Electronic supporting information

Tuning the flexibility in MOFs by SBU functionalization

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1. Linker synthesis

To a solution of potassium permanganate (39 g, 0.247 mmol, 6,5 eq.) in 250 mL water, 5,5´-dimethyl-2,2´-bipyridine (7 g, 0.038 mmol) was added and the mixture was heated for 2 h at 388 K. The reaction mixture was cooled down to room temperature and flittered trough Celite. The filtrate was cooled down to 277 K and acidified with HCl (conc.) until the precipitation of the product as white solid occurred. The solid was filtered (G5 frit) and washed with water. The obtained product was refluxed with acetone for 3 h and subjected to a hot filtration. The final product was dried overnight in vacuum. Yield: 8.03 g (90 %).

^{1}H-NMR (500 MHz, DMSO-d6, δ): 13.50 (br, 2 H); 9.19 (s, 2H); 8.57 (d, 2H); 8.45 (dd, 2H).

2. Thermodiffraction study.

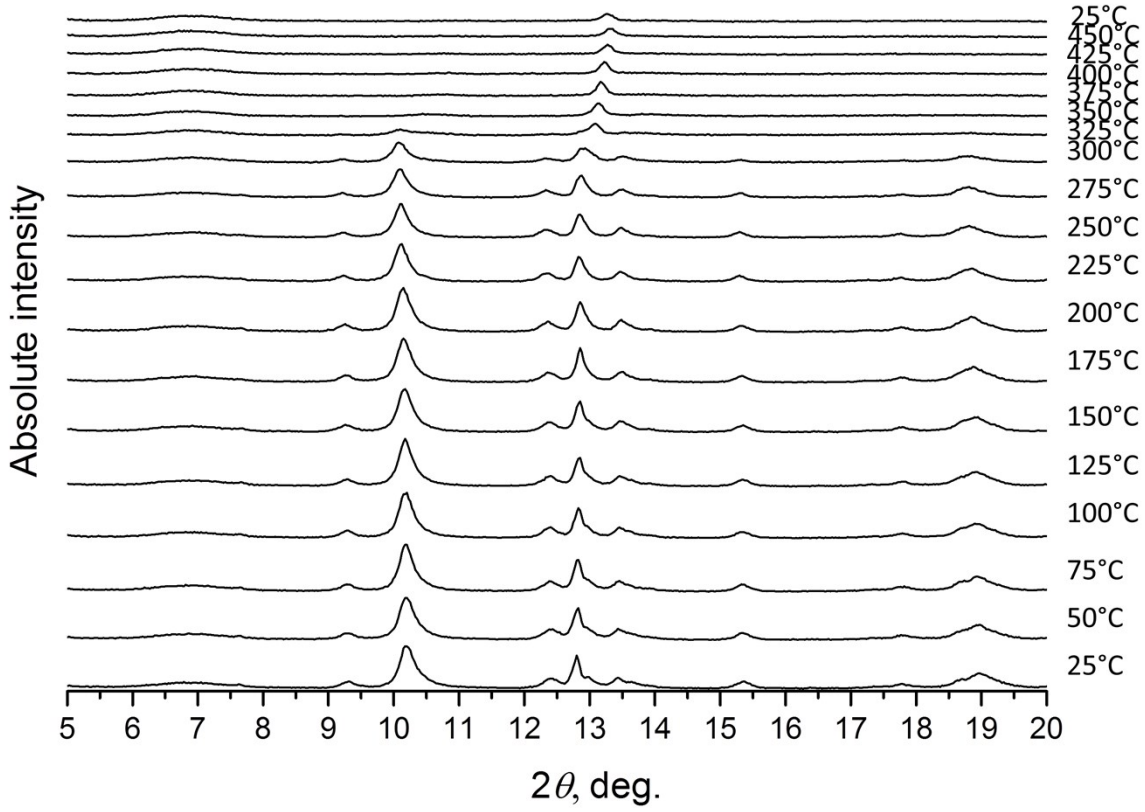

Figure S1. Temperature dependent PXRD measurements on **1'**.

3.TG analysis.

