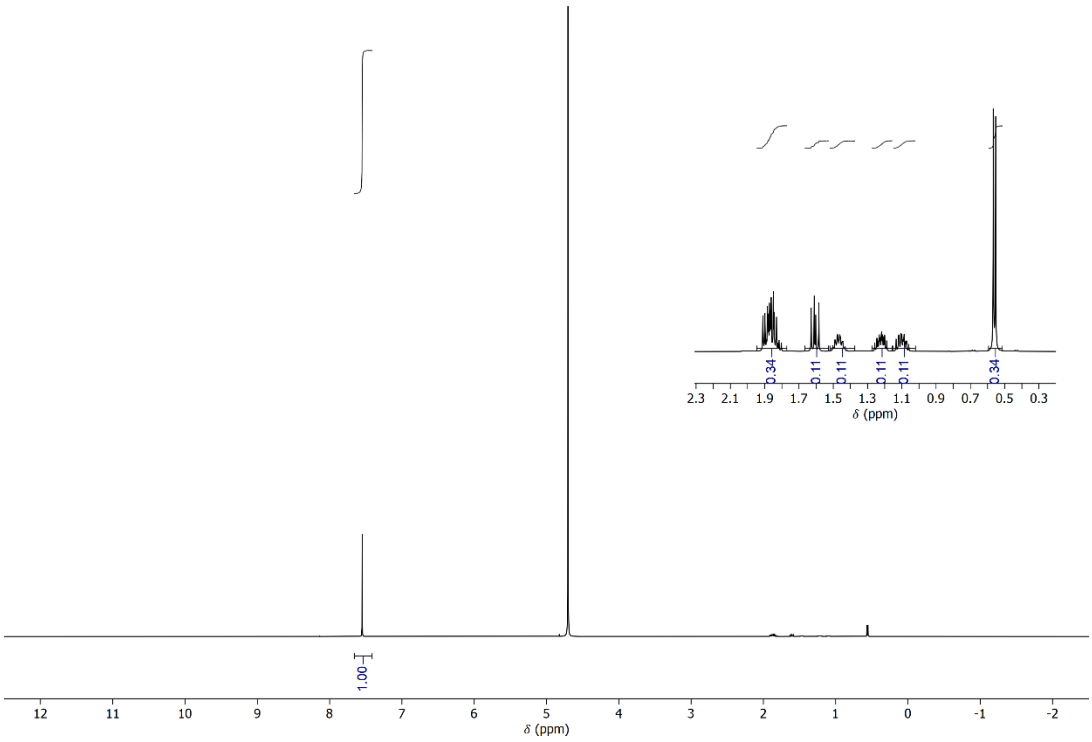

Figure S34. ^{1}H NMR spectrum of UiO-66-3Me-31 digested in K_3PO_4 in D_2O.

5. Solid state NMR

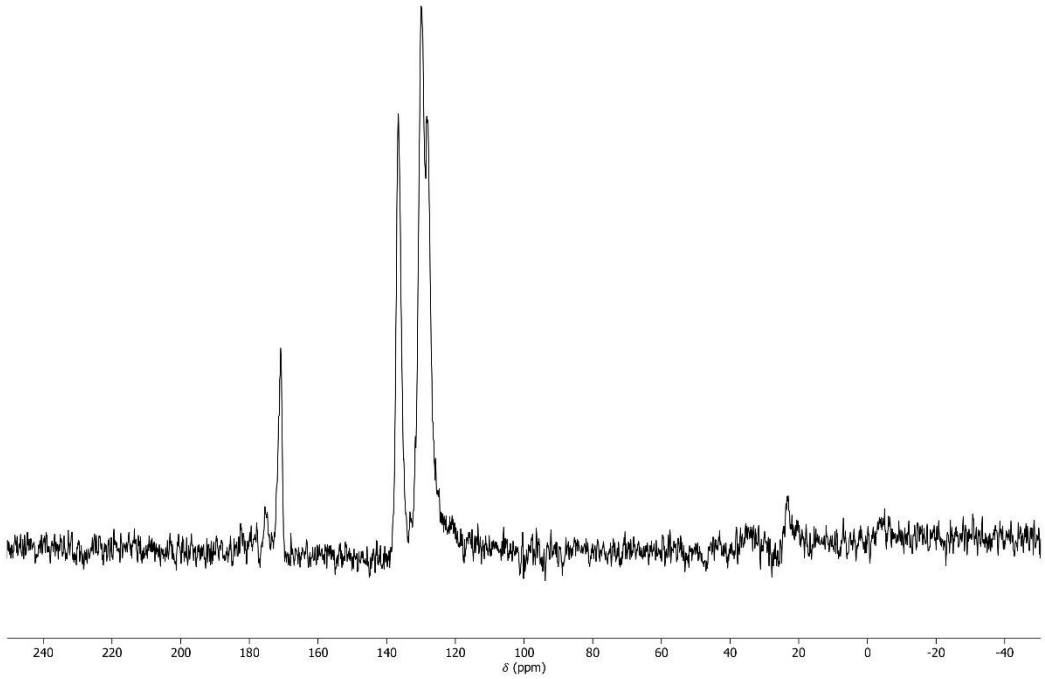

Figure S35. Solid state ^{13}C NMR spectrum of UiO-66-5.

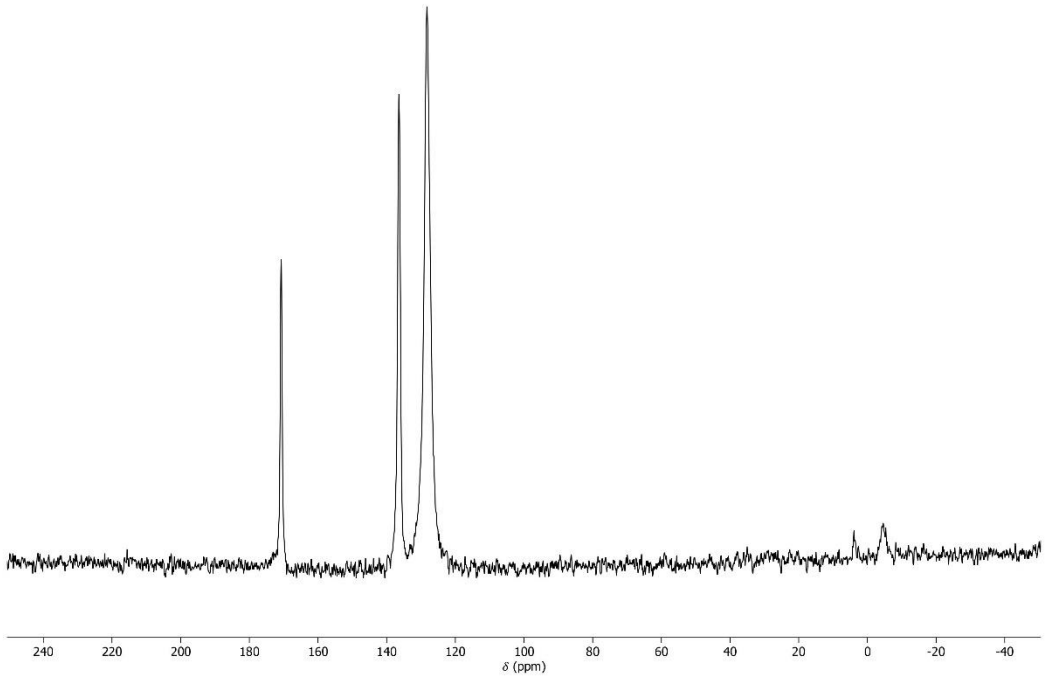

Figure S36. Solid state ^{13}C NMR spectrum UiO-66-5-th.

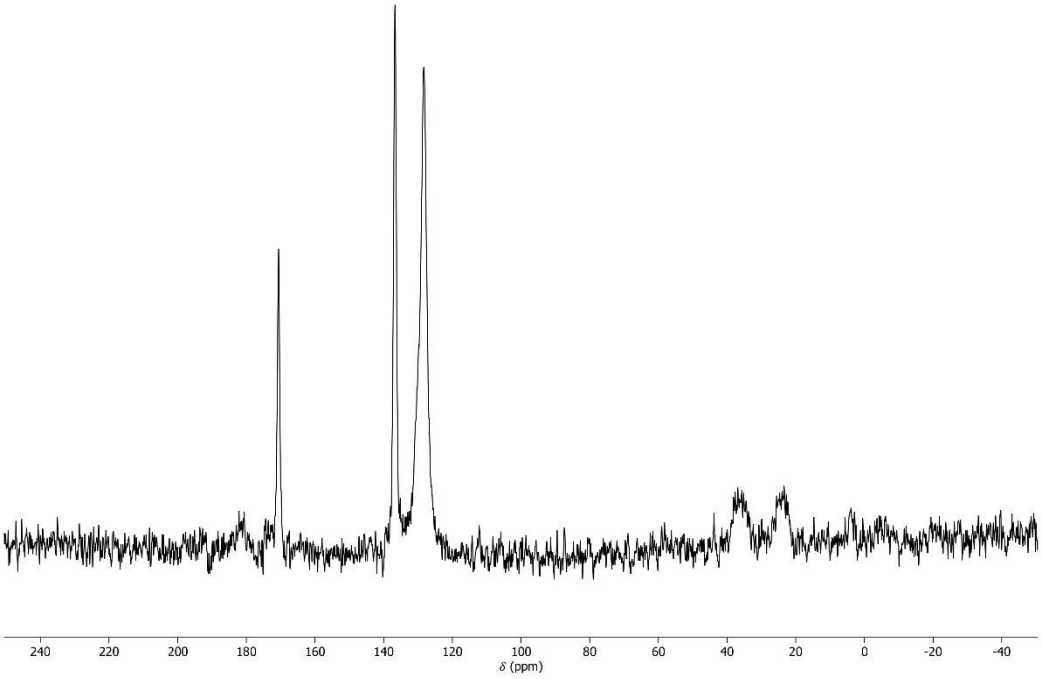

Figure S37. Solid state ^{13}C NMR spectrum of UiO-66-14.

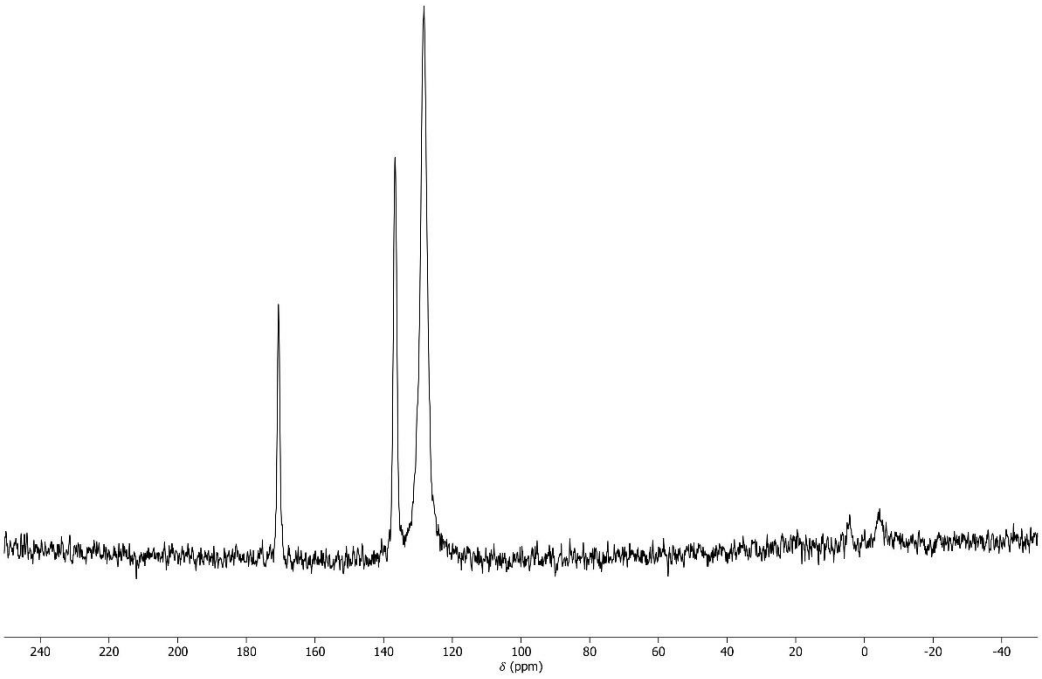

Figure S38. Solid state ^{13}C NMR spectrum of UiO-66-14-th.

