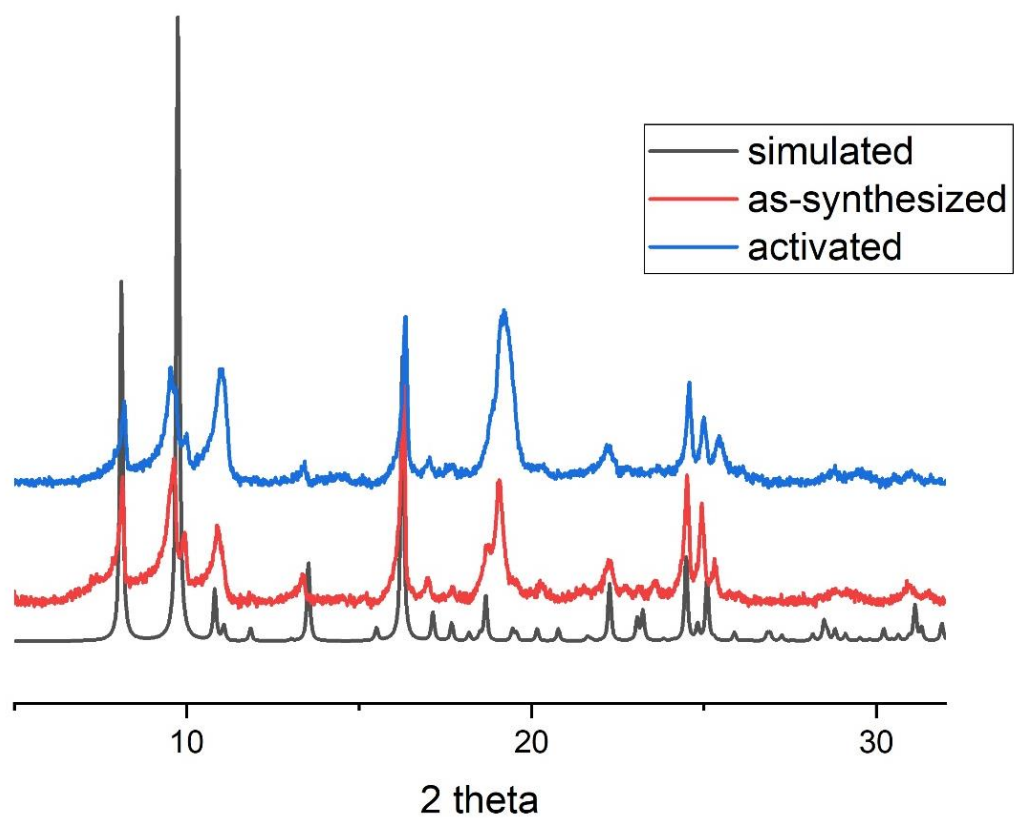


## Zn(II) and Co(II) 3D coordination polymers based on 2-iodoterephthalic acid and 1,2-bis(4-pyridyl)ethane: structures and sorption properties

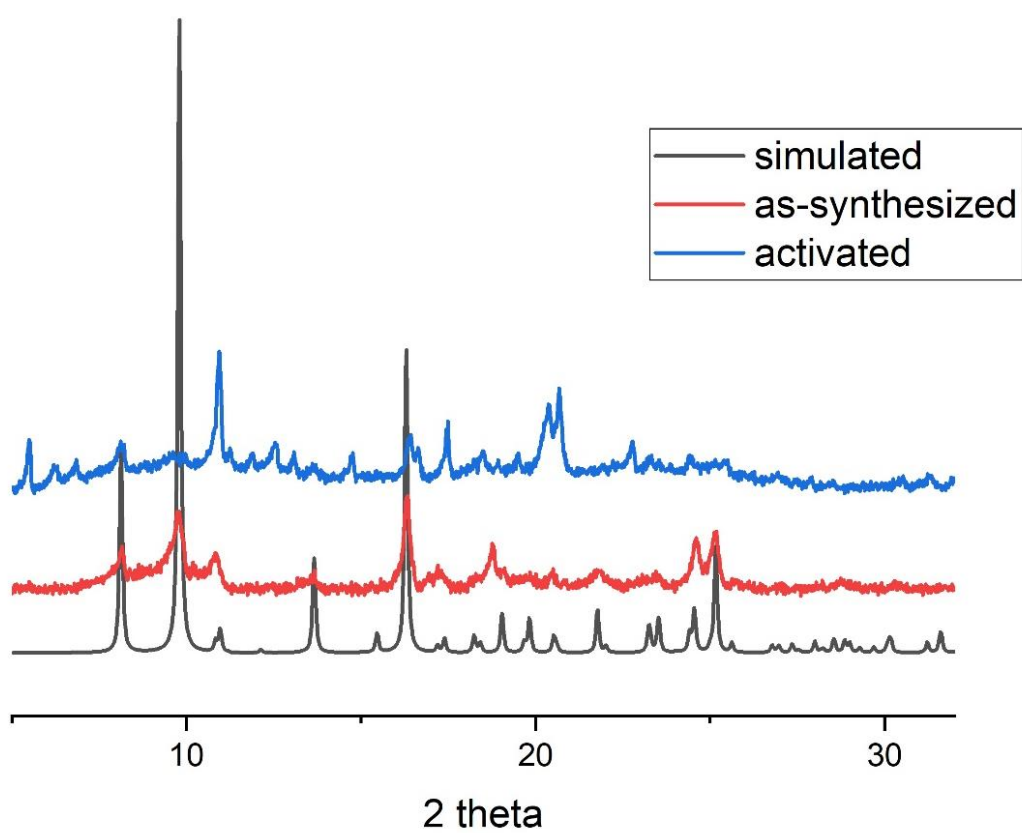
Alexander S. Zaguzin, Taisiya S. Sukhikh, Ilyas S. Sakhapov, Vladimir P. Fedin, Maxim N. Sokolov and Sergey A. Adonin

