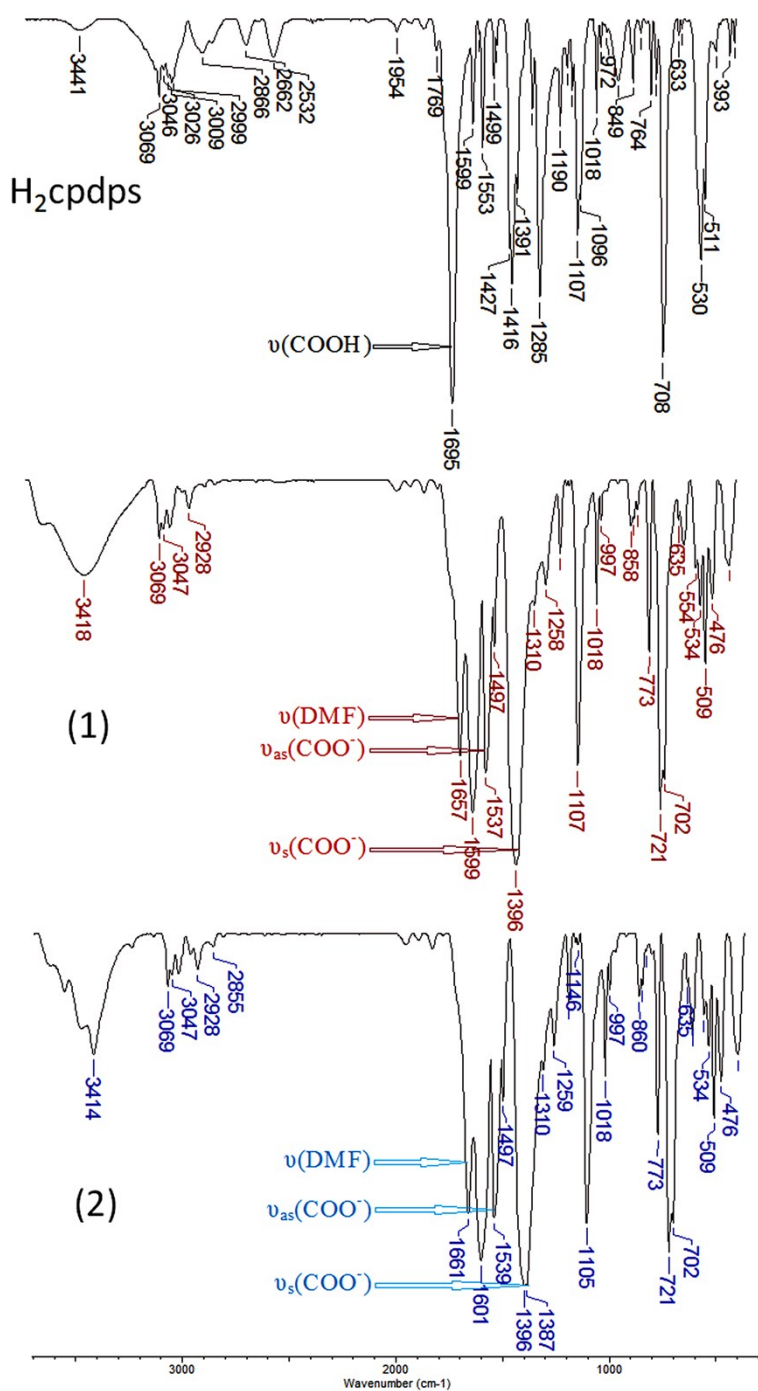


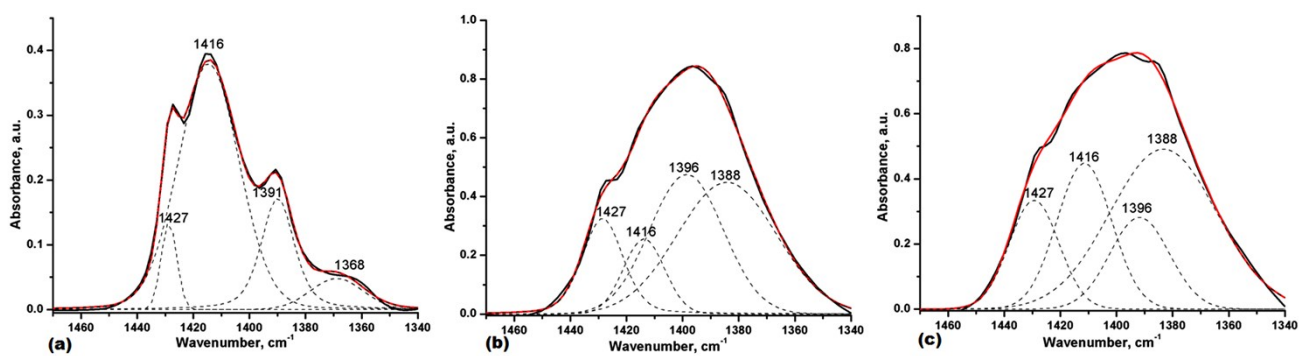
Supplementary information for:

*Metal-Organic Frameworks Based on Tri- and Penta-nuclear Manganese(II) Secondary Building Units Self-assembled by a V-Shaped Silicon-containing Dicarboxylate*