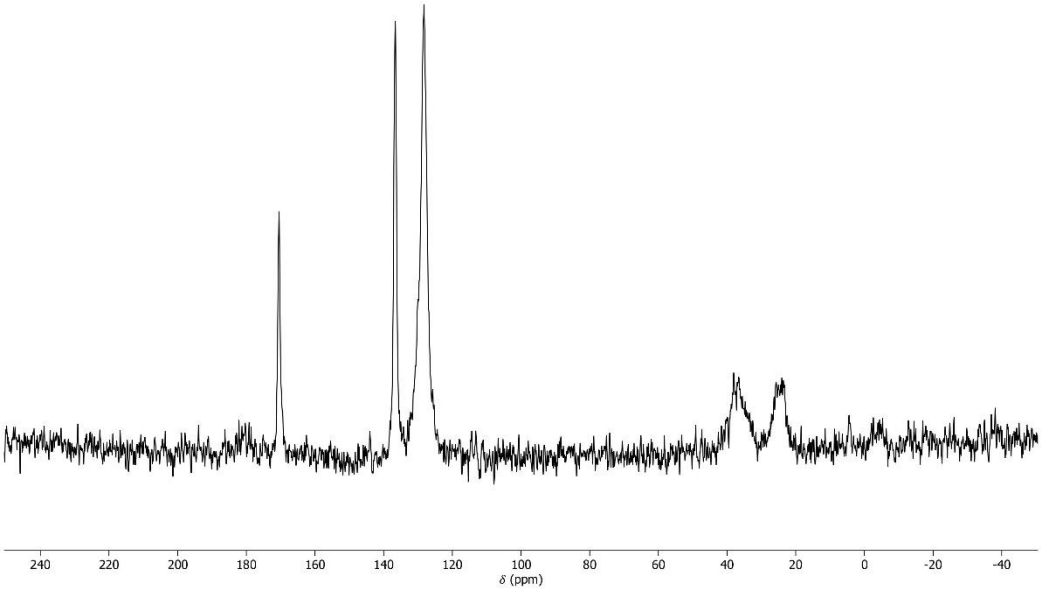

Figure S39. Solid state ^{13}C NMR spectrum of UiO-66-19

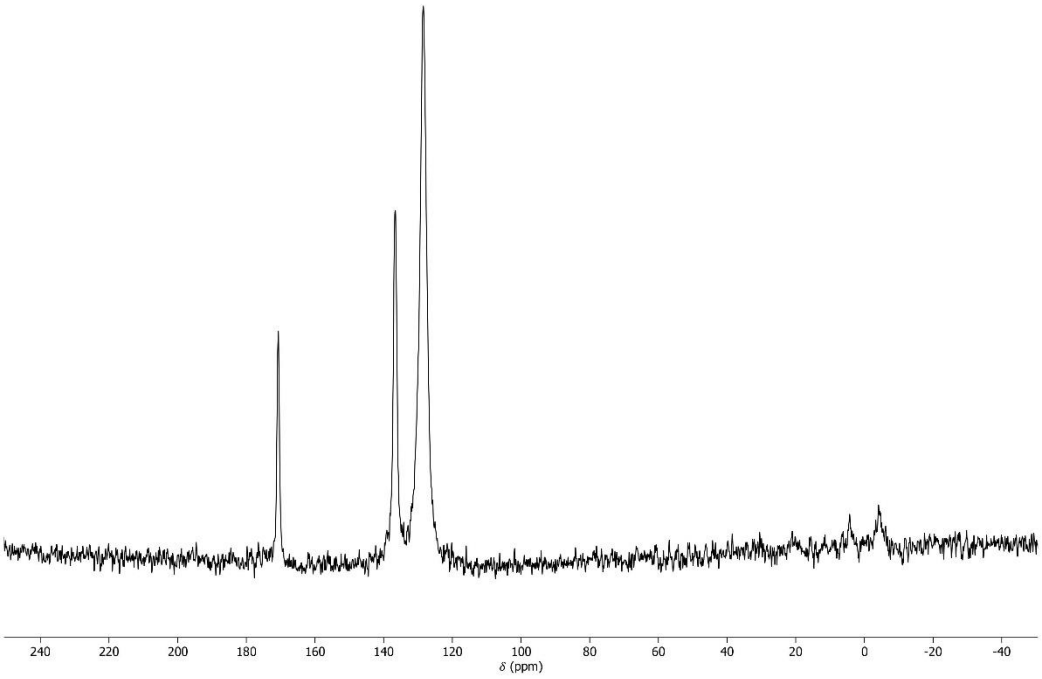

Figure S40. Solid state ^{13}C NMR spectrum of UiO-66-19-th

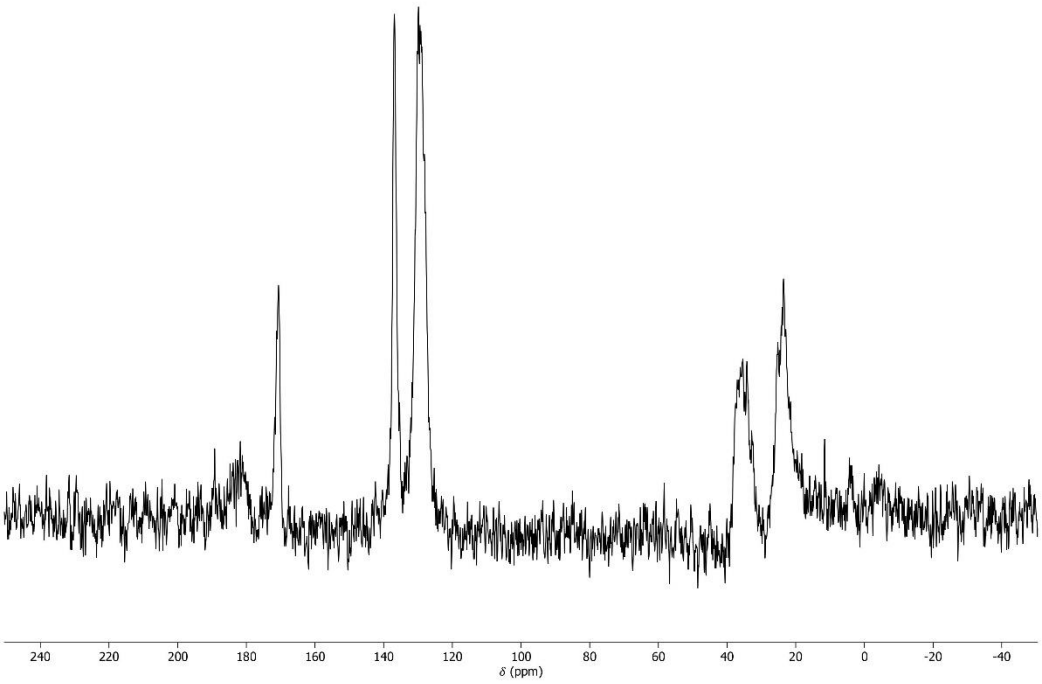

Figure S41. Solid state ^{13}C NMR spectrum of UiO-66-28.

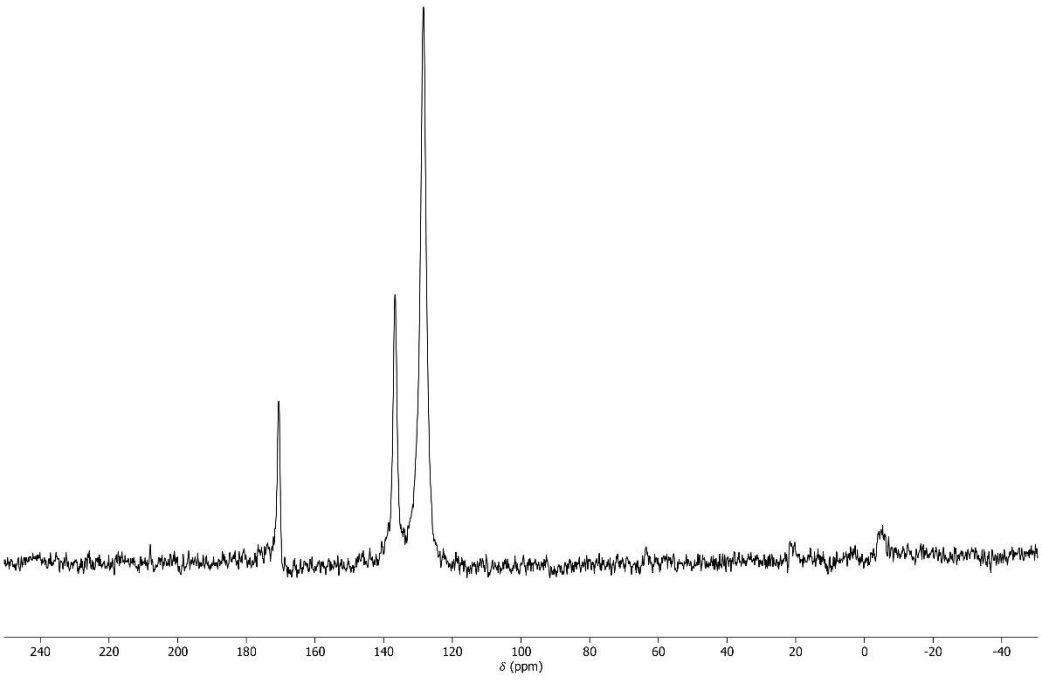

Figure S42. Solid state ^{13}C NMR spectrum of UiO-66-28-th.

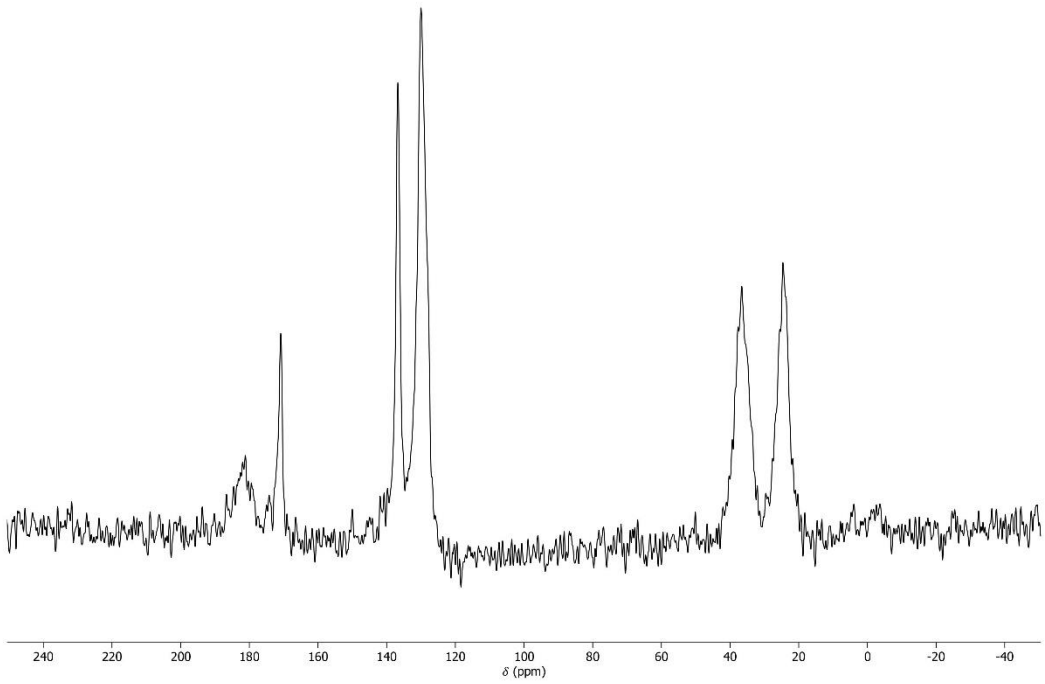

Figure S43. Solid state ^{13}C NMR spectrum of UiO-66-35.

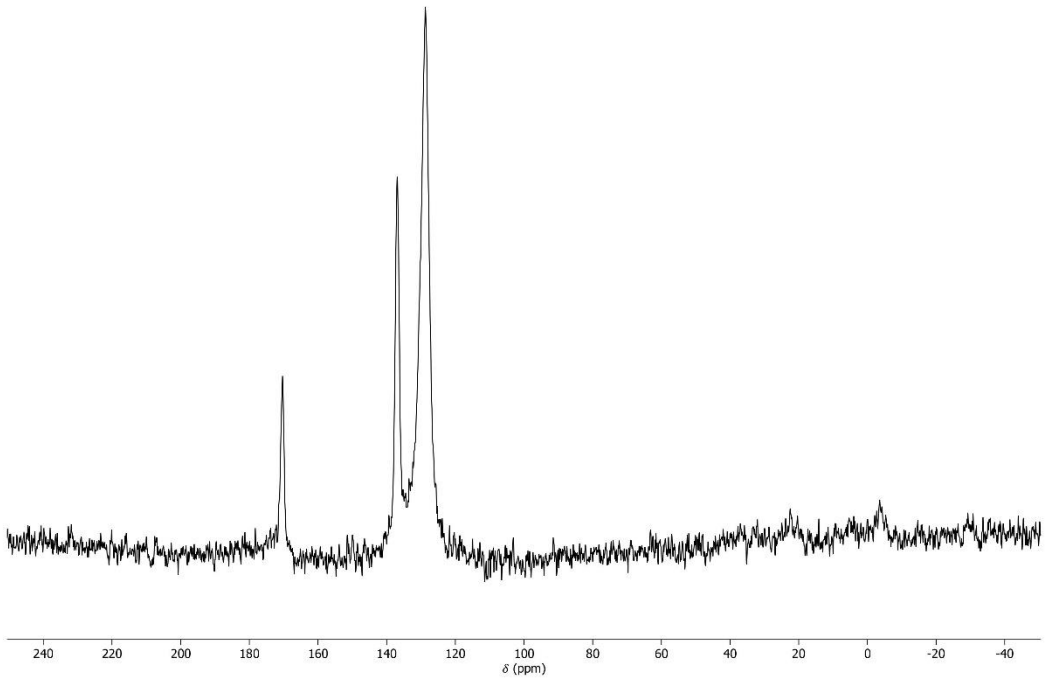

Figure S44. Solid state ^{13}C NMR spectrum of UiO-66-35-th.

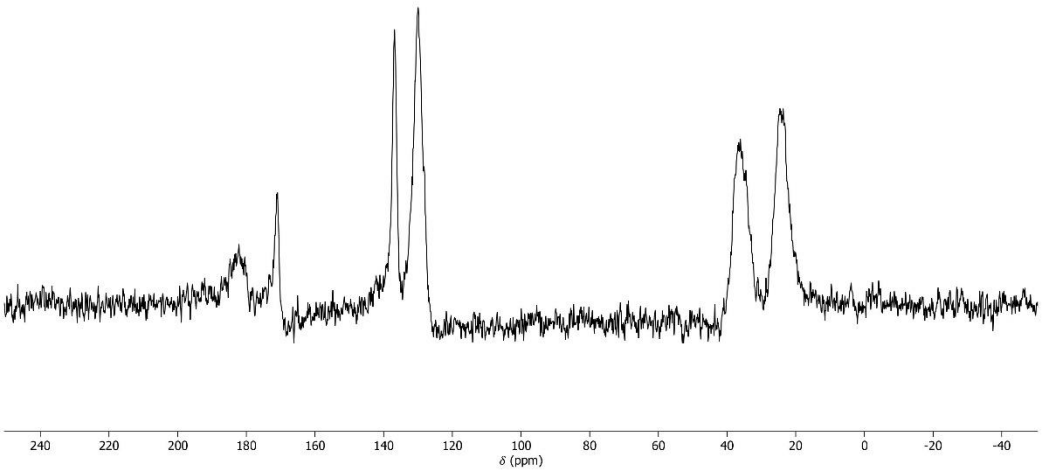

Figure S45. Solid state ^{13}C NMR spectrum of UiO-66-40.

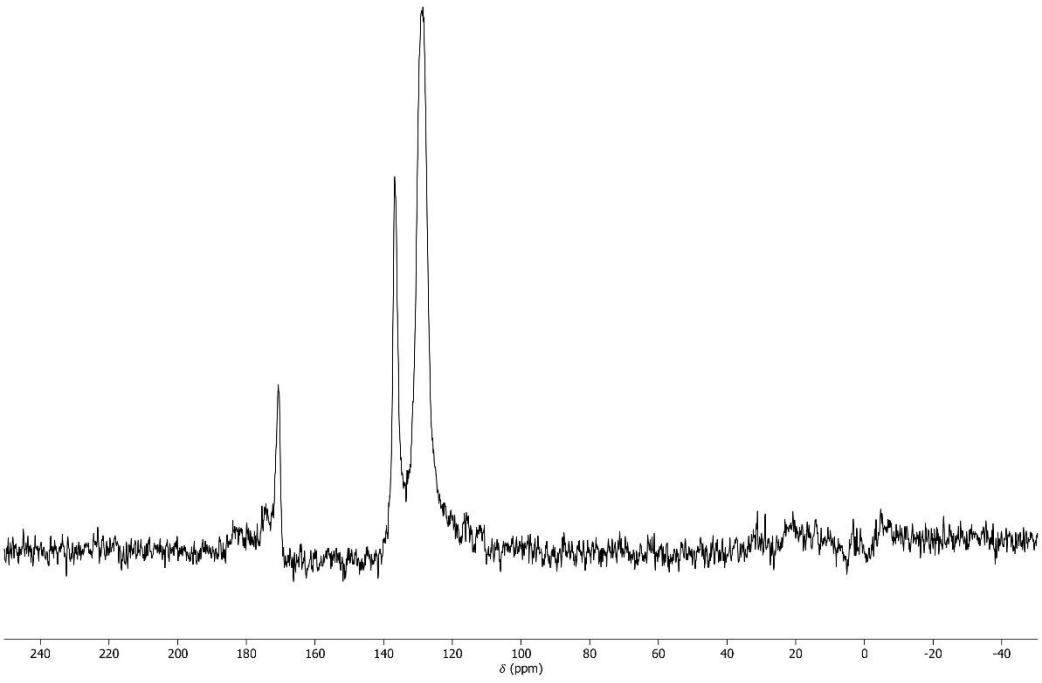

Figure S46. Solid state ^{13}C NMR spectrum of UiO-66-40-th.