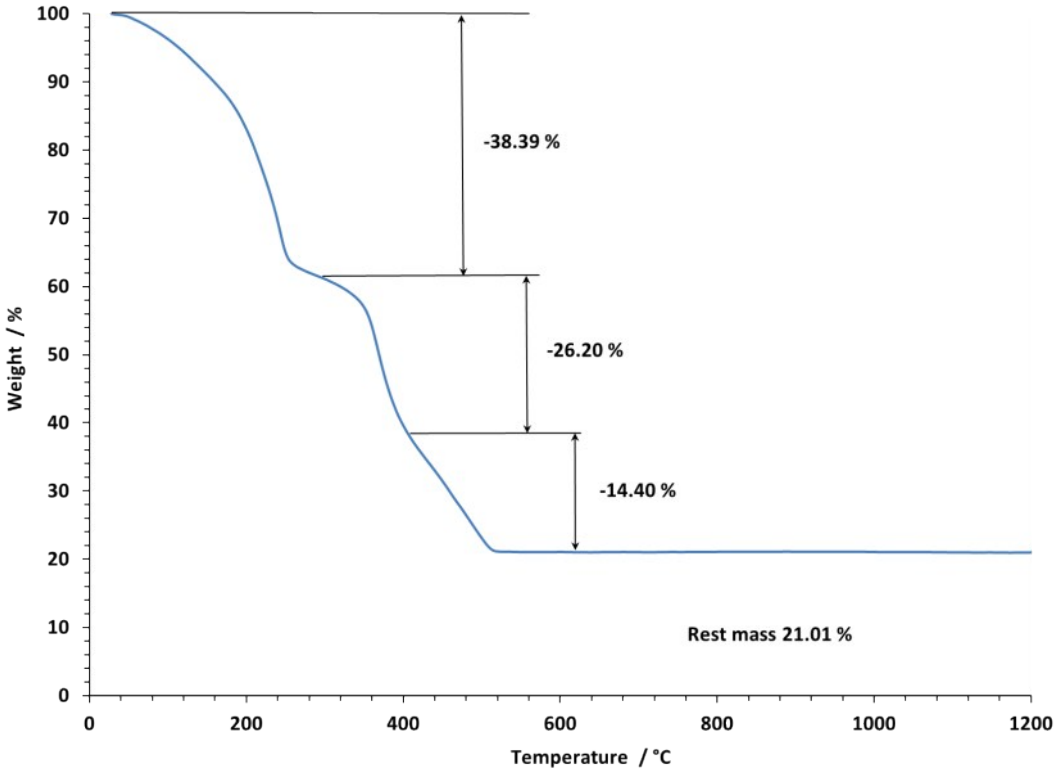

Figure S2. TG curve for **1.**

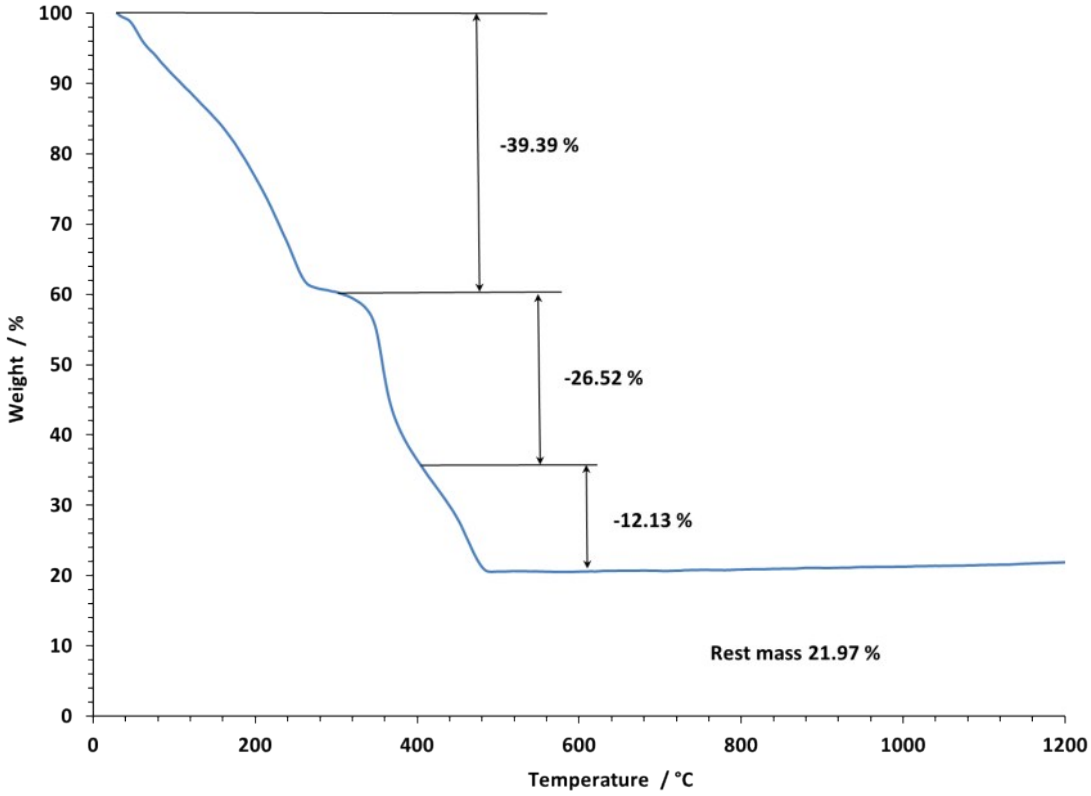