**Table S1.** Crystal data and structure refinement for **1** and **2**

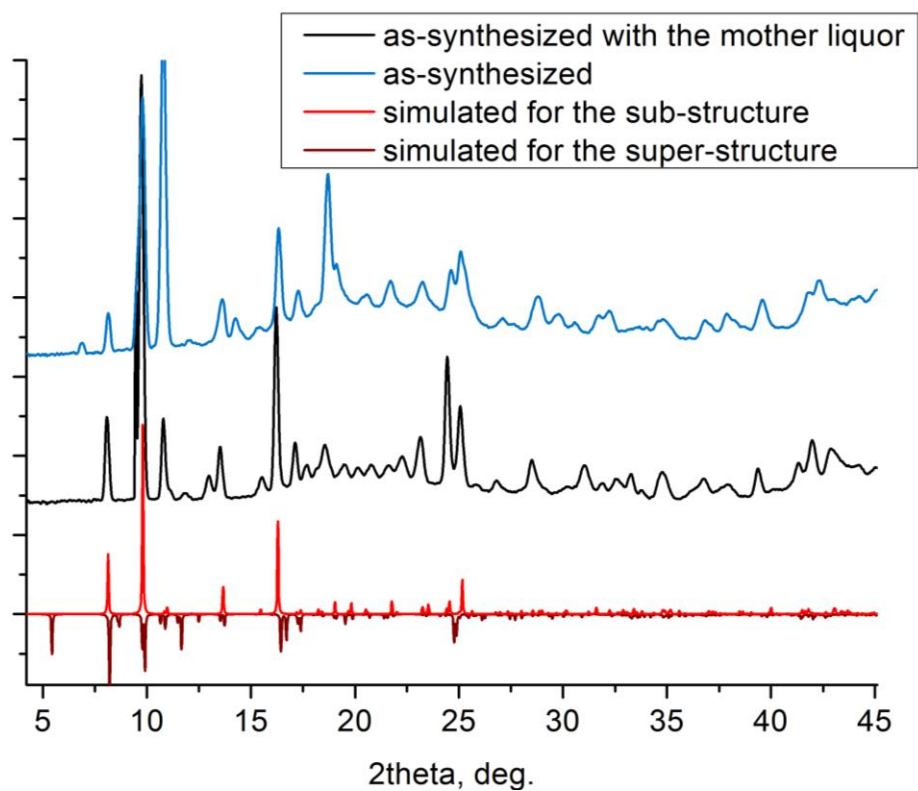
Identification code	<b>1</b>	<b>2</b>
Empirical formula	C <sub>31</sub> H <sub>23</sub> I <sub>2</sub> N <sub>3</sub> O <sub>9</sub> Zn <sub>2</sub>	C <sub>34</sub> Co <sub>2</sub> H <sub>30</sub> I <sub>2</sub> N <sub>4</sub> O <sub>10</sub>
Formula weight	966.06	1026.28
Temperature/K	150(2)	150(2)
Space group	C2/c	C2/c
a/Å	14.1684(4)	16.3143(14)
b/Å	16.5994(4)	14.5781(15)
c/Å	32.5179(8)	16.1189(16)
α/°	90	90
β/°	91.1000(10)	90.170(4)
γ/°	90	90
Volume/Å <sup>3</sup>	7646.4(3)	3833.6(6)
Z	8	4
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.678	1.778
μ/mm <sup>-1</sup>	2.919	2.535
F(000)	3744.0	2008.0
Crystal size/mm <sup>3</sup>	0.2 × 0.15 × 0.12	0.12 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	3.964 to 54.22	2.526 to 51.358
Index ranges	-18 ≤ h ≤ 18, -20 ≤ k ≤ 21, -41 ≤ l ≤ 41	-18 ≤ h ≤ 19, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	52403	9109
Independent reflections	8376 [R <sub>int</sub> = 0.0599, R <sub>sigma</sub> = 0.0369]	3593 [R <sub>int</sub> = 0.0415, R <sub>sigma</sub> = 0.0502]
Data/restraints/parameters	8376/127/447	3593/52/207
Goodness-of-fit on F <sup>2</sup>	1.046	1.046
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0818, wR <sub>2</sub> = 0.1967	R <sub>1</sub> = 0.0883, wR <sub>2</sub> = 0.2462
Final R indexes [all data]	R <sub>1</sub> = 0.0935, wR <sub>2</sub> = 0.2051	R <sub>1</sub> = 0.1016, wR <sub>2</sub> = 0.2632
Largest diff. peak/hole / e Å <sup>-3</sup>	2.75/-2.65	2.12/-1.29