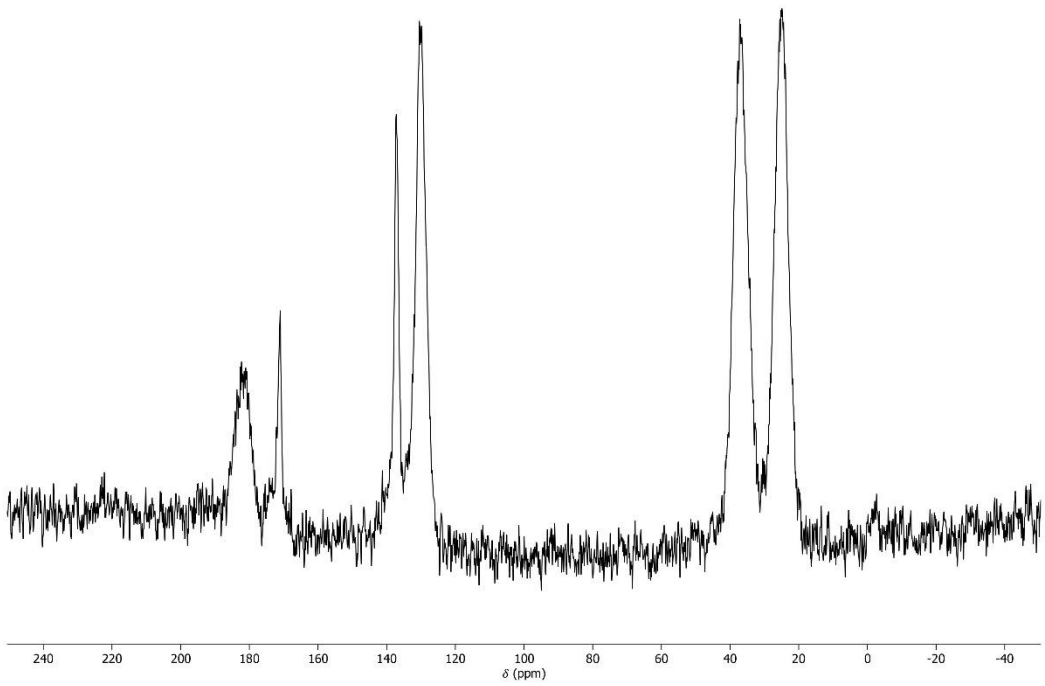

Figure S47. Solid state ^{13}C NMR spectrum of UiO-66-51.

6. Thermogravimetric Analysis

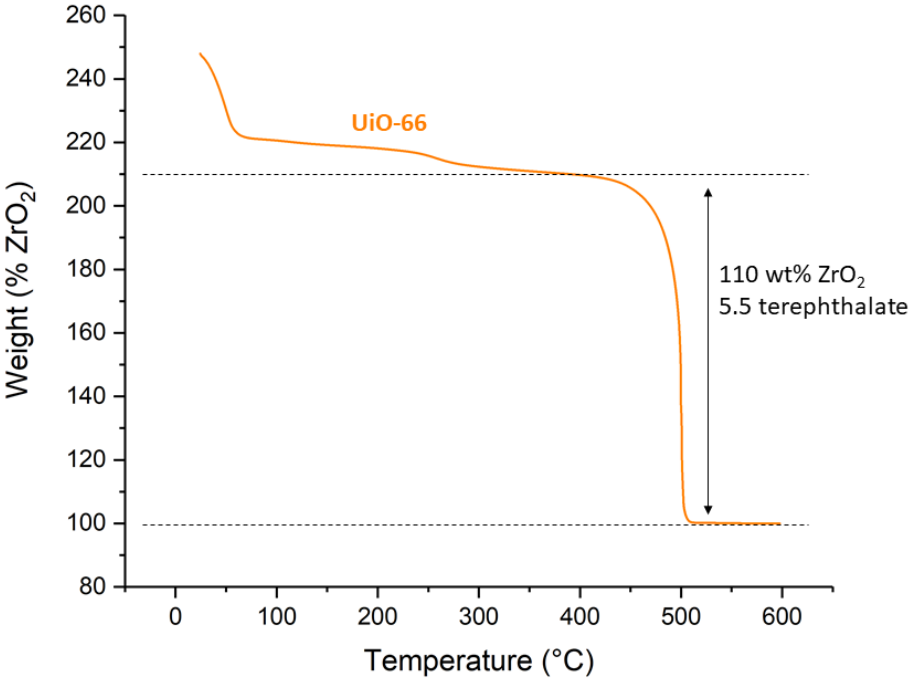

Figure S48. Thermogravimetric plots of UiO-66-0

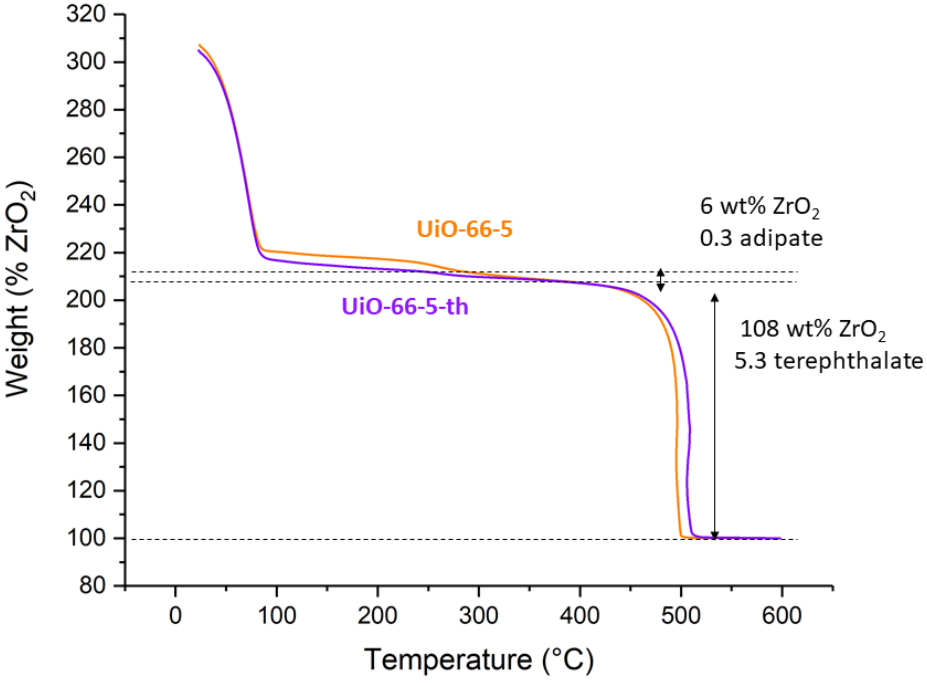

Figure S49. Thermogravimetric plots of UiO-66-5, before (orange) and after (purple) thermolysis.

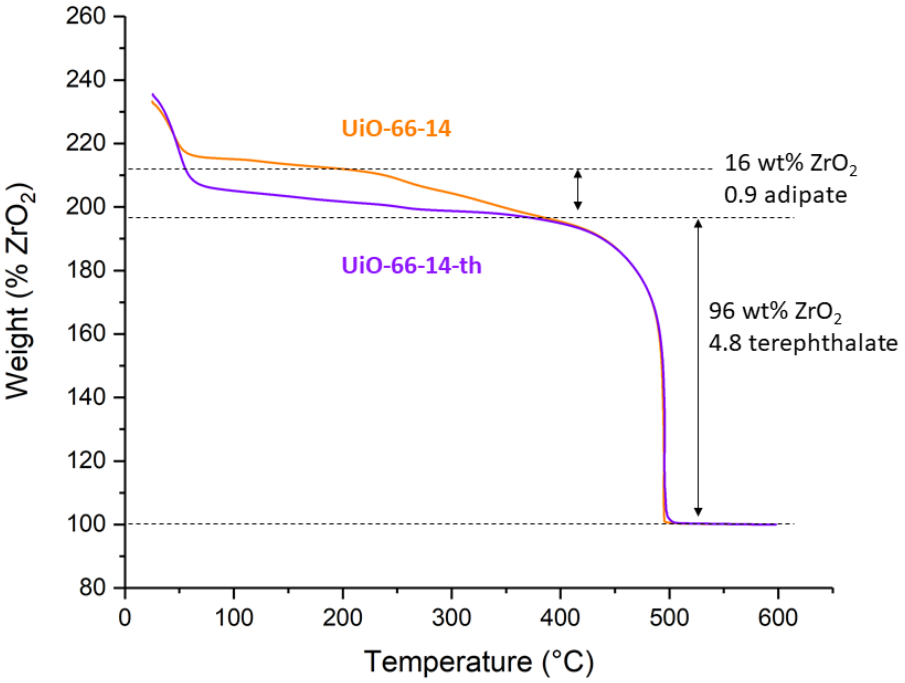

Figure S50. Thermogravimetric plots of UiO-66-14, before (orange) and after (purple) thermolysis.

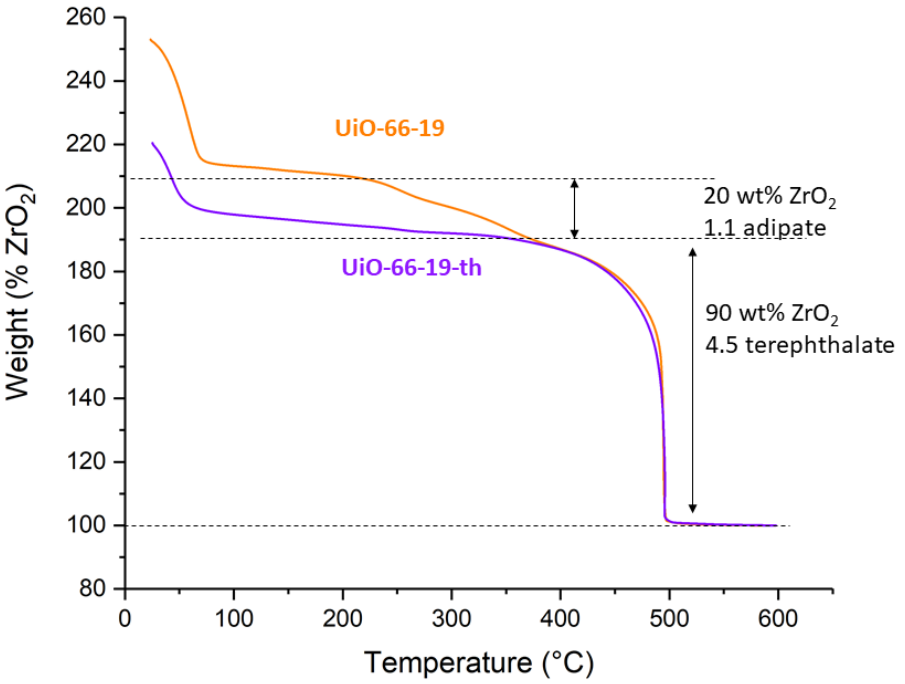

Figure S51. Thermogravimetric plots of UiO-66-19, before (orange) and after (purple) thermolysis.

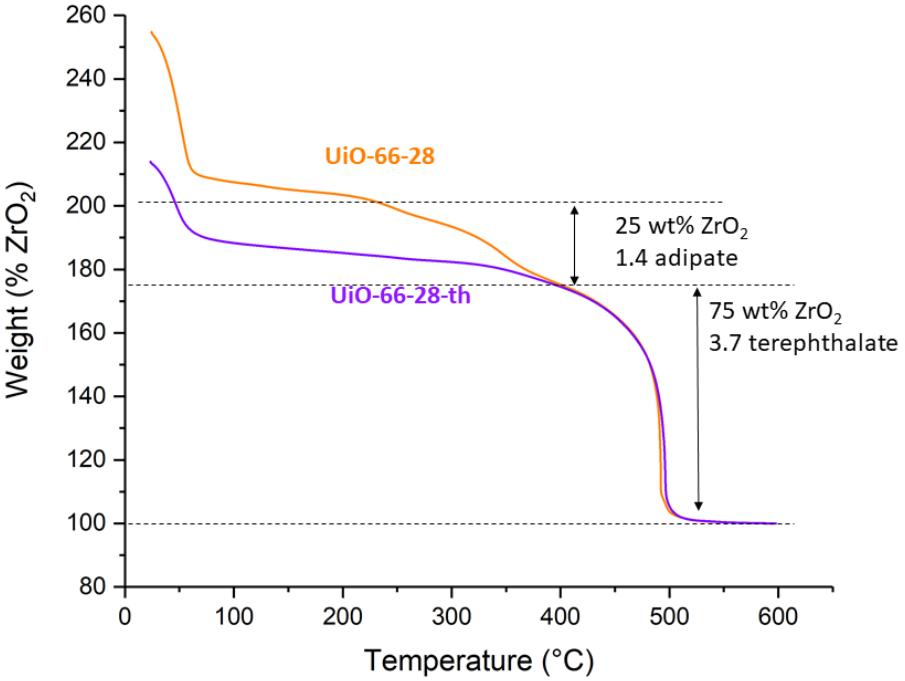

Figure S52. Thermogravimetric plots of UiO-66-28, before (orange) and after (purple) thermolysis.

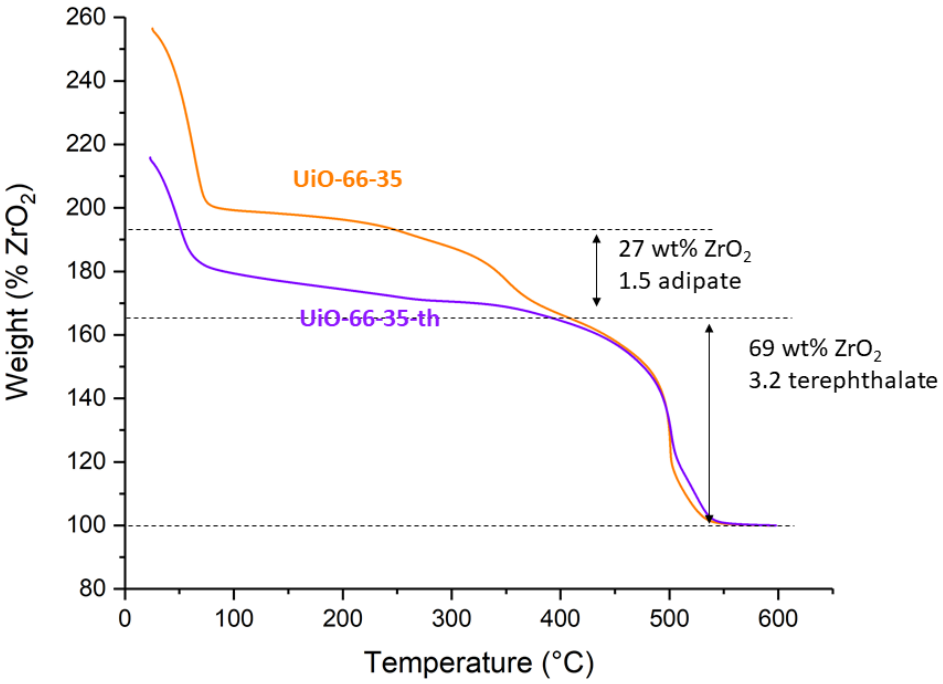

Figure S53. Thermogravimetric plots of UiO-66-35, before (orange) and after (purple) thermolysis.