Figure S3. TG curve for **2.**

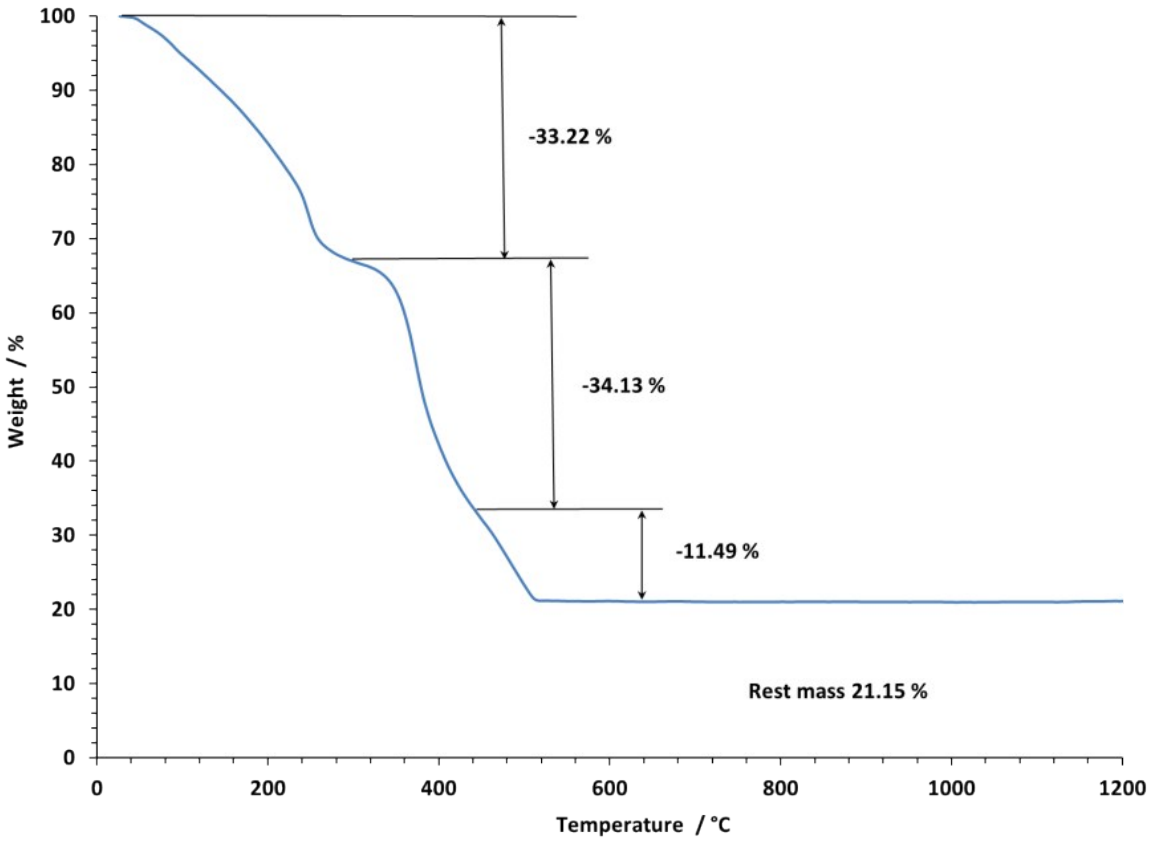

Figure S4. TG curve for **3.**

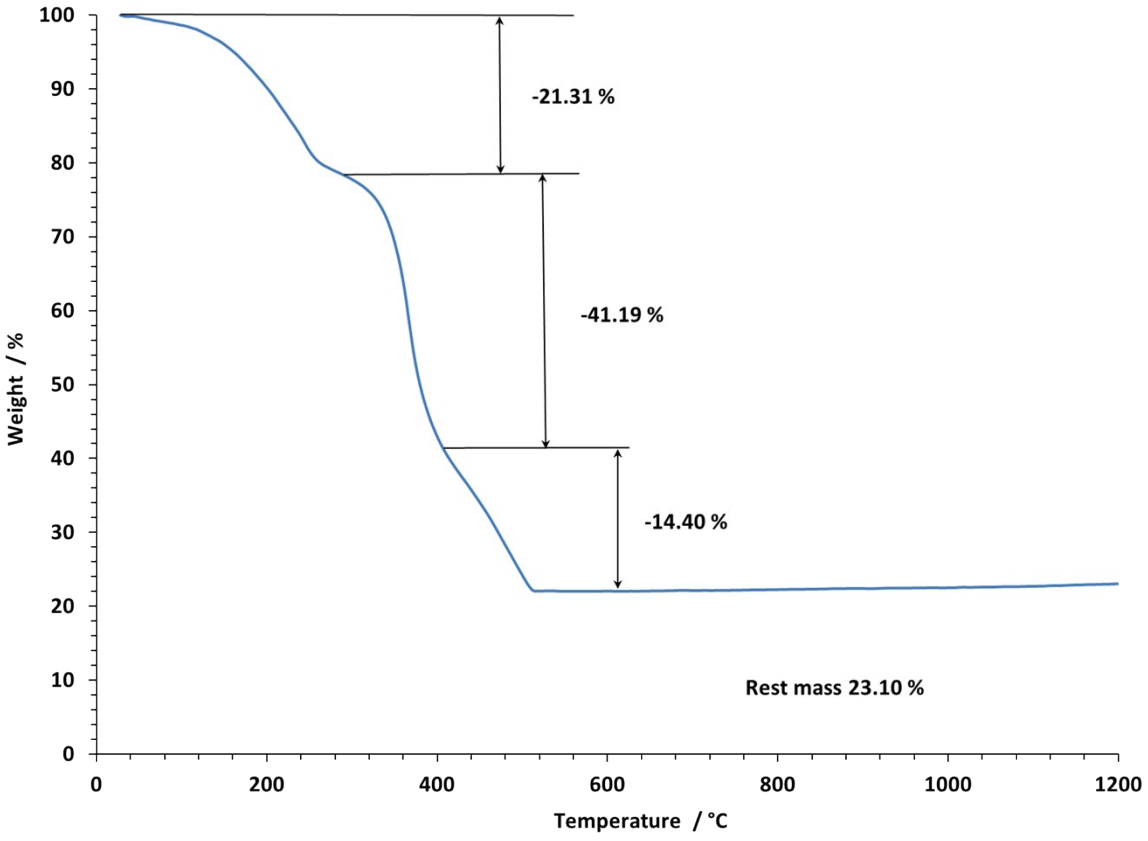