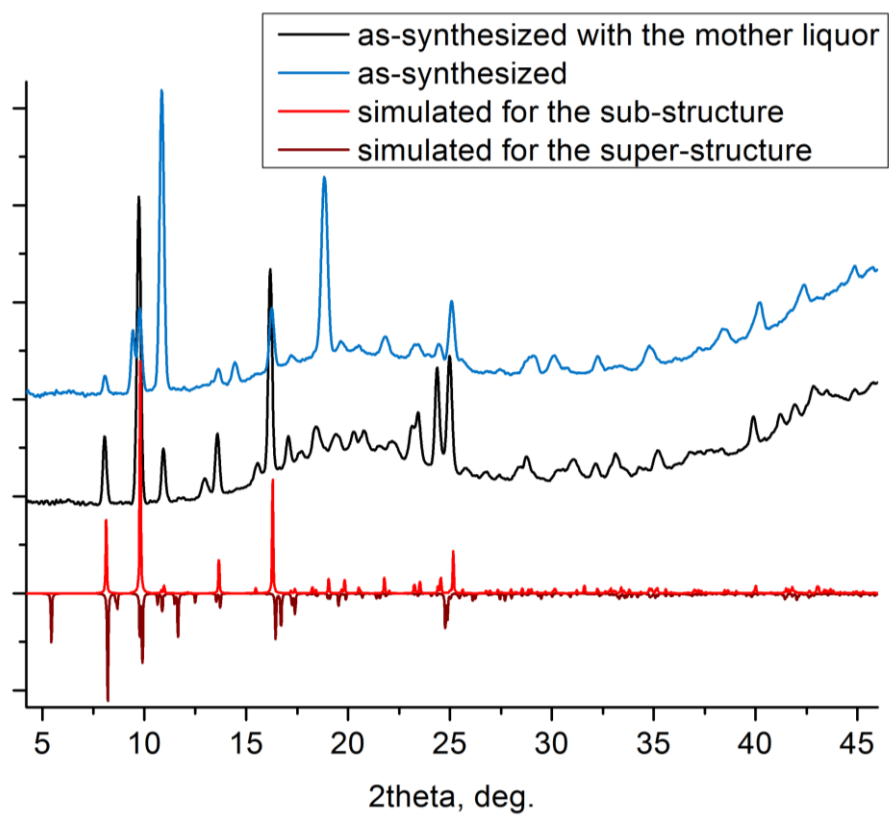
**Figure S1.** PXRD data for **1**



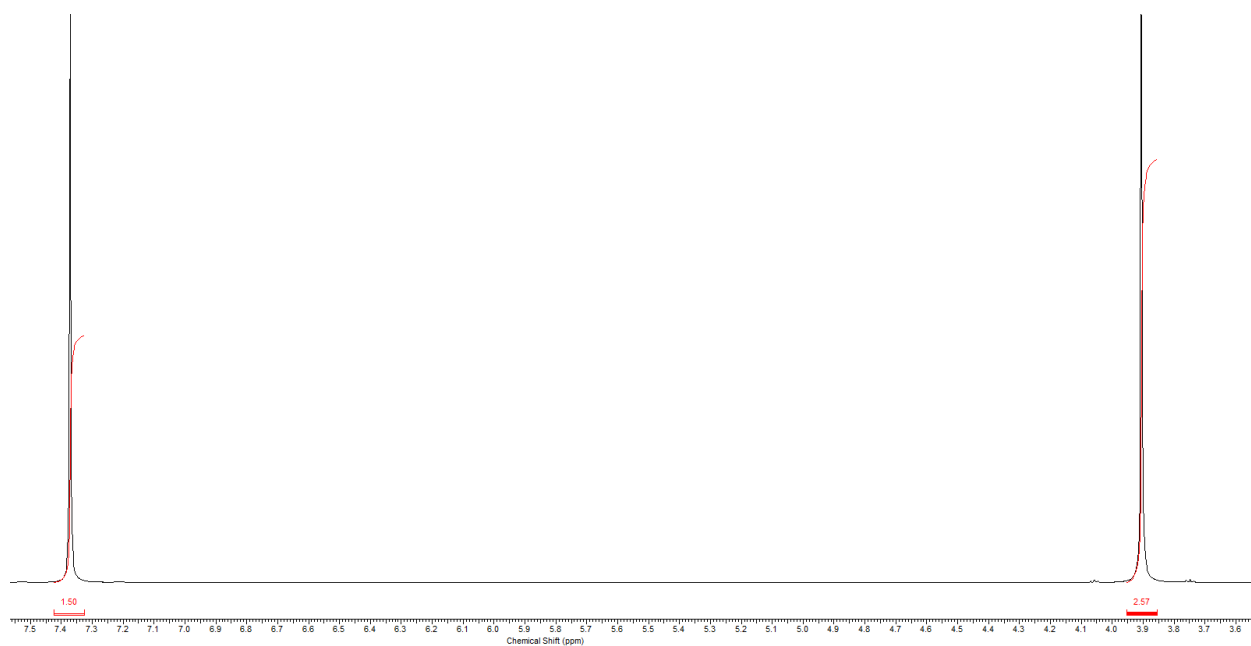
**Figure S2.** PXRD data for **2**