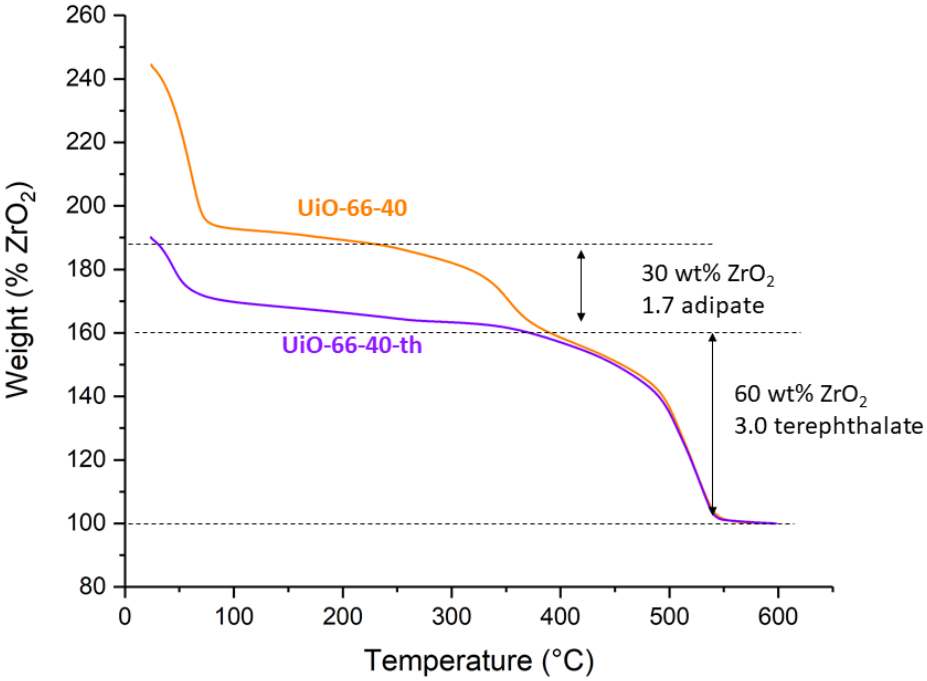

Figure S54. Thermogravimetric plots of UiO-66-40, before (orange) and after (purple) thermolysis.

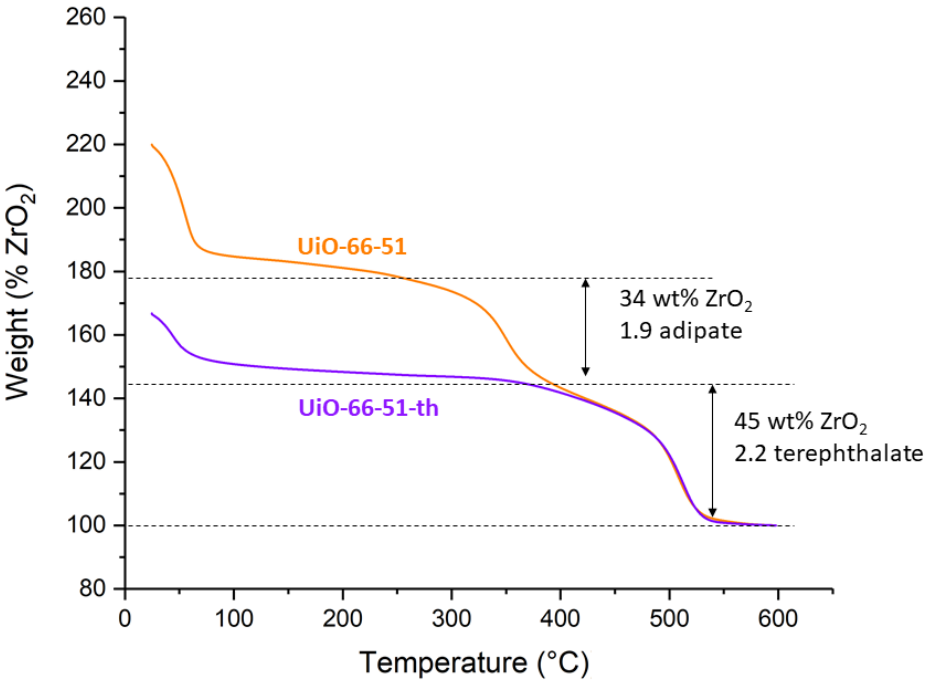

Figure S55. Thermogravimetric plots of UiO-66-51, before (orange) and after (purple) thermolysis.

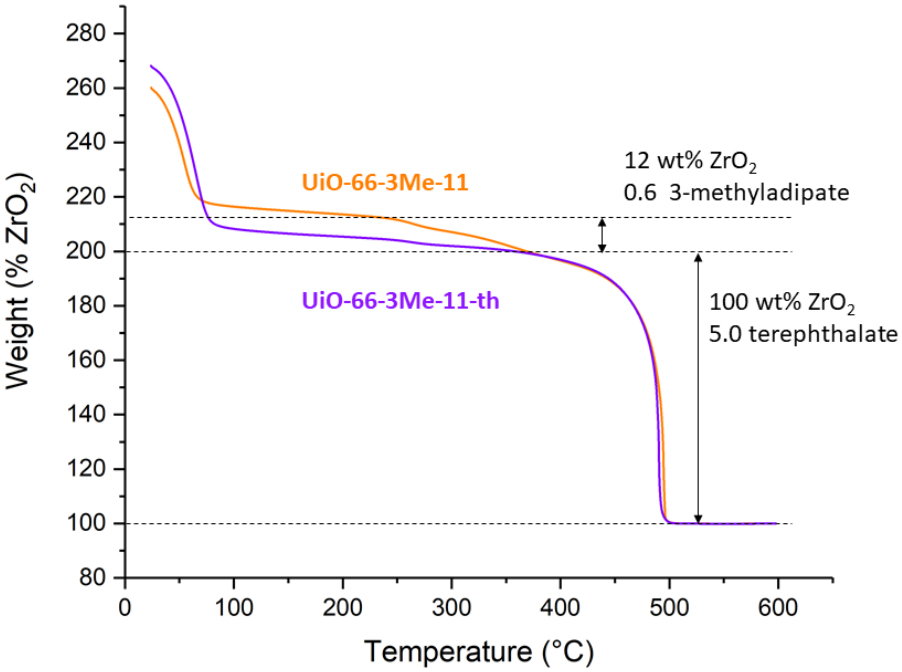

Figure S56. Thermogravimetric plots of UiO-66-3Me-11, before (orange) and after (purple) thermolysis.

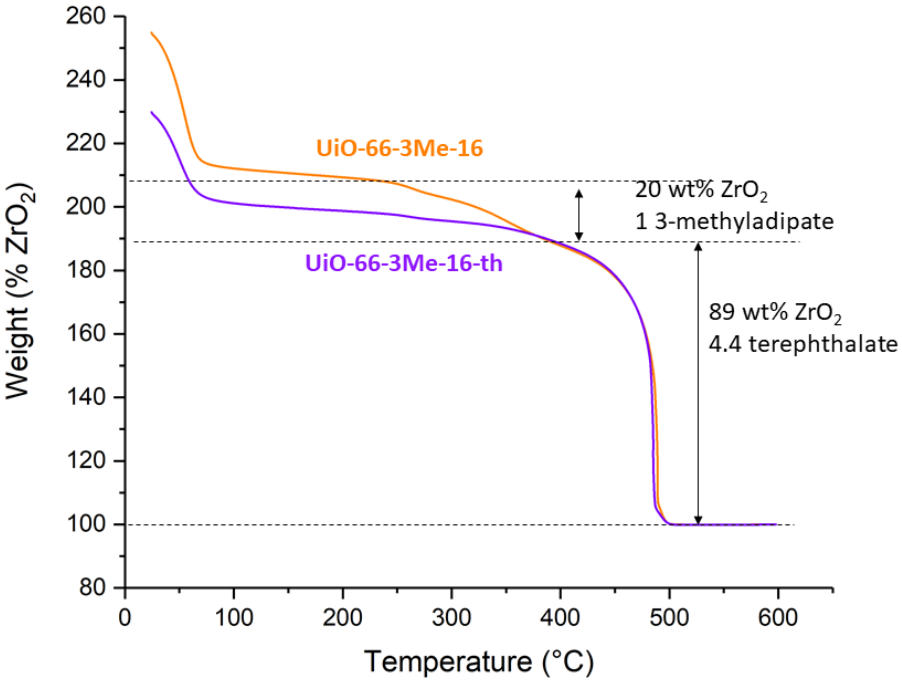

Figure S57. Thermogravimetric plots of UiO-66-3Me-16, before (orange) and after (purple) thermolysis.

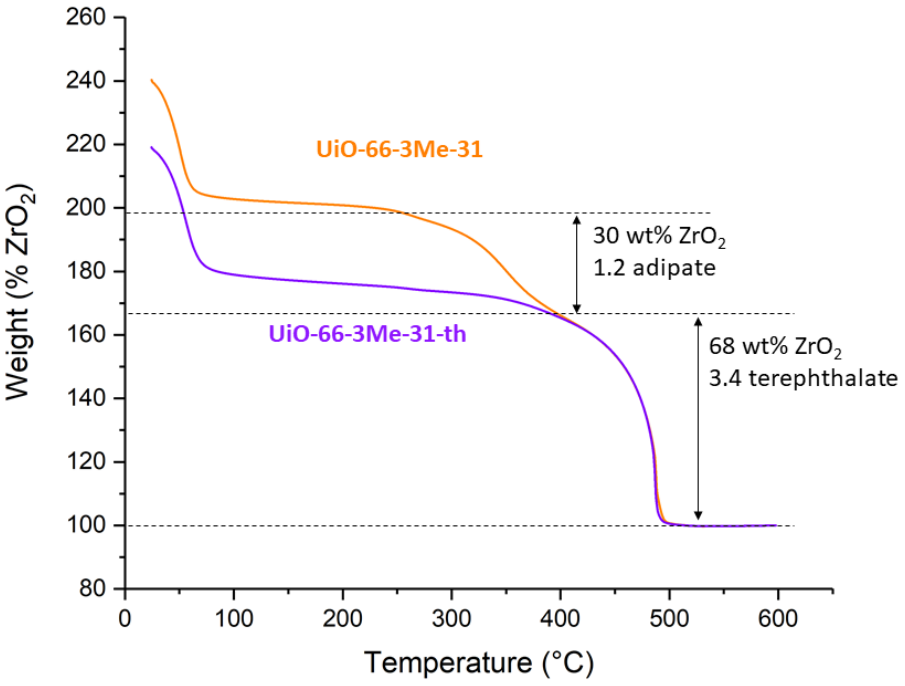

Figure S58. Thermogravimetric plots of UiO-66-3Me-31, before (orange) and after (purple) thermolysis.

7. Gas absorption isotherms

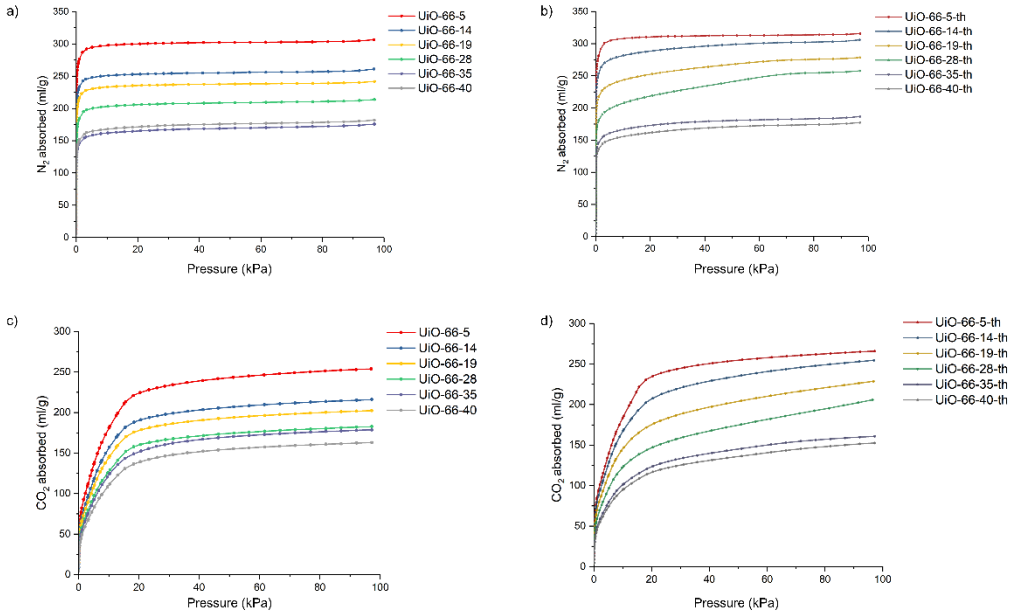

Figure S59: N_2 sorption isotherms of UiO-66-*x* before (a) and after (b) thermolysis, and CO_2 sorption isotherms of UiO-66-*x* before (c) and after (d) thermolysis.

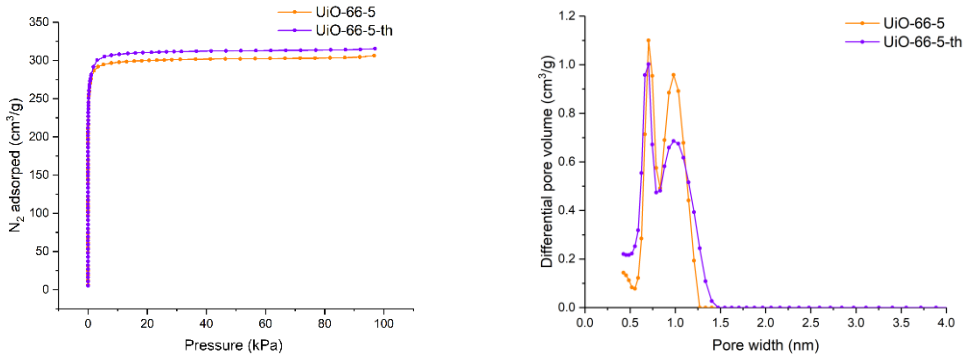

Figure S60: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-5 and UiO-66-5-th.

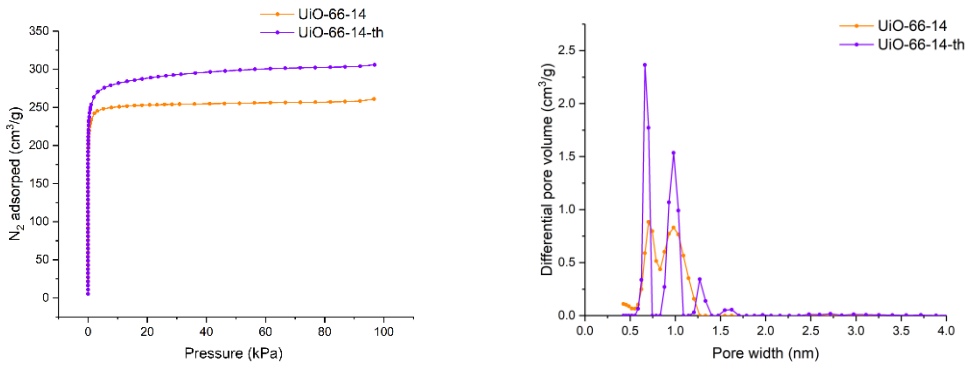

Figure S61: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-14 and UiO-66-14-th.

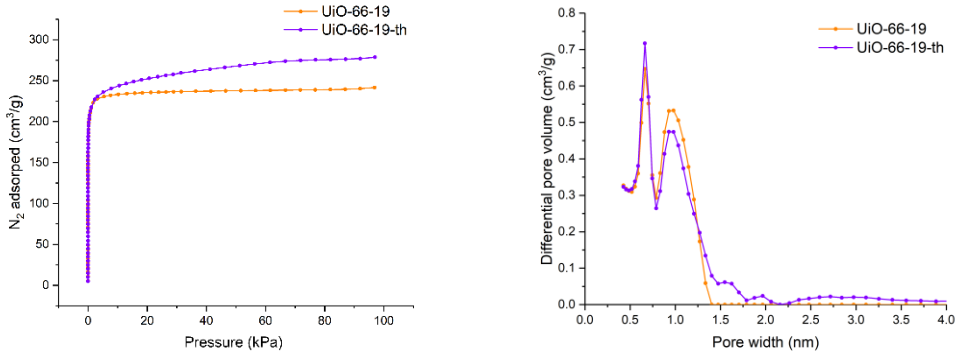

Figure S62: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-19 and UiO-66-19-th.