Figure S5. TG curve for **4.**

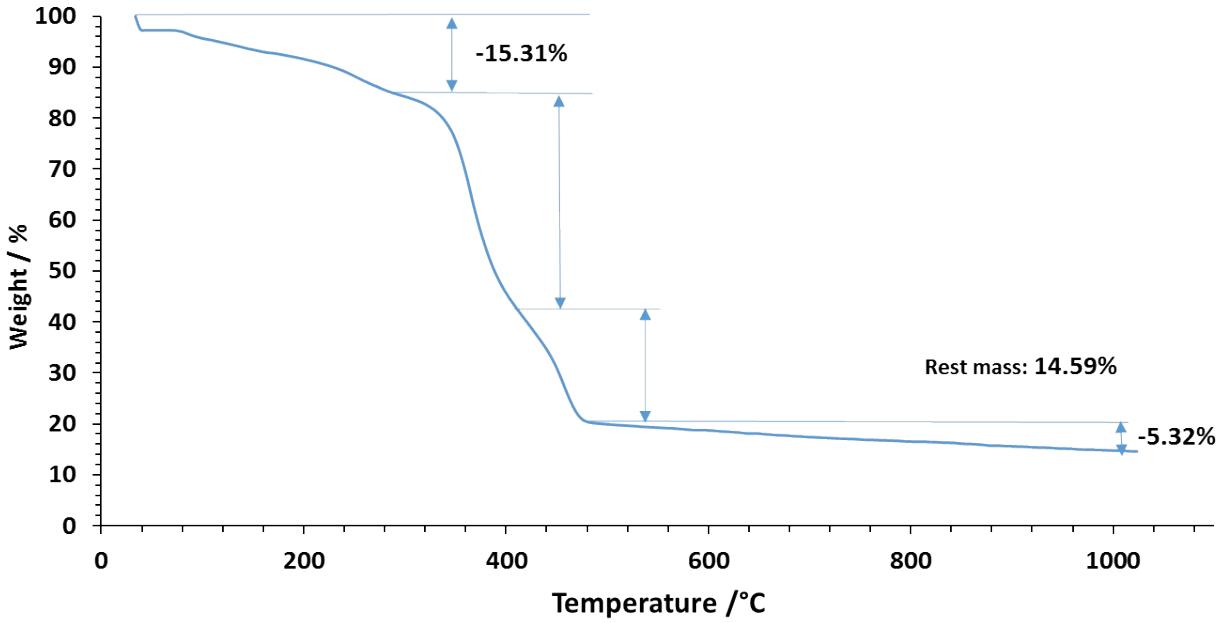

Figure S6. TG curve for **2'**.