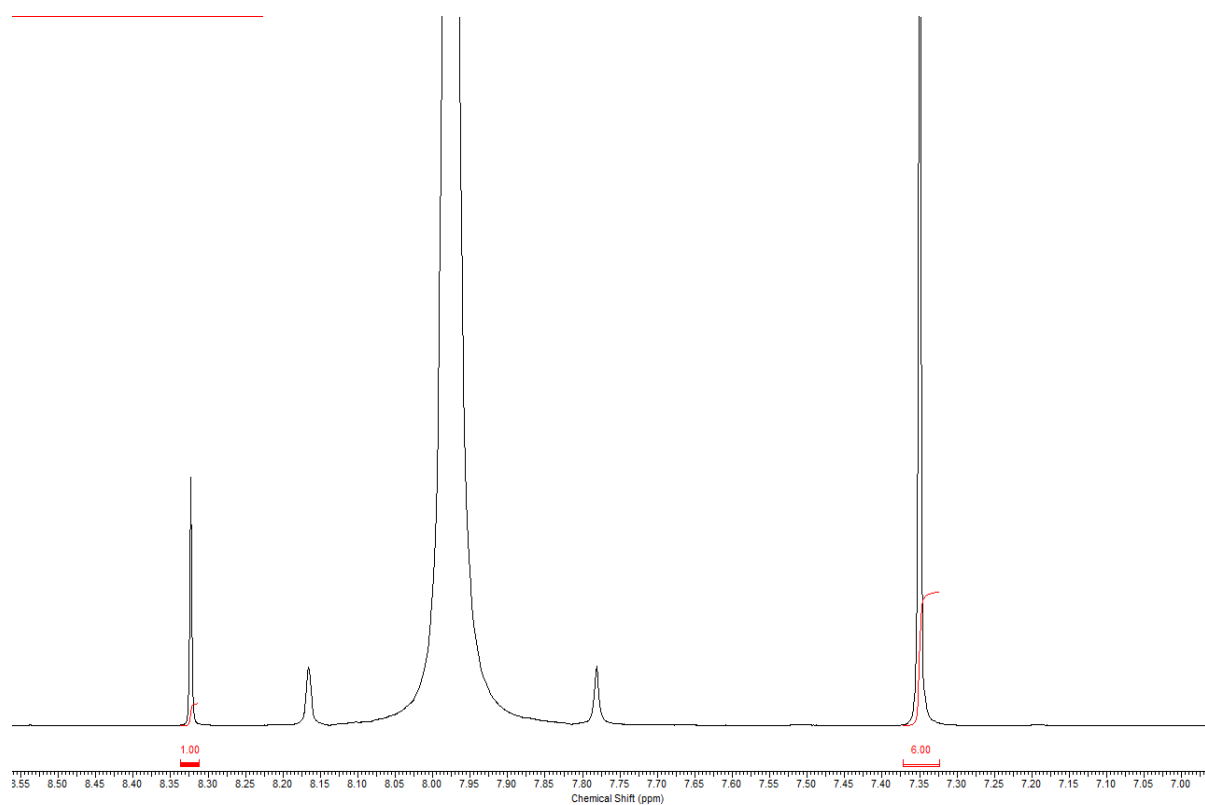
**Figure S3.** PXRD data for 1 at 150 K



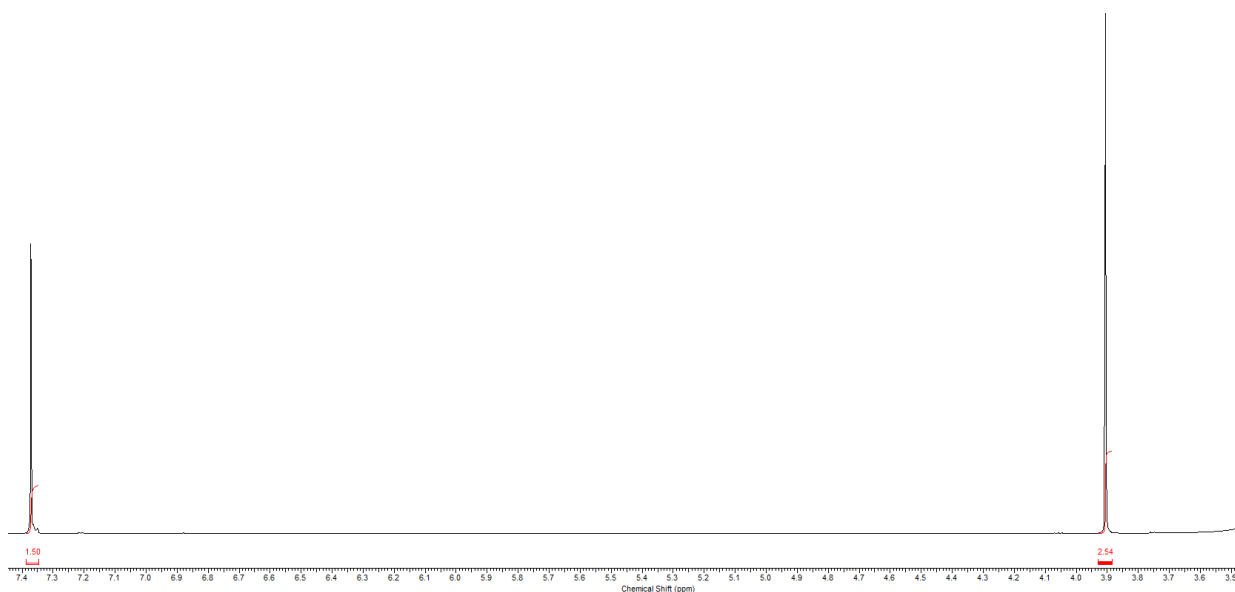
**Figure S4.** PXRD data for 2 at 150 K.