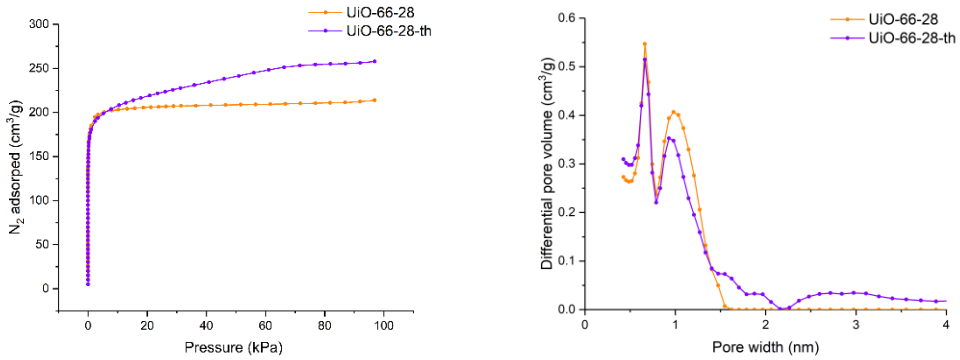

Figure S63: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-28 and UiO-66-28-th.

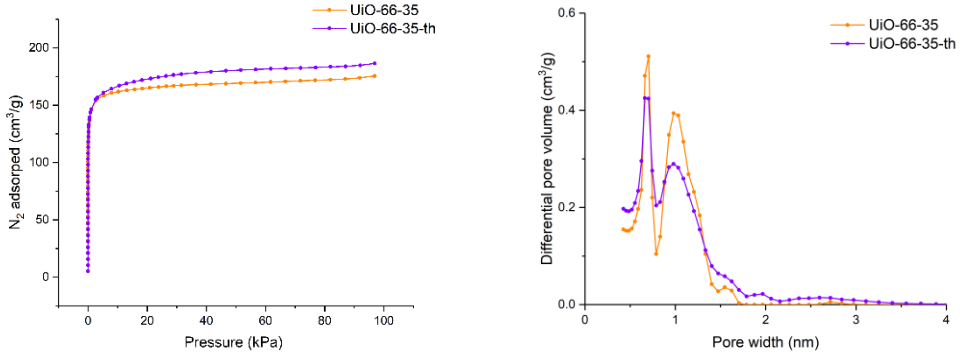

Figure S64: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-35 and UiO-66-35-th.

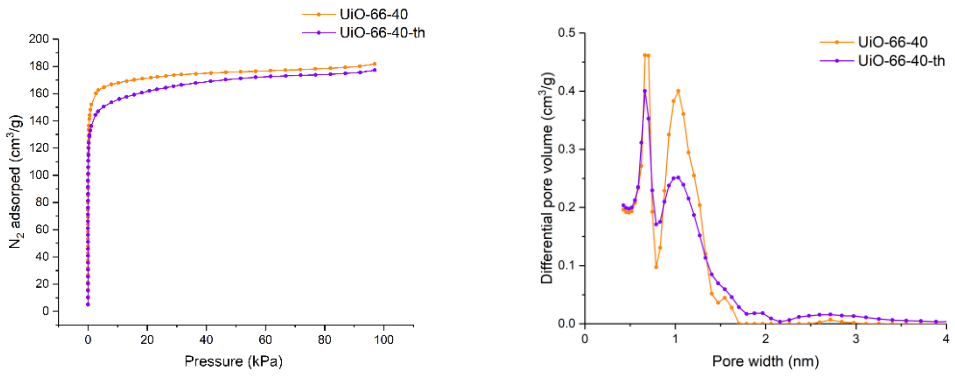

Figure S65: Nitrogen physisorption isotherms (left) and pore size distribution (right, NLDFT model) for UiO-66-40 and UiO-66-40-th.

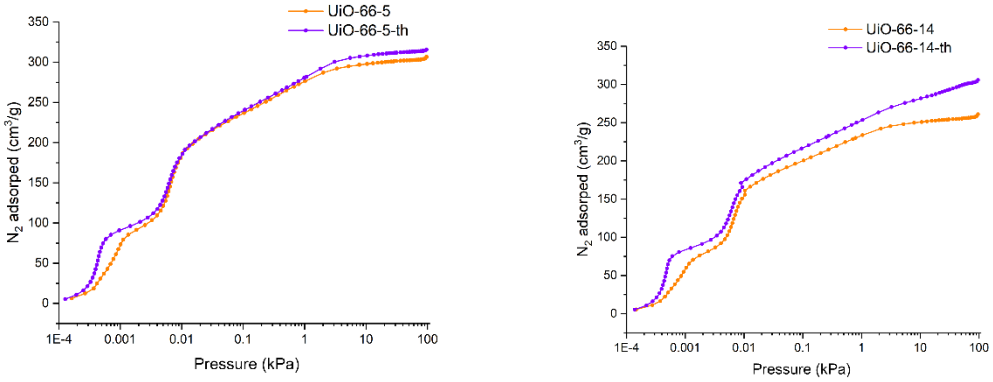

Figure S66: Nitrogen physisorption isotherms of UiO-66-5 (left) and UiO-66-14 (right) plotted on a logarithmic scale for pressure.

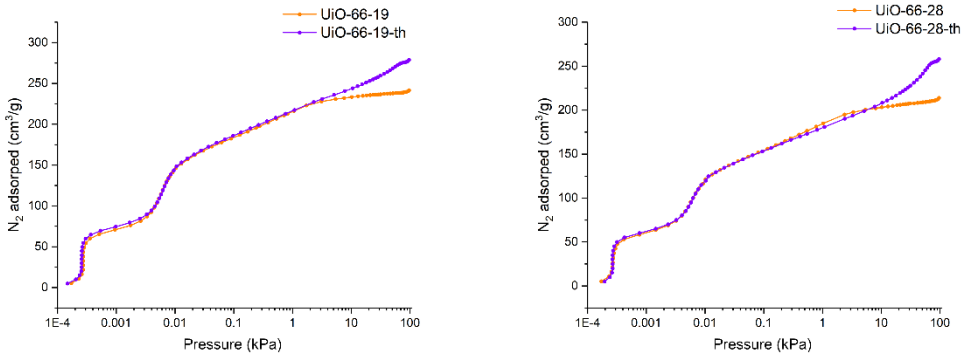

Figure S67: Nitrogen physisorption isotherms of UiO-66-19 (left) and UiO-66-28 (right) plotted on a logarithmic scale for pressure.

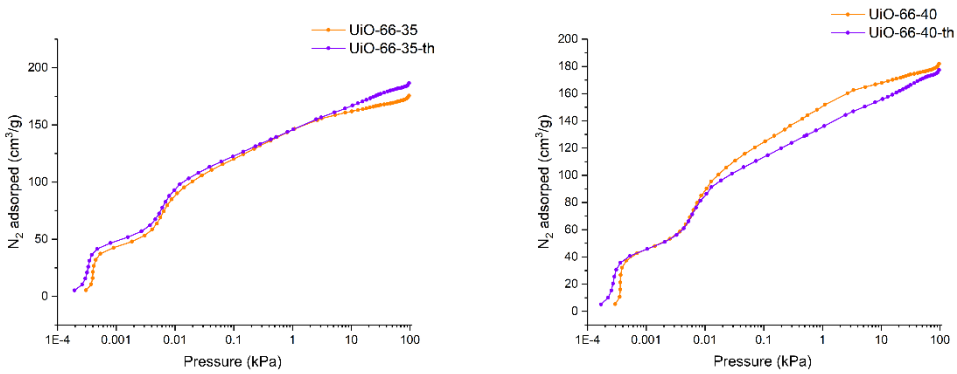

Figure S68: Nitrogen physisorption isotherms of UiO-66-35 (left) and UiO-66-40 (right) plotted on a logarithmic scale for pressure.

8. Computational Modeling

8.1 Computational details

All calculations were done using ORCA 5.0.3. The geometries of two $Zr_6O_4(OH)_4$ clusters bridged by one terephthalate were extracted from the crystal structure reported by Lillerud and coworkers.[3] The remaining terephthalates surrounding the clusters were truncated to formates, and the geometries were optimized with the coordinates of the formate carbon atoms fixed to replicate the rigidity of the framework. The bridging terephthalate was replaced with an adipate and a conformer search of the adipate was first done using the GFN2-xTB method of Grimme and Bannwarth.[4] The geometries of the conformers found were then reoptimized using the PBE functional[5] with an atom pairwise dispersion correction (D4),[6] together with the def2-SVP basis set[7] and effective core potentials for zirconium.[8] These calculations were performed using RI density fitting approximations with the def2/J Coulomb fitting basis set.[9] Single-point electronic energies were recalculated with the PBE0-D4 functional[10] and the def2-TZVPP basis set.

Three bridging conformers and one folded isomer was optimized, with the bridging conformers labelled herein as Zr_adipic_1 to Zr_adipic_3 and an isomer where the adipate is folded and does not bridge the two nodes, labelled as Zr_adipic_folded. The energies of the 4 structures and their structures are detailed in the following subsection.

8.2 Computed energies

Table S6: DFT-calculated gas phase electronic energies.

Structure	E_{el} (PBE-D4/def2-SVP) [kcal/mol]	E_{el} (PBE0-D4/def2-TZVPP) [kcal/mol]
Zr_terephthalate	-4102012.657	-4106030.681
Zr_adipic_1	-4055766.481	-4059747.101
Zr_adipic_2	-4055756.669	-4059741.286
Zr_adipic_3	-4055761.003	-4059739.572
Zr_adipic_folded	-4055761.264	-4059740.043
Terephthalic acid	-381715.2667	-382145.58
Adipic acid	-335470.9947	-335862.2938

8.3 Optimized Structures

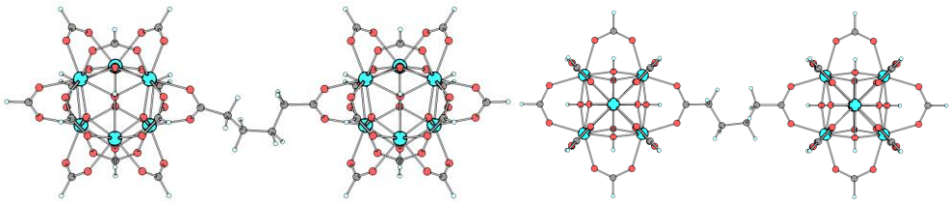

Figure S69: Optimized structure of Zr_adipic_1

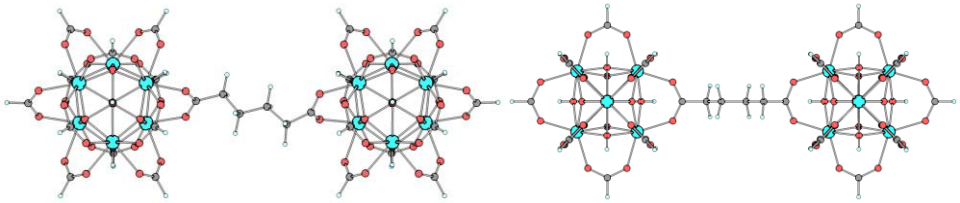

Figure S70: Optimized structure of Zr_adipic_2

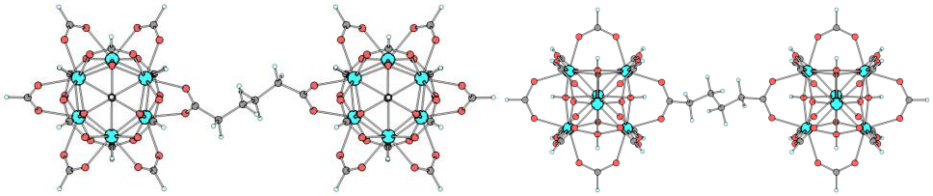

Figure S71: Optimized structure of Zr_adipic_3

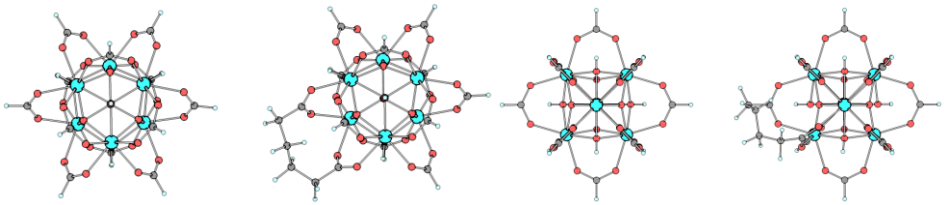

Figure S72: Optimized structure of Zr_adipic_folded

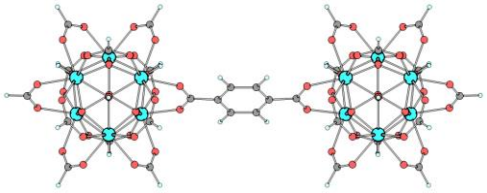

Figure S73: Optimized structure of Zr_terephthalate

Table S6: xyz coordinates of all computed structures

adipic_acid			
C	-1.09982	-0.8548	-1.36681
C	0.010502	0.009177	-0.76927
C	0.001848	0.000764	0.76165
H	-0.09058	1.051118	-1.14184
H	0.995541	-0.34339	-1.14343
C	1.112106	0.864828	1.359179
H	0.102971	-1.04117	1.134229
H	-0.98321	0.353286	1.135791
C	1.201189	0.93542	2.872257
H	1.033027	1.916785	1.007729
H	2.112432	0.529003	1.008593
C	-1.18905	-0.9252	-2.87988
H	-2.10012	-0.51896	-1.01617
H	-1.02076	-1.90679	-1.0154
O	-2.01669	-1.56936	-3.49441
O	-0.23287	-0.18333	-3.50019
O	0.246777	0.19128	3.492569
O	2.030047	1.578025	3.486772
H	0.408434	0.31635	4.453394
H	-0.39356	-0.30963	-4.46101

terephthalic_acid			
O	1.097909	-0.11809	-2.11017
O	-1.1638	-0.12297	-2.14036
C	-0.02925	-0.12493	-0.01824
C	1.207319	-0.1237	0.660414
H	2.141349	-0.12049	0.082008
C	-0.12029	-0.12201	-1.50994
C	-1.23395	-0.12901	0.712959
H	-2.18206	-0.12992	0.155647
O	-1.09861	-0.13669	4.880698
C	0.028543	-0.13062	2.788769
C	1.233246	-0.12657	2.057565
H	2.181355	-0.12576	2.614877
C	0.119594	-0.13361	4.280466
O	1.163105	-0.1332	4.910877
C	-1.20802	-0.13183	2.11011
H	-2.14205	-0.13499	2.688517
H	0.911253	-0.11647	-3.07359