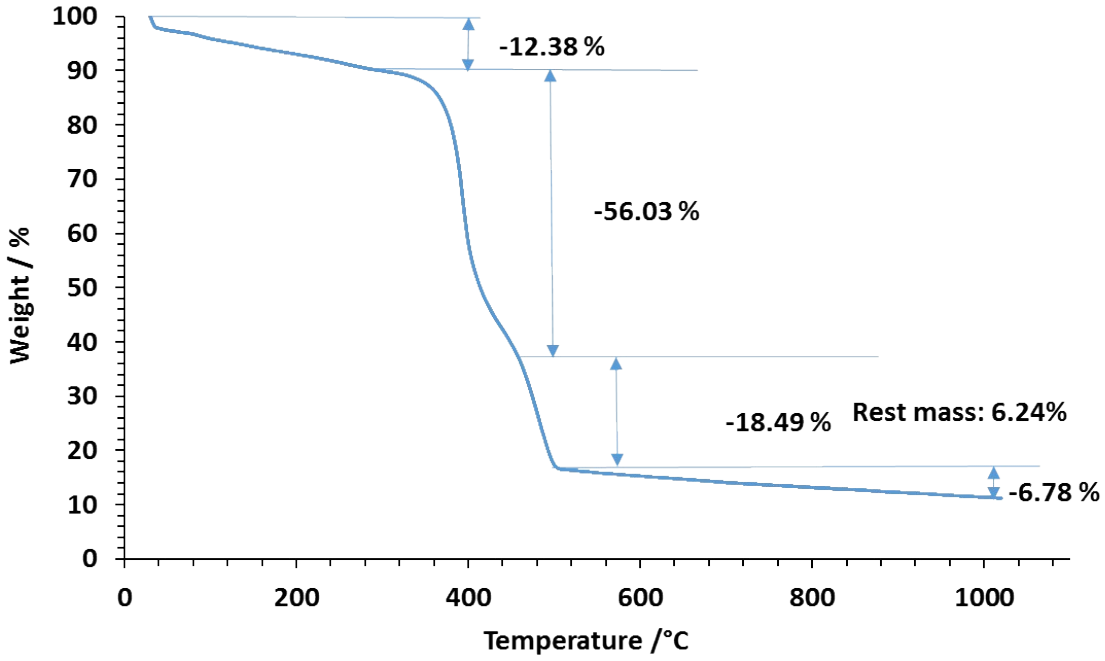

Figure S7. TG curve for **3'**.