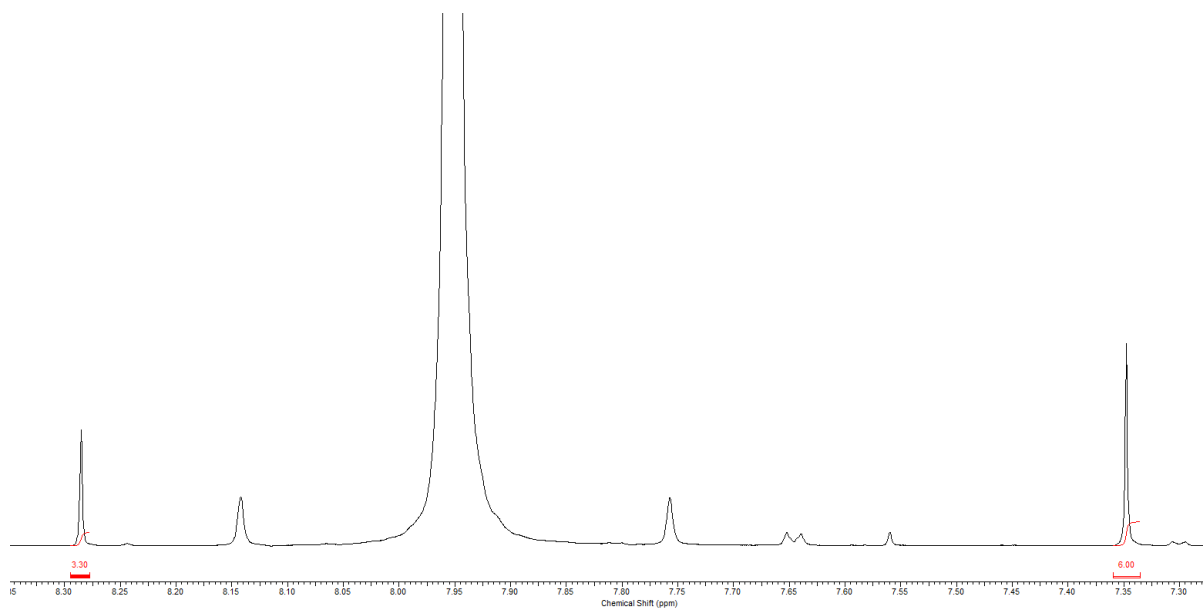
**Figure S5.**  $^1\text{H}$  NMR spectrum, sorption experiment with **2**, benzene:dichloroethane