H	-0.91195	-0.13857	5.844118

Zr_adipic_folded

C	-3.80131	-0.6522	10.94689
C	3.801313	0.652202	6.493378
C	-3.80131	-0.6522	-8.17661
C	3.801313	0.652202	-3.7231
C	0.652202	3.801313	-8.17661
C	-0.6522	-3.80131	-3.7231
C	0.652202	3.801313	10.94689
C	0.652202	3.801313	-3.7231
C	3.801313	0.652202	-8.17661
C	-3.80131	-0.6522	-3.7231
C	-0.6522	-3.80131	-8.17661
C	-3.14911	3.149111	-5.94986
C	-3.14911	3.149111	8.720136
C	-9.2E-09	1.36E-08	-10.4034
C	3.149111	-3.14911	-5.94985
C	3.149111	-3.14911	8.720136
C	0.652202	3.801313	6.493378
C	1.18E-09	-5.9E-11	13.17365
C	-3.80131	-0.6522	6.493378
C	-0.6522	-3.80131	10.94689
C	3.801313	0.652202	10.94689
Zr	-1.76915	-1.78623	8.701987
Zr	-1.24799	1.244274	10.47864
Zr	1.768289	1.764573	8.709065
Zr	1.24878	-1.25712	6.930127
Zr	-1.24866	1.251143	-7.71324
Zr	-1.77118	-1.77119	-5.94941
Zr	1.246631	-1.25161	-4.16686
Zr	1.767347	1.767448	-5.94171
Zr	-1.25149	1.246448	-4.16682
Zr	1.251019	-1.24852	-7.71353
Zr	-1.24639	1.245337	6.932315
Zr	1.248206	-1.25599	10.47686
O	-3.15344	0.3927	11.25099
O	-3.47746	-1.55944	10.12386
O	3.170627	-0.40637	6.197022
O	3.505445	1.524814	7.360568
O	-3.48591	-1.55388	-7.34487
O	-3.15044	0.389343	-8.4846
O	3.503783	1.527831	-4.58669
O	3.163967	-0.402	-3.42342
O	-0.41375	3.175866	-8.4536
O	1.531019	3.503247	-7.3147
O	0.401121	-3.16732	-3.42375
O	-1.55695	-3.47769	-4.54728
O	1.532362	3.502485	10.08627
O	-0.41295	3.173628	11.22308
O	1.527451	3.503849	-4.58719
O	0.989865	0.990009	-7.92729
O	-0.40157	3.163609	-3.42275
O	3.503318	1.530989	-7.31462
O	0.979685	0.979376	-3.93202
O	3.175648	-0.41355	-8.45379
O	-2.39075	0.408816	-5.94521
O	0.409022	-2.39058	-5.94549
O	-2.73579	2.778091	-4.81146
O	0.788387	-0.82197	-9.84907
O	2.770558	-2.74349	-7.08831
O	-3.16775	0.401488	-3.42454
O	0.389244	-3.15033	-8.4846
O	-0.73398	-0.73414	-7.41477
O	-0.73746	-0.73813	-4.47486
O	1.77854	-0.30458	-5.93718
O	-0.30448	1.778737	-5.93733
O	-3.47729	-1.55743	-4.54686
O	-1.55381	-3.48602	-7.34472
O	-2.74383	2.770399	-7.08842
O	-2.73824	2.777535	7.580846
O	-2.74215	2.767907	9.857392
O	2.777742	-2.73625	-4.81141
O	-0.82208	0.788288	-9.84911
O	0.987903	0.984402	10.69349
O	0.981028	0.975461	6.707171
O	0.398479	-2.40306	8.695506
O	-2.38258	0.40147	8.712051
O	2.778361	-2.74133	7.579655
O	-0.82655	0.782673	12.61738
O	3.504298	1.530586	10.08392
O	1.524316	3.505799	7.360868
O	-0.73344	-0.74371	10.17044
O	-0.7486	-0.75132	7.217104
O	-0.3032	1.775907	8.704433
O	1.773833	-0.31114	8.704527
O	-1.54007	-3.50486	10.09003
O	-3.50326	-1.54306	7.340058
O	2.769182	-2.74184	9.857215
O	-0.40057	3.163072	6.18981
O	-3.16722	0.399863	6.194399
O	0.379196	-3.14204	11.26422
O	3.175286	-0.41391	11.22229
O	0.790307	-0.82013	12.61932
H	3.914266	-3.96762	-5.94993
H	-0.79914	-4.77392	-8.71323
H	-0.80726	-4.77205	-3.18462
H	-4.77195	-0.80748	-3.18457
H	4.750772	0.827124	-3.15451
H	0.827274	4.750905	-3.15482
H	-3.96772	3.914141	-5.94976
H	0.836213	4.739663	-8.76063
H	4.739808	0.836083	-8.76043
H	0.026108	0.026102	-11.5232
H	-4.77396	-0.79912	-8.71317
H	0.834165	4.74067	11.53004
H	-3.96624	3.915835	8.722652
H	-4.77681	-0.79705	11.479
H	0.028254	0.030218	14.29339
H	0.828733	4.750287	5.924292
H	4.745677	0.834901	5.918399
H	-4.75728	-0.81874	5.931166
H	-0.80615	-4.76671	11.49437
H	3.915768	-3.96632	8.723533
H	4.738292	0.836981	11.53301
H	-3.34846	0.576276	-5.9444
H	1.390462	1.39057	-8.71745
H	0.576641	-3.34827	-5.94477
H	1.359471	1.358995	-3.12093
H	-3.341	0.564742	8.707136
H	1.322568	1.312785	5.860654
H	0.530442	-3.36257	8.600792
H	1.387995	1.382485	11.48511
C	-0.16091	-0.16156	-1.46584
O	0.709799	-0.89968	-2.01747
O	-0.90013	0.706362	-2.01964
C	-0.91726	-0.92908	3.032474
C	-1.74947	-2.17611	3.438064
C	-0.92722	-3.4698	3.656623
H	-2.51936	-2.34566	2.657591
H	-2.32431	-1.92303	4.355263
C	-1.31092	-4.26354	4.919536
H	0.149943	-3.22128	3.737581
H	-1.0315	-4.12965	2.771124
C	-0.82752	-3.56292	6.180503
H	-0.8155	-5.25823	4.89111
H	-2.40136	-4.4405	4.999868
C	-0.30965	-0.31965	4.281207
H	-1.57049	-0.17282	2.557594
H	-0.11823	-1.21836	2.319144
O	-0.91448	0.674214	4.805781
O	0.711648	-0.89351	4.786888
O	0.375936	-3.13606	6.159658
O	-1.62569	-3.41663	7.161708
H	-0.28764	-0.28869	-0.35922

Zr_adipic_1

C	-3.80131	-0.6522	10.94689
C	3.801313	0.652202	6.493378
C	-3.80131	-0.6522	-8.17661

C	3.801313	0.652202	-3.7231
C	0.652202	3.801313	-8.17661
C	-0.6522	-3.80131	-3.7231
C	0.652202	3.801313	10.94689
C	-0.6522	-3.80131	6.493378
C	0.652202	3.801313	-3.7231
C	3.801313	0.652202	-8.17661
C	-3.80131	-0.6522	-3.7231
C	-0.6522	-3.80131	-8.17661
C	-3.14911	3.149111	-5.94986
C	-3.14911	3.149111	8.720136
C	4.67E-09	-2.3E-08	-10.4034
C	3.149111	-3.14911	-5.94986
C	3.149111	-3.14911	8.720136
C	0.652202	3.801313	6.493378
C	1.33E-08	-3E-08	13.17365
C	-3.80131	-0.6522	6.493378
C	-0.6522	-3.80131	10.94689
C	3.801313	0.652202	10.94689
Zr	-1.77293	-1.77244	8.722708
Zr	-1.24858	1.251023	10.48791
Zr	1.769013	1.769512	8.717284
Zr	1.24619	-1.25153	6.95345
Zr	-1.24789	1.251433	-7.71831
Zr	-1.77221	-1.77173	-5.95195
Zr	1.248087	-1.24929	-4.18317
Zr	1.770001	1.770676	-5.94451
Zr	-1.25154	1.249776	-4.18231
Zr	1.250789	-1.24763	-7.71821
Zr	-1.25114	1.245906	6.950312
Zr	1.250464	-1.24815	10.48844
O	-3.15109	0.388746	11.25768
O	-3.4853	-1.55562	10.11763
O	3.167257	-0.40463	6.198758
O	3.506997	1.527898	7.358787
O	-3.48635	-1.55445	-7.34546
O	-3.15004	0.38769	-8.48864
O	3.509253	1.525826	-4.59067
O	3.162927	-0.40158	-3.42382
O	-0.41313	3.175843	-8.45564
O	1.533234	3.50394	-7.31708
O	0.409509	-3.17779	-3.43515
O	-1.55809	-3.47576	-4.54615
O	1.532178	3.504581	10.08601
O	-0.41236	3.17524	11.22717
O	-1.55685	-3.47807	7.318648
O	0.403264	-3.17005	6.19741
O	1.526695	3.50861	-4.5901
O	0.991109	0.990839	-7.93291
O	-0.40346	3.165374	-3.42746
O	3.503638	1.532896	-7.31679
O	0.981883	0.982698	-3.95095
O	3.175901	-0.41306	-8.45616
O	-2.39175	0.409575	-5.95308
O	0.409449	-2.39099	-5.95242
O	-2.73398	2.783526	-4.81117
O	0.788047	-0.8233	-9.85114
O	2.769667	-2.74498	-7.08867
O	-3.18175	0.412384	-3.4399
O	0.388172	-3.15045	-8.48818
O	-0.73331	-0.7335	-7.41929
O	-0.73979	-0.73948	-4.48574
O	1.785515	-0.30215	-5.94781
O	-0.30173	1.785291	-5.94853
O	-3.47369	-1.55961	-4.54434
O	-1.55478	-3.48542	-7.34622
O	-2.74509	2.769128	-7.08863
O	-2.73897	2.777124	7.581348
O	-2.74363	2.771255	9.859044
O	2.781905	-2.7343	-4.81122
O	-0.82295	0.787934	-9.85062
O	0.990539	0.99069	10.7037
O	0.98491	0.984568	6.725966
O	0.408567	-2.39328	8.722931
O	-2.39386	0.408792	8.722146
O	2.778633	-2.73796	7.581214
O	-0.82347	0.787284	12.62069
O	3.503642	1.53305	10.0872
O	1.529248	3.506767	7.357542
O	-0.73407	-0.73399	10.18982
O	-0.73764	-0.73732	7.261418
O	-0.30362	1.784747	8.718611
O	1.78556	-0.30365	8.719404
O	-1.55541	-3.48496	10.11751
O	-3.47959	-1.55679	7.319385
O	2.770331	-2.7444	9.858927
O	-0.40529	3.167528	6.201277
O	-3.16672	0.400658	6.19513
O	0.38855	-3.15101	11.2583
O	3.175653	-0.41271	11.22689
O	0.788095	-0.82336	12.62159
H	3.91278	-3.96922	-5.95048
H	-0.79769	-4.77631	-8.70963
H	-0.81614	-4.76633	-3.17629
H	-4.76491	-0.81839	-3.17448
H	4.747698	0.829103	-3.14958
H	0.830842	4.746169	-3.14762
H	-3.96985	3.912127	-5.95109
H	0.833943	4.741718	-8.75837
H	4.741863	0.834222	-8.75804
H	0.02713	0.027498	-11.5233
H	-4.77611	-0.79775	-8.71002
H	0.834302	4.741684	11.52861
H	-3.96658	3.915619	8.720792
H	-4.77633	-0.79752	11.47998
H	0.027489	0.028146	14.2936
H	0.830733	4.746247	5.917821
H	4.746681	0.831365	5.918633
H	-4.77089	-0.80836	5.952915
H	-0.81106	-4.76966	5.95138
H	-0.79753	-4.7766	11.47948
H	3.915243	-3.96696	8.720929
H	4.742254	0.833913	11.52782
H	-3.34903	0.578903	-5.95029
H	1.393036	1.391797	-8.72215
H	0.5791	-3.34822	-5.94988
H	1.336702	1.337734	-3.11777
H	-3.35114	0.578193	8.721847
H	1.365056	1.364699	5.91578
H	0.577606	-3.35062	8.722751
H	1.391227	1.391471	11.49365
O	0.680022	-0.91138	-2.07751
O	-0.91983	0.68847	-2.08313
C	-0.27556	-0.26654	-1.53667
O	-0.87536	0.722853	4.840734
C	-0.09736	-0.10319	4.261982
O	0.722011	-0.88144	4.849884
C	-0.69694	-0.66114	-0.14552
H	-1.00732	0.271424	0.364791
H	-1.63615	-1.24898	-0.26205
C	0.348523	-1.4469	0.644359
H	0.456213	-2.46372	0.215692
H	1.340267	-0.963	0.508255
C	0.02837	-1.51714	2.13738
H	-0.91134	-2.08703	2.309956
H	0.83023	-2.06669	2.669882
C	-0.10588	-0.12211	2.754815
H	0.763977	0.501238	2.440996
H	-1.01321	0.41426	2.420121

Zr_adipic_2

C	-3.80131	-0.6522	10.94689
C	3.801313	0.652202	6.493378
C	-3.80131	-0.6522	-8.17661
C	3.801313	0.652202	-3.7231
C	0.652202	3.801313	-8.17661
C	-0.6522	-3.80131	-3.7231
C	0.652202	3.801313	10.94689
C	-0.6522	-3.80131	6.493378
C	0.652202	3.801313	-3.7231