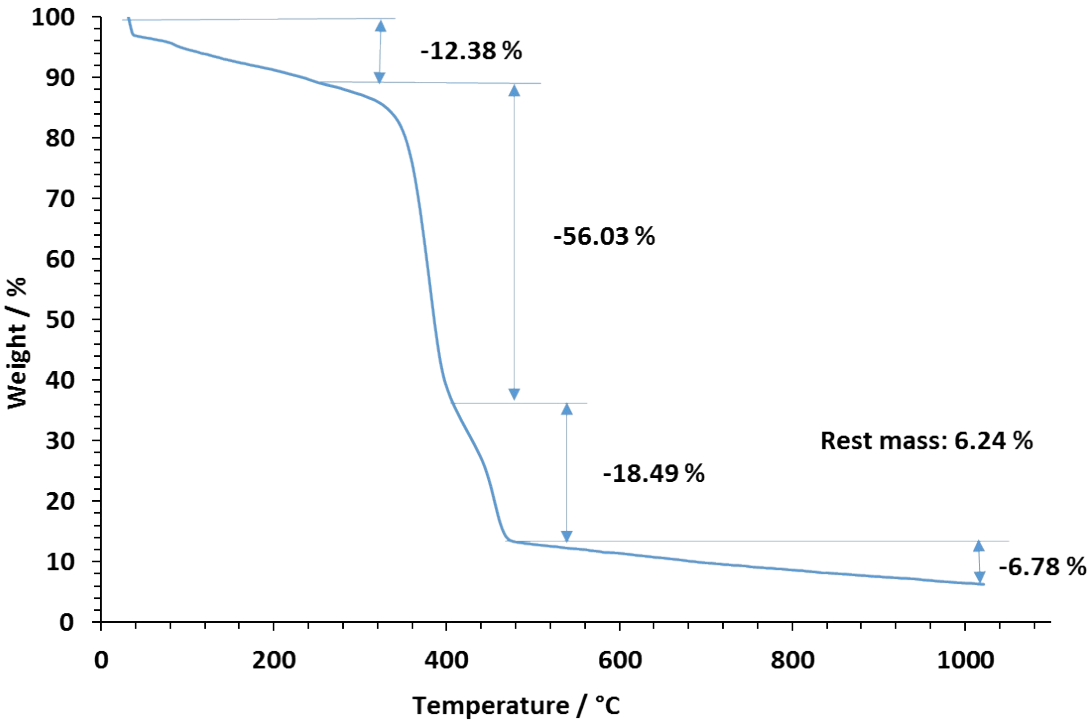

Figure S8. TG curve for **4'**.

4. IR-spectra.

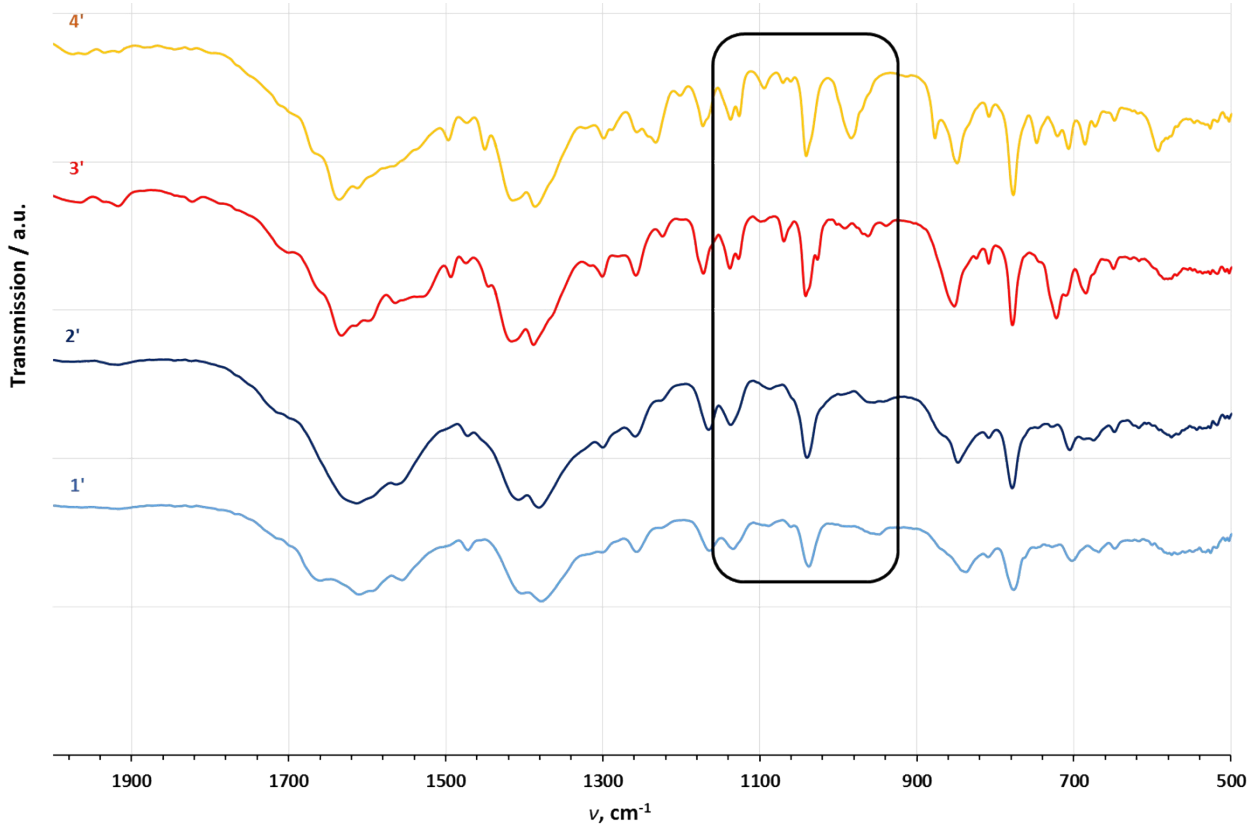

Figure S9. IR spectra for compounds **1'**- **4'**. The region containing vibrations of phenyl ring is highlighted.