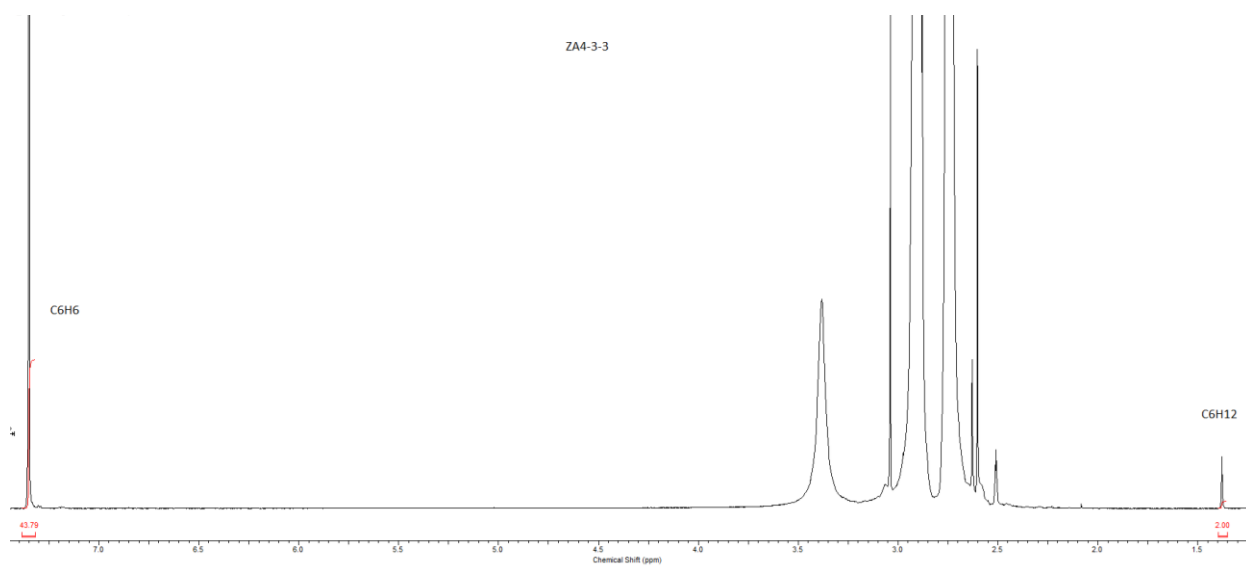
**Figure S6.**  $^1\text{H}$  NMR spectrum, sorption experiment with **2**, benzene:chloroform



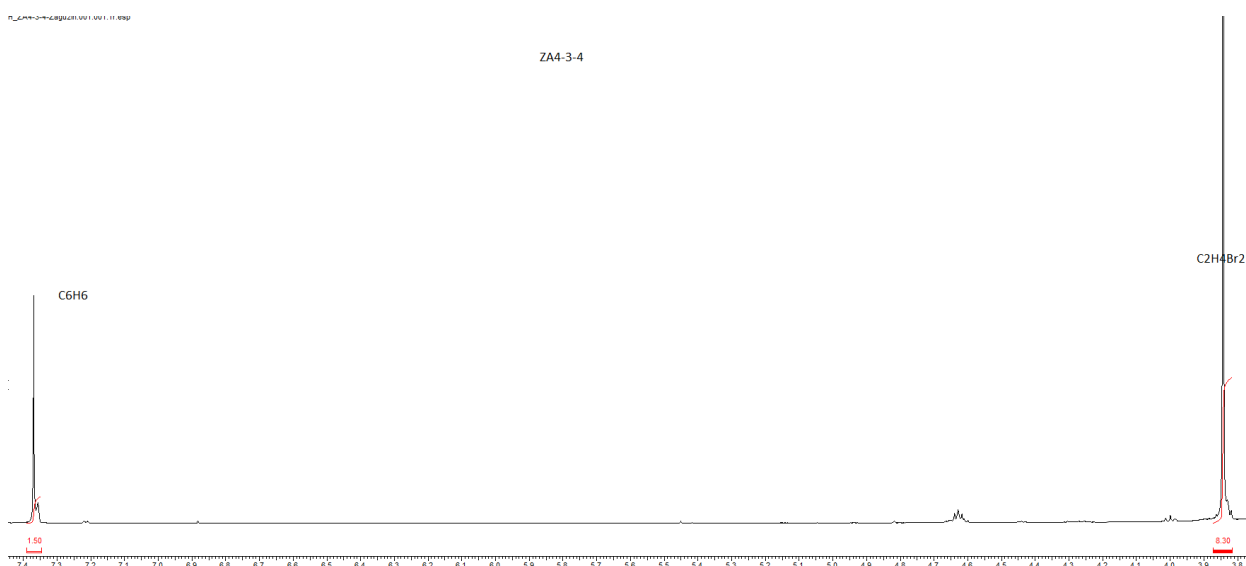
**Figure S7.**  $^1\text{H}$  NMR spectrum, sorption experiment with **1**, benzene: dichloroethane