C	3.801313	0.652202	-8.17661
C	-3.80131	-0.6522	-3.7231
C	-0.6522	-3.80131	-8.17661
C	-3.14911	3.149111	-5.94986
C	-3.14911	3.149111	8.720136
C	-1.1E-08	1.66E-08	-10.4034
C	3.149111	-3.14911	-5.94986
C	3.149111	-3.14911	8.720136
C	0.652202	3.801313	6.493378
C	-1.8E-08	5.57E-09	13.17365
C	-3.80131	-0.6522	6.493378
C	-0.6522	-3.80131	10.94689
C	3.801313	0.652202	10.94689
Zr	-1.77376	-1.77389	8.728098
Zr	-1.24782	1.250809	10.49749
Zr	1.773944	1.773873	8.719666
Zr	1.254892	-1.25418	6.981457
Zr	-1.24973	1.25016	-7.72571
Zr	-1.77368	-1.77372	-5.95768
Zr	1.248956	-1.25666	-4.20475
Zr	1.769923	1.769852	-5.95919
Zr	-1.25676	1.248946	-4.20431
Zr	1.250223	-1.24972	-7.72566
Zr	-1.25413	1.254872	6.981129
Zr	1.250856	-1.24777	10.49739
O	-3.14864	0.384527	11.26524
O	-3.48708	-1.55415	10.11582
O	3.160589	-0.40103	6.197446
O	3.513176	1.524158	7.364294
O	-3.48454	-1.55636	-7.34927
O	-3.15192	0.387781	-8.49119
O	3.504624	1.534518	-4.58255
O	3.176717	-0.41385	-3.44854
O	-0.40952	3.174035	-8.46284
O	1.532595	3.505188	-7.31643
O	0.400728	-3.16521	-3.42825
O	-1.55536	-3.48074	-4.55145
O	1.534421	3.503673	10.08909
O	-0.41173	3.175864	11.22983
O	-1.56141	-3.468	7.311291
O	0.432629	-3.20586	6.242542
O	1.534554	3.504363	-4.58238
O	0.991544	0.991475	-7.94324
O	-0.41371	3.176595	-3.44813
O	3.505427	1.532501	-7.31624
O	0.992209	0.991959	-3.98949
O	3.174331	-0.40983	-8.46232
O	-2.40039	0.409368	-5.96266
O	0.409434	-2.40026	-5.96258
O	-2.74433	2.773911	-4.81104
O	0.78782	-0.8238	-9.85314
O	2.773577	-2.74255	-7.08874
O	-3.16524	0.400791	-3.42817
O	0.387609	-3.15174	-8.49138
O	-0.734	-0.7341	-7.42593
O	-0.72961	-0.72977	-4.52108
O	1.791279	-0.30536	-5.96574
O	-0.30528	1.791094	-5.96561
O	-3.48057	-1.55528	-4.55137
O	-1.55631	-3.48478	-7.3491
O	-2.74284	2.773213	-7.08872
O	-2.72681	2.79188	7.582455
O	-2.74717	2.768381	9.859141
O	2.774042	-2.74432	-4.811
O	-0.82363	0.788179	-9.85331
O	0.99314	0.993008	10.71092
O	0.981215	0.980948	6.737277
O	0.412348	-2.39371	8.737453
O	-2.39383	0.412321	8.737401
O	2.792028	-2.7268	7.582414
O	-0.82242	0.789333	12.62356
O	3.503848	1.534364	10.08896
O	1.524252	3.512979	7.364092
O	-0.73208	-0.7322	10.19616
O	-0.73723	-0.73746	7.282215
O	-0.2986	1.791457	8.733624
O	1.791574	-0.29879	8.733692
O	-1.55413	-3.4873	10.11566
O	-3.46782	-1.56142	7.311149
O	2.768633	-2.74699	9.859159
O	-0.40072	3.160253	6.196905
O	-3.20572	0.432546	6.242385
O	0.384388	-3.14853	11.26536
O	3.176172	-0.41202	11.22934
O	0.789038	-0.82254	12.62343
H	3.917743	-3.96469	-5.95059
H	-0.79638	-4.77852	-8.70626
H	-0.80986	-4.76833	-3.17873
H	-4.76837	-0.80978	-3.17879
H	4.739683	0.836025	-3.13815
H	0.835752	4.740059	-3.13867
H	-3.96428	3.918168	-5.9506
H	0.832079	4.745261	-8.75346
H	4.744767	0.832494	-8.75414
H	0.027539	0.027454	-11.5235
H	-4.7785	-0.79646	-8.70629
H	0.832236	4.744601	11.52469
H	-3.97472	3.906879	8.720728
H	-4.77886	-0.79563	11.47605
H	0.025569	0.025519	14.29381
H	0.830199	4.744315	5.914774
H	4.743802	0.830699	5.914085
H	-4.7488	-0.83628	5.92266
H	-0.83652	-4.7486	5.922381
H	-0.79563	-4.77886	11.47605
H	3.90656	-3.97503	8.720741
H	4.744162	0.832611	11.5253
H	-3.35785	0.577417	-5.96362
H	1.389225	1.390307	-8.73566
H	0.577025	-3.35781	-5.96319
H	1.417318	1.417483	-3.22604
H	-3.3509	0.582399	8.727334
H	1.323449	1.323728	5.893671
H	0.582153	-3.35083	8.727095
H	1.393302	1.393891	11.50108
O	0.762233	-0.84141	-2.12846
O	-0.84101	0.762291	-2.12825
C	0.097367	0.097037	-1.58519
O	-0.96425	0.634558	4.917481
C	-0.42242	-0.4225	4.460431
O	0.6345	-0.9643	4.917648
C	0.405956	0.405371	-0.16179
H	1.473106	0.190965	0.043651
H	0.191871	1.472552	0.04383
C	-0.48017	-0.48063	0.709504
H	-1.54935	-0.28448	0.480871
H	-0.28445	-1.54984	0.48058
C	-0.16628	-0.16723	2.148334
H	0.915609	-0.34407	2.331055
H	-0.34204	0.914837	2.331124
C	-0.96314	-0.96329	3.177519
H	-2.04779	-0.75961	3.093098
H	-0.76003	-2.04809	3.093462

Zr_adipic_3

C	-3.80131	-0.6522	10.94689
C	3.801313	0.652202	6.493378
C	-3.80131	-0.6522	-8.17661
C	3.801313	0.652202	-3.7231
C	0.652202	3.801313	-8.17661
C	-0.6522	-3.80131	-3.7231
C	0.652202	3.801313	10.94689
C	-0.6522	-3.80131	6.493378
C	0.652202	3.801313	-3.7231
C	3.801313	0.652202	-8.17661
C	-3.80131	-0.6522	-3.7231
C	-0.6522	-3.80131	-8.17661
C	-3.14911	3.149111	-5.94986
C	-3.14911	3.149111	8.720136
C	-1.1E-08	4.91E-08	-10.4034

C	3.149111	-3.14911	-5.94986
C	3.149111	-3.14911	8.720136
C	0.652202	3.801313	6.493378
C	-3.2E-08	2.05E-08	13.17365
C	-3.80131	-0.6522	6.493378
C	-0.6522	-3.80131	10.94689
C	3.801313	0.652202	10.94689
Zr	-1.76999	-1.76979	8.719688
Zr	-1.24923	1.250524	10.4809
Zr	1.761604	1.761986	8.715228
Zr	1.237032	-1.24982	6.916199
Zr	-1.24762	1.251336	-7.70801
Zr	-1.76937	-1.77001	-5.94751
Zr	1.250498	-1.25207	-4.16371
Zr	1.76768	1.767341	-5.93712
Zr	-1.24598	1.242988	-4.15336
Zr	1.251298	-1.2474	-7.71156
Zr	-1.25632	1.24496	6.927102
Zr	1.251025	-1.24965	10.47695
O	-3.15217	0.391064	11.25254
O	-3.48506	-1.55432	10.11615
O	3.166878	-0.40242	6.192038
O	3.498841	1.530935	7.351958
O	-3.48685	-1.55263	-7.34294
O	-3.15037	0.390116	-8.48186
O	3.505963	1.52471	-4.59012
O	3.164835	-0.40127	-3.4199
O	-0.41497	3.176553	-8.45063
O	1.53075	3.50387	-7.31428
O	0.416417	-3.18811	-3.44255
O	-1.55997	-3.46979	-4.54183
O	1.52871	3.504118	10.08233
O	-0.412	3.174291	11.22656
O	-1.55333	-3.48198	7.321831
O	0.386419	-3.15114	6.172273
O	1.523296	3.507158	-4.59128
O	0.99015	0.991422	-7.92328
O	-0.39627	3.158519	-3.41265
O	3.503866	1.530677	-7.31428
O	0.979904	0.976124	-3.92731
O	3.176081	-0.41424	-8.45241
O	-2.38612	0.408912	-5.93999
O	0.409981	-2.3875	-5.94548
O	-2.73167	2.780084	-4.81196
O	0.790658	-0.81979	-9.84888
O	2.768637	-2.744	-7.08789
O	-3.17389	0.405321	-3.42665
O	0.388463	-3.14948	-8.48523
O	-0.73372	-0.73372	-7.41331
O	-0.74101	-0.74438	-4.46194
O	1.778146	-0.30329	-5.93523
O	-0.30395	1.774668	-5.92939
O	-3.47615	-1.55659	-4.54655
O	-1.55207	-3.48724	-7.34215
O	-2.74535	2.769031	-7.08858
O	-2.74601	2.770307	7.58063
O	-2.7409	2.772585	9.858161
O	2.784697	-2.73229	-4.81111
O	-0.81953	0.790075	-9.84765
O	0.989698	0.987953	10.69534
O	0.982589	0.986427	6.712215
O	0.407773	-2.39153	8.707939
O	-2.39366	0.40805	8.713206
O	2.769999	-2.7406	7.581733
O	-0.82078	0.790035	12.61949
O	3.504397	1.529065	10.08261
O	1.536377	3.494225	7.346277
O	-0.73543	-0.73573	10.18556
O	-0.73352	-0.73104	7.251735
O	-0.30956	1.778819	8.706641
O	1.775583	-0.3102	8.700144
O	-1.55398	-3.48617	10.11527
O	-3.47909	-1.55415	7.320682
O	2.772395	-2.74363	9.859165
O	-0.41277	3.179434	6.208871
O	-3.15831	0.391926	6.17928
O	0.391631	-3.15203	11.25031
O	3.175737	-0.41389	11.22283
O	0.789066	-0.82042	12.61781
H	3.910628	-3.97111	-5.95149
H	-0.8001	-4.77307	-8.71452
H	-0.82201	-4.76377	-3.17372
H	-4.76993	-0.81212	-3.18161
H	4.749812	0.829884	-3.15347
H	0.825026	4.753528	-3.15835
H	-3.96898	3.912825	-5.94921
H	0.837227	4.737696	-8.76349
H	4.738564	0.836691	-8.76231
H	0.021751	0.022511	-11.5234
H	-4.77179	-0.8007	-8.71658
H	0.83658	4.739903	11.53051
H	-3.96258	3.919768	8.721407
H	-4.77309	-0.8002	11.48481
H	0.02408	0.02313	14.29367
H	0.832894	4.749079	5.922932
H	4.754937	0.825808	5.930594
H	-4.77767	-0.8013	5.963753
H	-0.79529	-4.78069	5.967848
H	-0.80085	-4.77162	11.48719
H	3.91886	-3.96337	8.718524
H	4.73779	0.837784	11.53347
H	-3.34375	0.576708	-5.93609
H	1.386855	1.39147	-8.71563
H	0.575853	-3.34545	-5.93965
H	1.31882	1.314463	-3.0801
H	-3.35185	0.572556	8.716742
H	1.407634	1.413967	5.949658
H	0.573479	-3.34956	8.711224
H	1.387976	1.38489	11.48844
C	-0.3464	-0.38576	-1.52177
O	0.677468	-0.94787	-2.03798
O	-0.91583	0.648547	-2.00786
C	-0.96388	-1.02862	-0.28642
H	-0.49558	-2.02272	-0.14796
H	-2.03175	-1.18431	-0.54858
C	-0.886	-0.20887	1.013638
H	-1.20774	0.833707	0.801516
H	-1.6271	-0.61529	1.734535
O	0.750245	-0.81173	4.755991
C	0.118048	0.16138	4.224966
O	-0.83447	0.7951	4.79214
C	0.620182	0.699337	2.887943
H	0.111799	1.66519	2.699101
H	1.696615	0.912368	3.06725
C	0.507747	-0.20995	1.651976
H	0.811418	-1.24379	1.923552
H	1.251321	0.134303	0.901399

Zr_terephtalate

Zr	1.756731	2.22E-08	10.47687
Zr	-1.9E-08	-2.48439	8.720136
Zr	-1.75673	2.38E-08	6.963405
Zr	-2.9E-09	2.484393	8.720136
Zr	-8.9E-09	2.484393	-5.94985
Zr	-1.8E-08	-2.48439	-5.94985
Zr	1.756731	-1.2E-08	-4.19312
Zr	-1.75673	-1.8E-08	-7.70659
Zr	-1.75673	7.95E-09	10.47687
Zr	1.756731	3.18E-08	6.963405
Zr	1.756731	-1.1E-08	-7.70659
Zr	-1.75673	-1.7E-08	-4.19312
O	1.340818	-3.56543	10.15049
C	2.145907	-3.157	11.04055
O	2.476803	-1.95844	11.2883
O	-1.4315	3.567485	7.381307
C	-2.3211	3.159852	6.5756
O	-2.5705	1.96127	6.245314
O	-2.5718	1.961066	-3.47513
C	-2.32448	3.159326	-3.80821
O	-1.43637	3.56668	-4.61563

O	2.476004	-1.95855	-8.51956	C	-2.32076	3.156081	-8.09612
C	2.143332	-3.15675	-8.2728	C	-2.14608	-3.15714	-8.26965
O	1.336038	-3.56447	-7.38435	O	2.572175	1.961731	6.246872
O	1.434774	3.563866	-7.28715	C	2.32386	3.159966	6.578945
C	2.323163	3.155744	-8.09413	O	1.434923	3.566977	7.385751
O	2.569716	1.957353	-8.42675	O	2.473726	-1.96021	6.145003
O	2.569662	1.957987	11.19547	C	2.140985	-3.15821	6.394019
C	2.320543	3.156619	10.86594	O	1.335526	-3.56462	7.284329
O	1.430194	3.565024	10.06116	O	1.989999	-1.40592	8.718762
O	-1.33618	-3.56397	-4.51525	O	0.000357	1.410121	6.739046
C	-2.14307	-3.15827	-3.62581	O	-1.98939	-1.40624	8.721728
O	-2.47708	-1.96055	-3.37743	O	-0.00087	1.404786	10.70981
O	-2.47753	-1.96038	6.14869	O	-3.90738	0.067634	7.582534
C	-2.14479	-3.15842	6.397594	O	1.136833	-0.06833	12.62637
O	-1.33957	-3.56505	7.288023	O	0.000621	-1.04221	10.19289
O	3.907139	0.068351	-7.08452	O	-1.47149	1.041053	8.722276
O	0.000844	1.404414	-7.93976	O	1.470989	1.041111	8.722259
C	4.465879	0.126034	-5.94814	O	-0.00029	-1.0391	7.256049
O	3.907759	0.066952	-4.81113	O	-1.43546	3.563876	10.05659
O	1.13619	-0.07012	-9.8565	O	-1.33615	-3.56552	10.15406
O	1.989903	-1.40551	-5.95083	C	-2.32475	3.155618	10.86251
C	-0.00042	-0.12798	-10.4149	O	-2.57206	1.957123	11.19405
O	-1.13684	-0.06943	-9.8559	O	-1.1363	-0.06614	12.62729
O	2.476418	-1.96103	-3.37734	O	-3.90731	0.066223	9.855892
O	-0.0007	1.410103	-3.96756	O	-2.47366	-1.959	11.29097
C	2.144081	-3.15883	-3.62732	C	-2.14221	-3.15739	11.04347
O	1.339611	-3.56497	-4.51882	C	-4.46577	0.125364	8.719448
O	-1.9893	-1.40541	-5.94947	C	0.000384	-0.12553	13.18548
O	2.570521	1.961631	-3.47432	H	2.786191	-1.96494	8.721795
O	-2.56911	1.957321	-8.42617	H	-0.00155	1.96252	11.50694
O	-2.47625	-1.95855	-8.51808	H	-2.78592	-1.96478	8.724709
O	1.13217	-0.06335	-2.08204	H	0.001942	1.965842	5.940533
O	-3.90636	0.068122	-7.08455	H	2.786718	-1.96365	-5.95365
O	-1.47055	1.041629	-5.95158	H	-0.00098	1.965996	-3.16918
O	0.000572	-1.03866	-4.48529	H	0.001445	1.962066	-8.73694
O	0.000294	-1.04055	-7.42072	H	-2.78597	-1.96375	-5.95146
O	1.473107	1.042837	-5.9512	H	2.95216	3.945289	11.34894
O	-1.13309	-0.06279	-2.08209	H	2.954794	3.949536	6.096393
C	-0.00046	-0.16185	-0.00901	H	-2.95169	3.949082	6.092034
C	1.224089	-0.17294	0.687743	H	-2.95735	3.944125	11.34449
H	2.161018	-0.16937	0.113079	H	5.580994	0.228509	8.717763
C	-0.00042	-0.10138	-1.49739	H	2.627945	-3.94551	11.67309
C	-1.22488	-0.17432	0.687922	H	0.000831	-0.23001	14.30051
H	-2.16191	-0.17175	0.113415	H	2.621299	-3.94809	5.76179
O	-1.13239	-0.06239	4.852993	H	-2.62518	-3.9482	5.765287
C	-0.00025	-0.16091	2.779526	H	-2.6243	-3.94617	11.67564
C	1.224201	-0.17228	2.082586	H	-5.5808	0.230288	8.71955
H	2.161226	-0.16871	2.657088	H	2.623886	-3.94914	-2.99524
C	5.78E-05	-0.09946	4.267762	H	5.580918	0.230836	-5.94838
O	1.13276	-0.05855	4.852147	H	2.953204	3.949295	-3.32356
C	-1.22479	-0.17392	2.082798	H	2.95555	3.944327	-8.57627
H	-2.16175	-0.17134	2.657426	H	2.625418	-3.94573	-8.90472
O	-3.90771	0.066754	-4.81135	H	-0.00084	-0.23246	-11.5299
C	-4.46574	0.124831	-5.94841	H	-2.9525	3.944457	-8.57942
C	2.32158	3.159994	-3.80571	H	-2.95594	3.948583	-3.3258
O	1.431545	3.567629	-4.61097	H	-5.58093	0.227643	-5.94906
O	3.906809	0.069139	9.853765	H	-2.62347	-3.94862	-2.99425
C	4.465839	0.125036	8.717521	H	-2.62932	-3.94593	-8.90089
O	3.907823	0.065558	7.580414				
O	-1.3403	-3.56516	-7.37999				
O	-1.43121	3.56461	-7.29069				