5. PXRD patterns

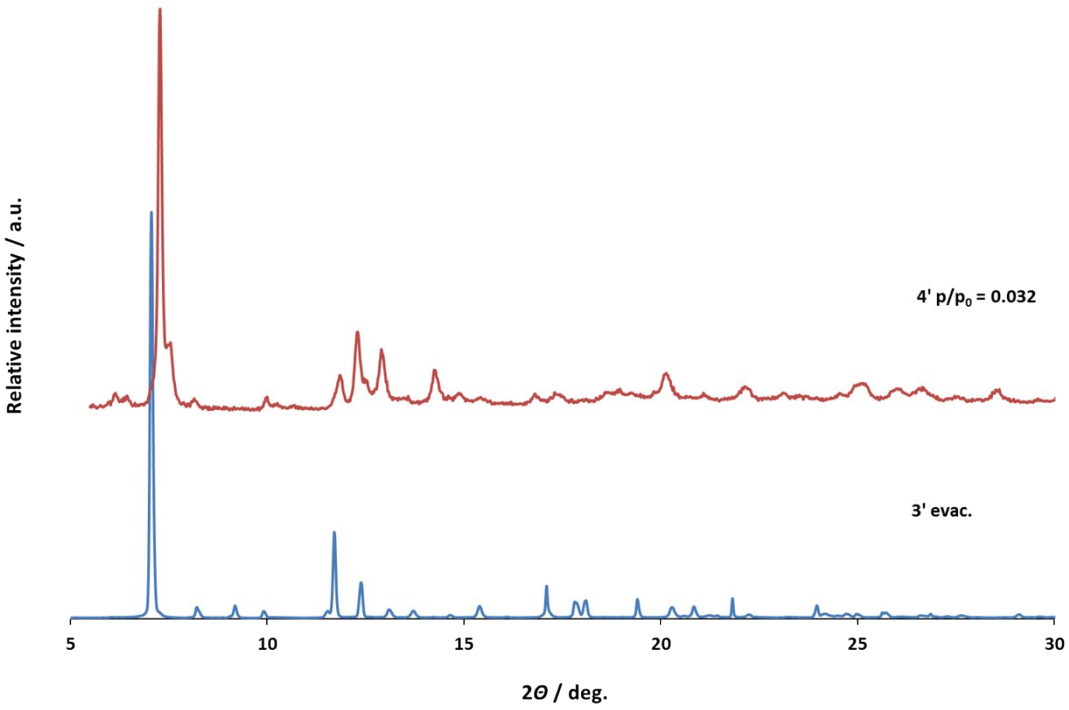

Figure S10. Comparison of the PXRD patterns of **3'** (evacuated) and **4'** (p/p_0 = 0.032).

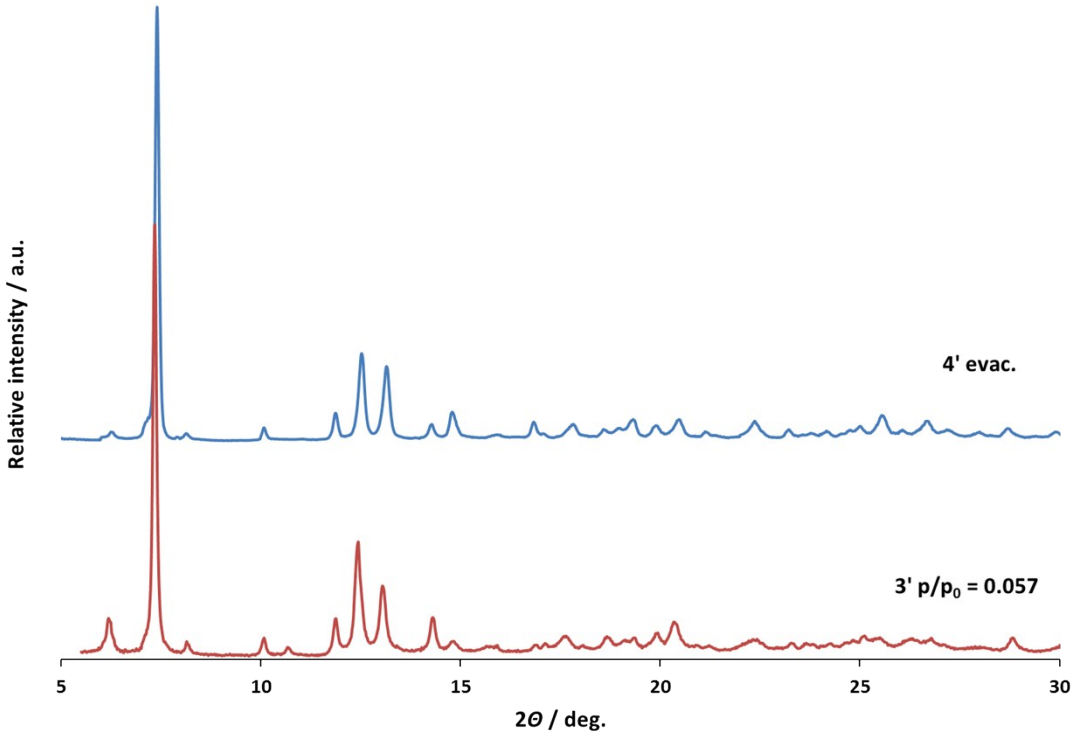

Figure S11. Comparison of the PXRD patterns of **3'** (p/p_0 = 0.057) and **4'** (evacuated).