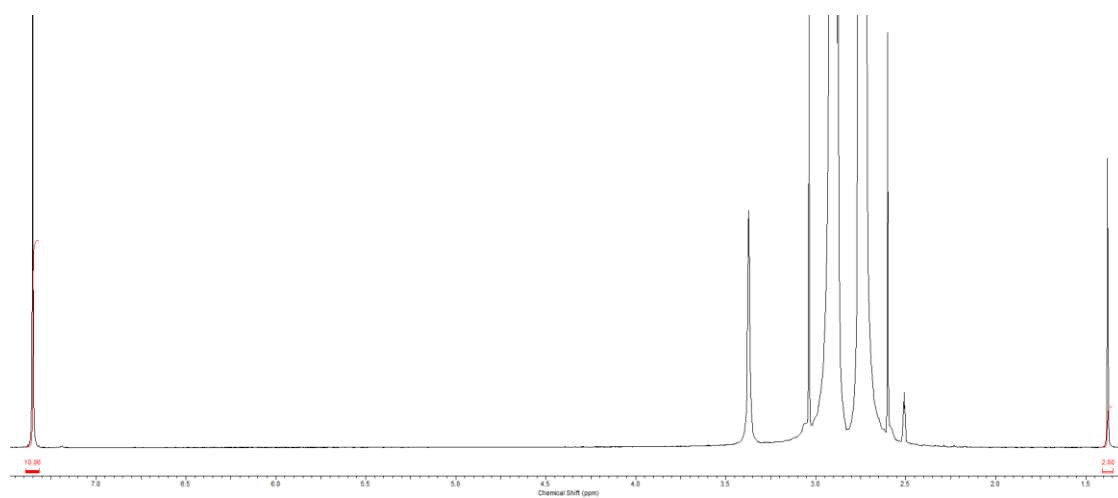
**Figure S8.**  $^1\text{H}$  NMR spectrum, sorption experiment with **1**, benzene: chloroform



**Figure S9.**  $^1\text{H}$  NMR spectrum, sorption experiment with **1**, benzene:cyclohexane



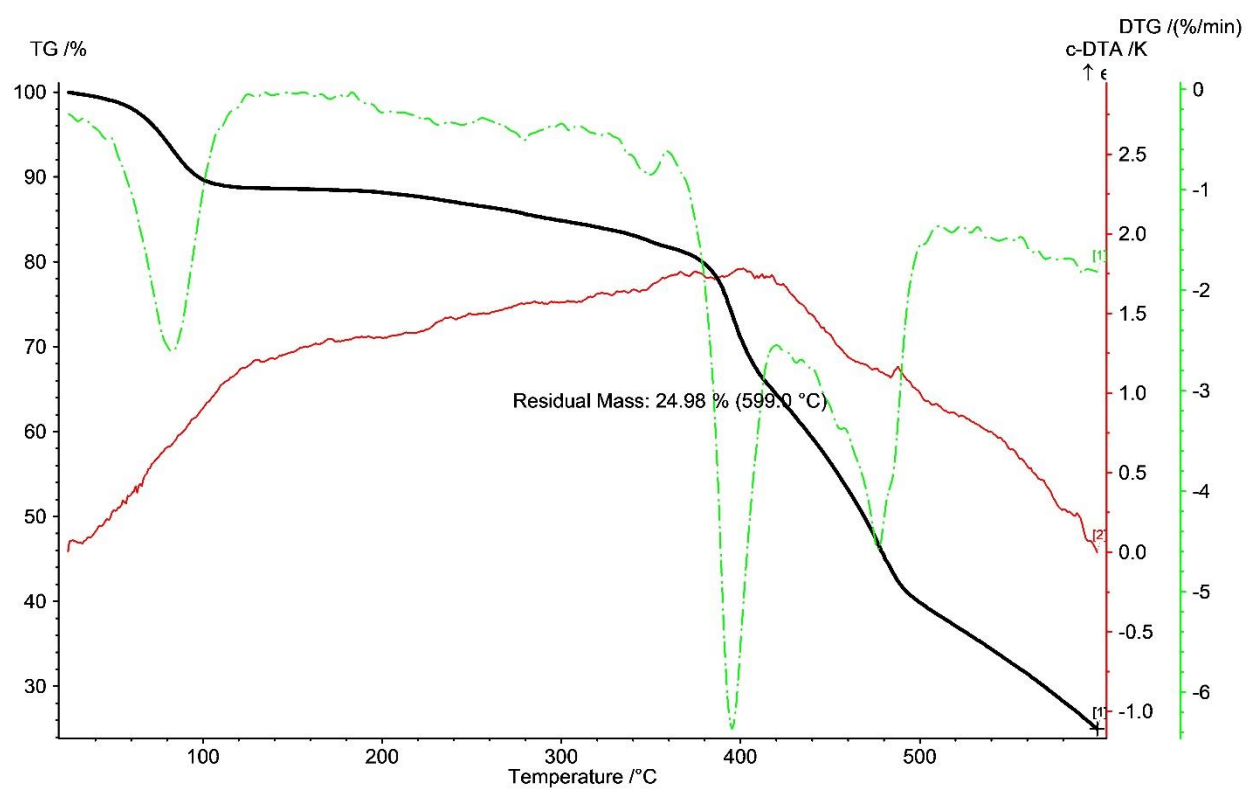
**Figure S10.**  $^1\text{H}$  NMR spectrum, sorption experiment with **1**, benzene:dibromoethane