9. Infrared spectra

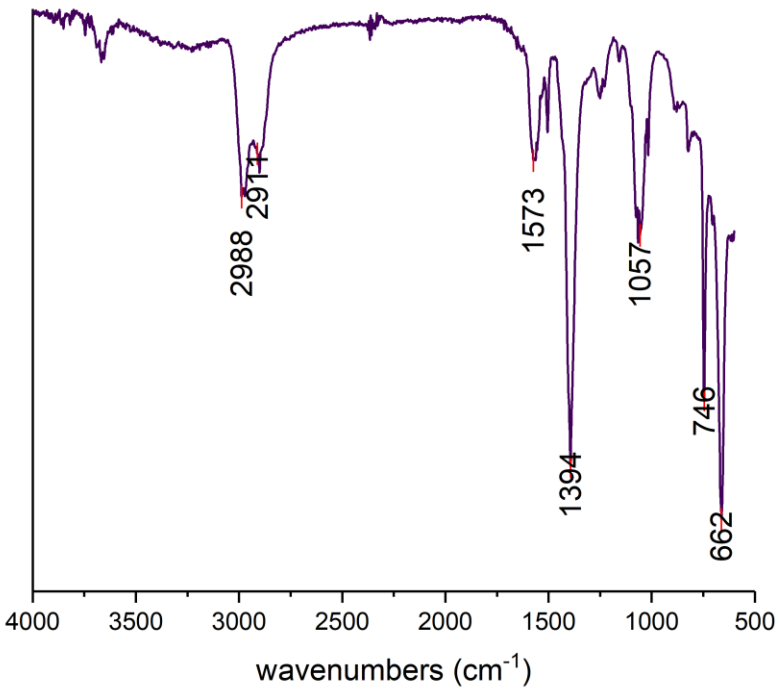

Figure S74: Infrared spectrum of UiO-66-0

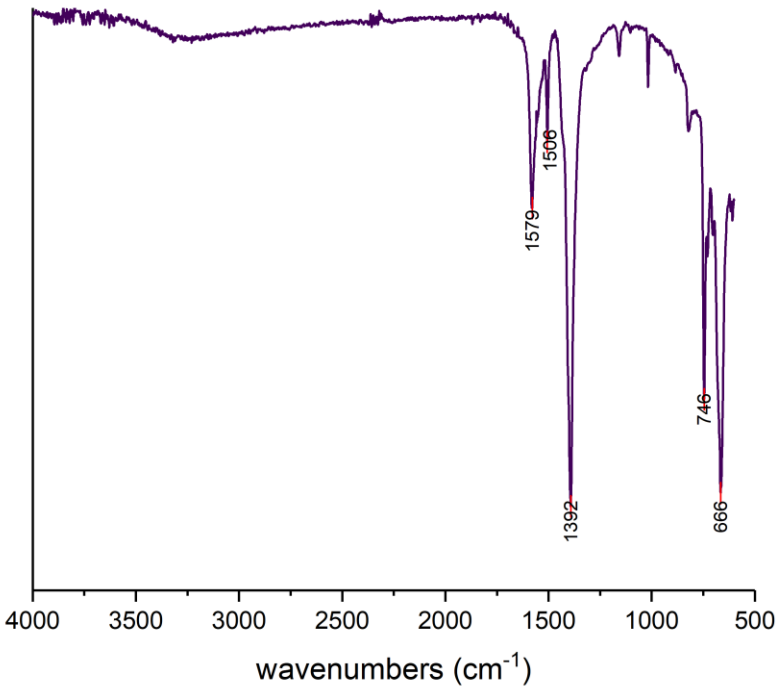

Figure S75: Infrared spectrum of UiO-66-5

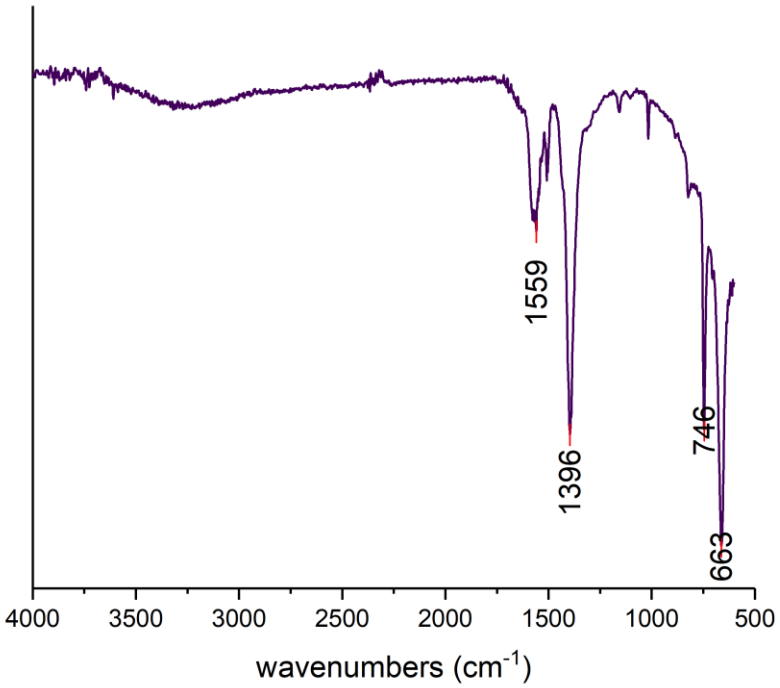

Figure S76: Infrared spectrum of UiO-66-14

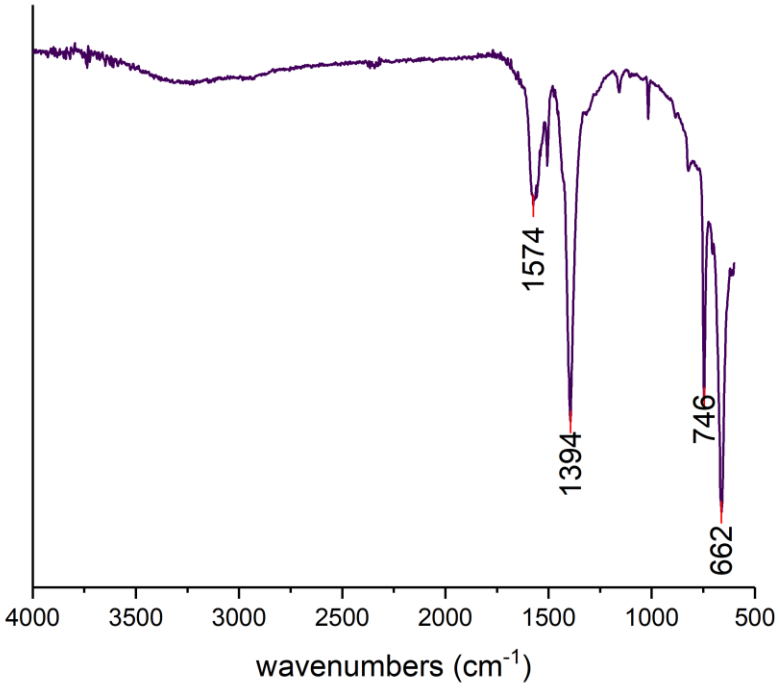

Figure S77: Infrared spectrum of UiO-66-19

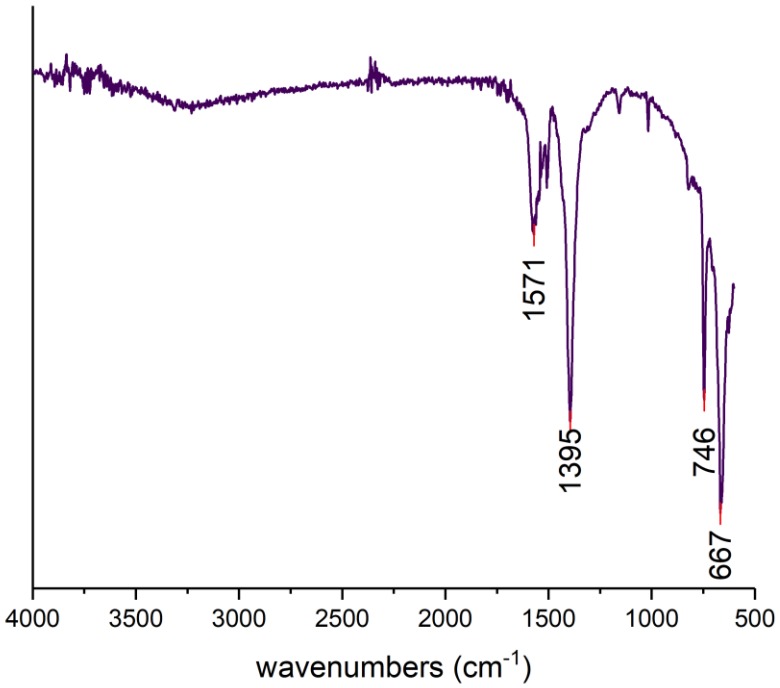

Figure S78: Infrared spectrum of UiO-66-28

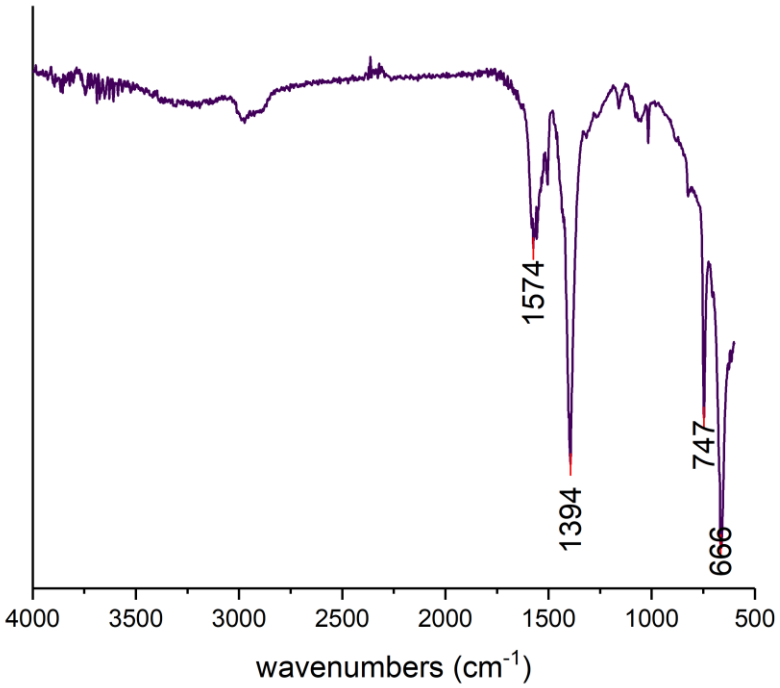

Figure S79: Infrared spectrum of UiO-66-35

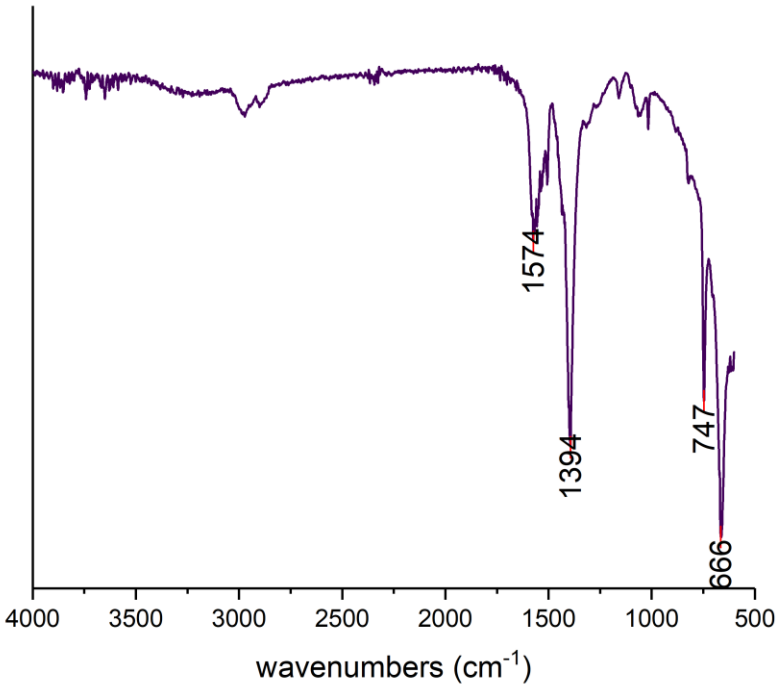

Figure S80: Infrared spectrum of UiO-66-40

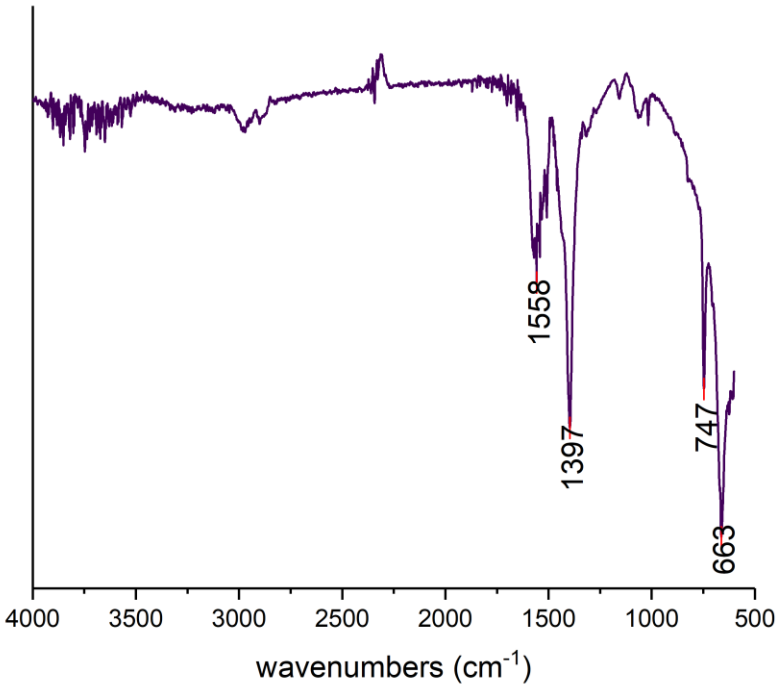

Figure S81: Infrared spectrum of UiO-66-51

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