7. Crystallographic data

Table S1. Experimental crystallographic data for **1** - **4**.

	1	**2**	**3**	**4**
Empirical formula	$C_{26}H_{14}N_4O_{12}Zn_3$	$C_{28}H_{18}N_4O_{12}Zn_3$	$C_{38}H_{22}N_4O_{12}Zn_3$	$C_{42}H_{26}N_4O_{12}Zn_3$
Formula weight	770.58	798.57	922.77	974.84
Temperature, K	296	296	296	296
Crystal size, mm	0.08x0.08x0.09	0.06x0.06x0.07	0.04x0.04x0.06	0.05x0.05x0.06
Crystal system, space group	Tetragonal, $P4_32_12$ *(No. 96)*			
Unit cell dimensions, Å	*a* = 15.320(2) *c* = 23.240(5)	*a* = 15.300(2) *c* = 23.280(5)	*a* = 15.160(2) *c* = 23.030(5)	*a* = 15.270(2) *c* = 23.050(5)
Volume, Å^3	5454.5(18)	5449.6(18)	5292.9(18)	5374.6(18)
Z	4	4	4	4
Calculated density, g/cm^3	0.938	0.973	1.158	1.205
Absorption coefficient, mm^{-1}	2.428	2.434	2.520	2.487
Tmin, Tmax	0.811, 0.829	0.848, 0.868	0.863, 0.906	0.865, 0.886
ϑ range, deg	2.6 – 36.2	2.0 – 36.2	2.0 – 35.7	2.0 – 35.7
Radiation wavelength, *Å*	0.88561 (Synchrotron)			
Limiting indices	-16 ≤ *h* ≤ 19 -13 ≤ *k* ≤ 19 -29 ≤ *l* ≤ 16	-19 ≤ *h* ≤ 7 -20 ≤ *k* ≤ 20 -30 ≤ *l* ≤ 23	-19 ≤ *h* ≤ 19 -19 ≤ *k* ≤ 19 -27 ≤ *l* ≤ 29	-13 ≤ *h* ≤ 19 -17 ≤ *k* ≤ 17 -28 ≤ *l* ≤ 30
Reflections collected / unique	12822 / 5847	19800 / 6337	40505 / 6196	20740 / 6207
R(int)	0.0194	0.0275	0.0556	0.0314
Data / parameters	5847 / 205	6337 / 215	6196 / 247	6207 / 265
Flack parameter	0.511(11)	0.508(11)	0.252(17)	0.560(14)
Final residual parameters after applying SQUEEZE routine				
SU (max) last refinement cycle	0.000	0.001	0.000	0.001
SQUEEZEd electrons / unit cell	241	1245	962	680
GooF on F^2 [I>2$\sigma(I)$]	1.089	1.100	1.078	1.100
GooF on F^2 (all data)	1.089	1.099	1.079	1.123
R1 [I>2$\sigma(I)$]	0.0287	0.0313	0.0515	0.0377
wR2 [I>2$\sigma(I)$]	0.0847	0.0911	0.1480	0.1150
R1 (all data)	0.0295	0.0332	0.0607	0.0410
wR2 (all data)	0.0852	0.0960	0.1546	0.1195
Largest diff. peak / hole, *e*Å^{-3}	0.569 / -0.543	0.629 / -0.532	0.656 / -0.764	0.500 / -0.756
Final residual parameters before applying SQUEEZE routine				
SU (max) last refinement cycle	0.000	0.000	0.007	0.001
F(000)	1536	1600	1856	1968
GooF on F^2 [I>2$\sigma(I)$]	1.177	1.171	1.136	1.098

GooF on F^2 (all data)	1.177	1.171	1.136	1.117
R1 [$I>2\sigma(I)$]	0.0381	0.0427	0.0571	0.0446
wR2 [$I>2\sigma(I)$]	0.1295	0.1495	0.1723	0.1409
R1 (all data)	0.0390	0.0469	0.0693	0.0497
wR2 (all data)	0.1301	0.1542	0.1803	0.1458
Largest diff. peak / hole, eÅ^{-3}	0.628 / -0.569	0.926 / -0.954	1.055 / -0.910	0.970 / -1.063