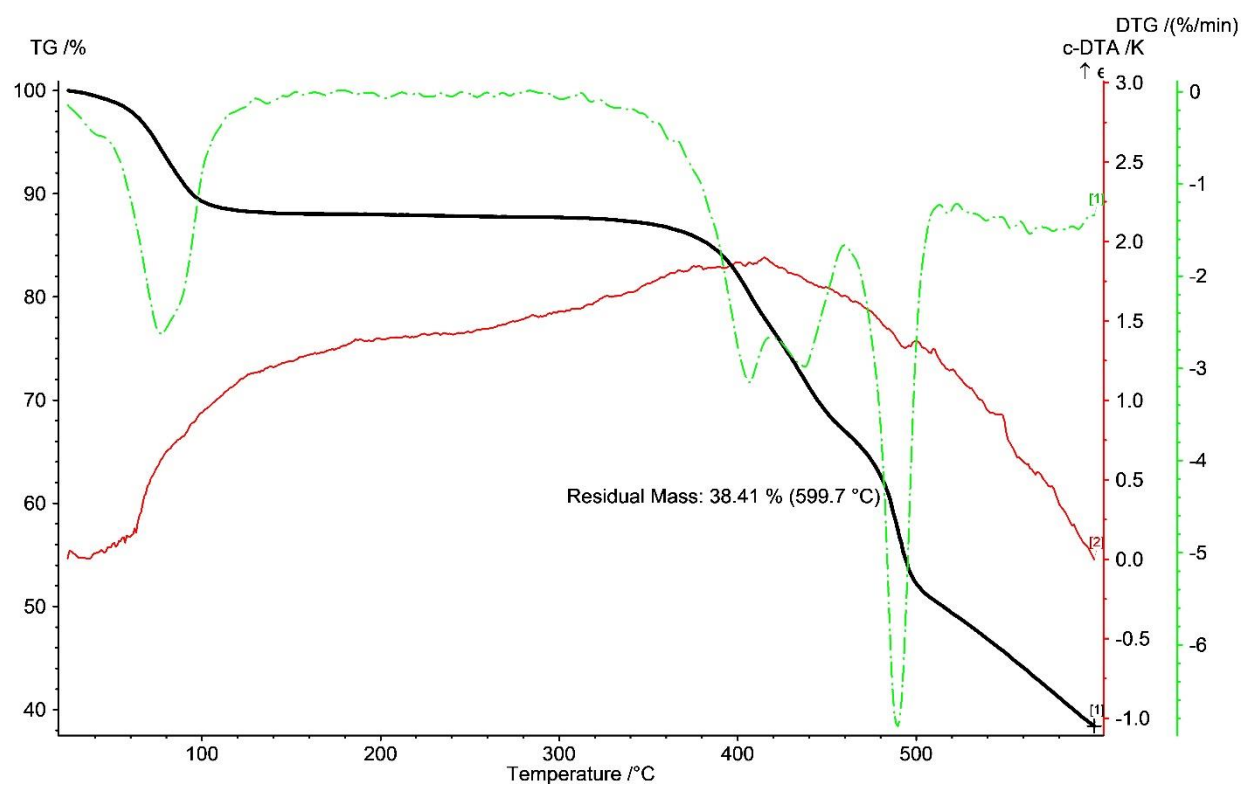
**Figure S11.**  $^1\text{H}$  NMR spectrum, sorption experiment with **2**, benzene: cyclohexane



**Figure S12.**  $^1\text{H}$  NMR spectrum, sorption experiment with **2**, benzene:dibromoethane



**Figure S13.** TGA data for as-synthesized **1**



**Figure S14.** TGA data for as-synthesized **2**