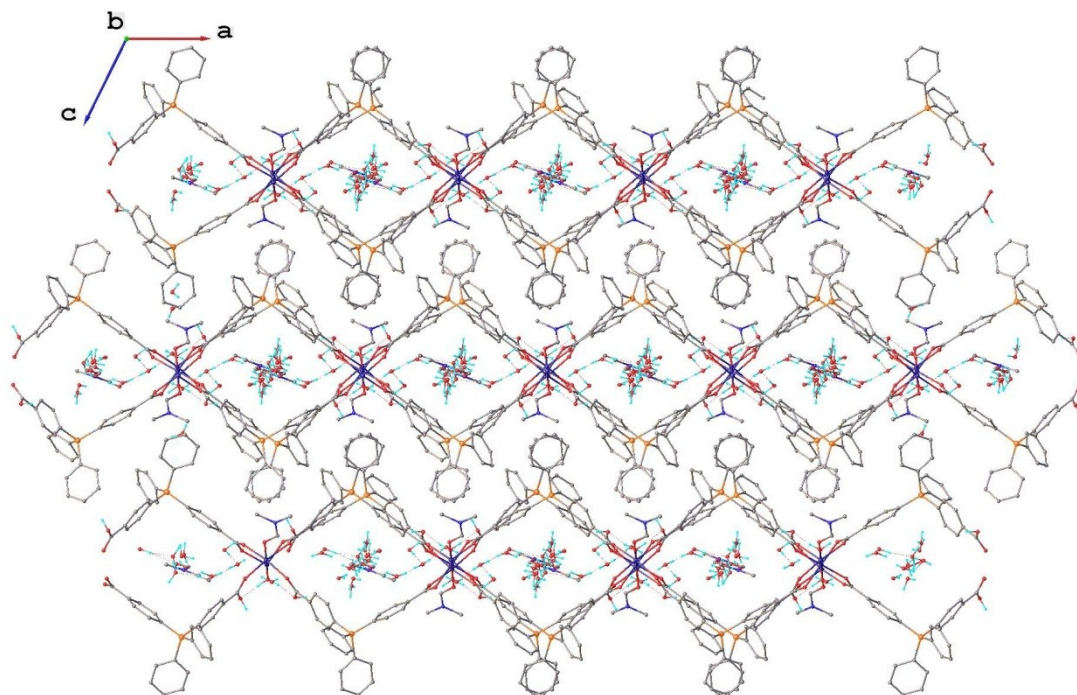
Angelica Vlad, Mirela-Fernanda Zaltariov, Sergiu Shova, Ghenadie Novitchi, Cyrille Train, Maria Cazacu



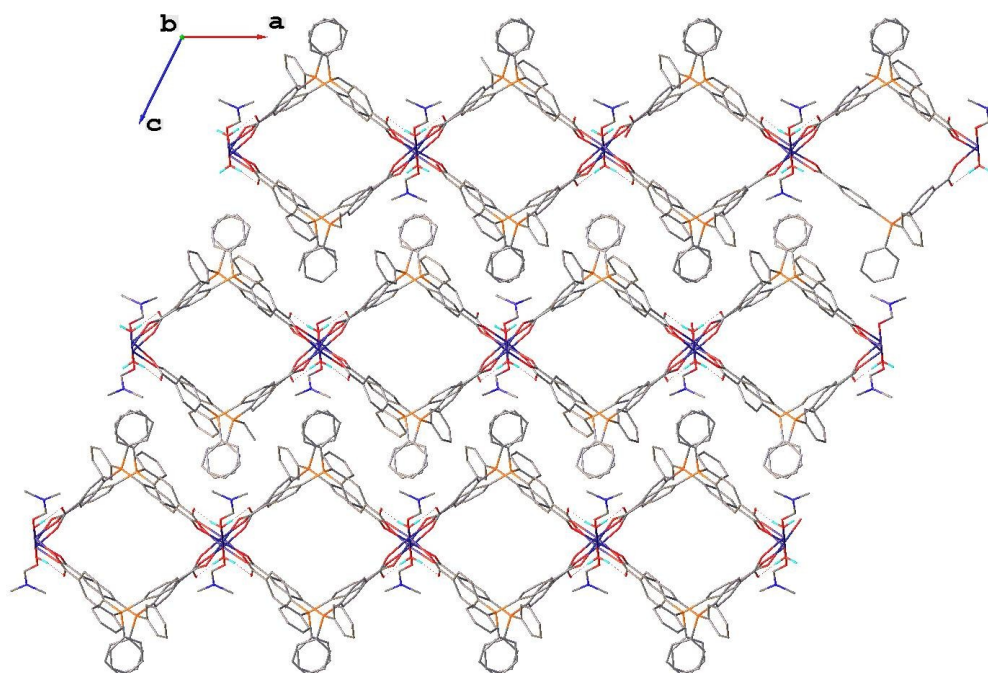
**Figure S1.** Comparative FTIR spectra of the carboxylic acid (H<sub>2</sub>cpdps) and manganese(II) complexes **1** and **2**.



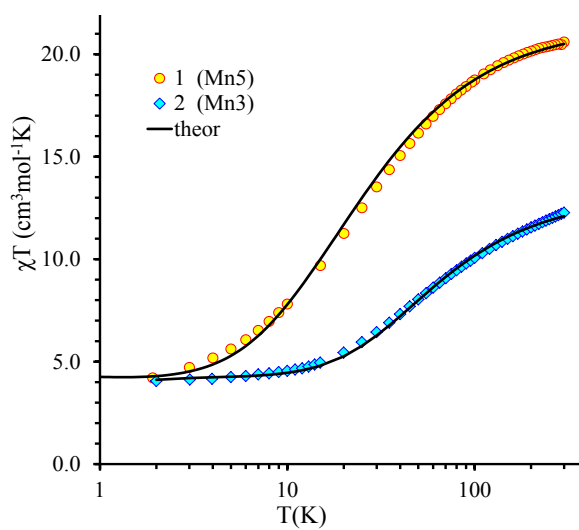
**Figure S2.** Deconvoluted FTIR spectra in the range 1470-1340 cm<sup>-1</sup> for H<sub>2</sub>cpdps – (a) and manganese(II) complexes **1** – (b) and **2** – (c).



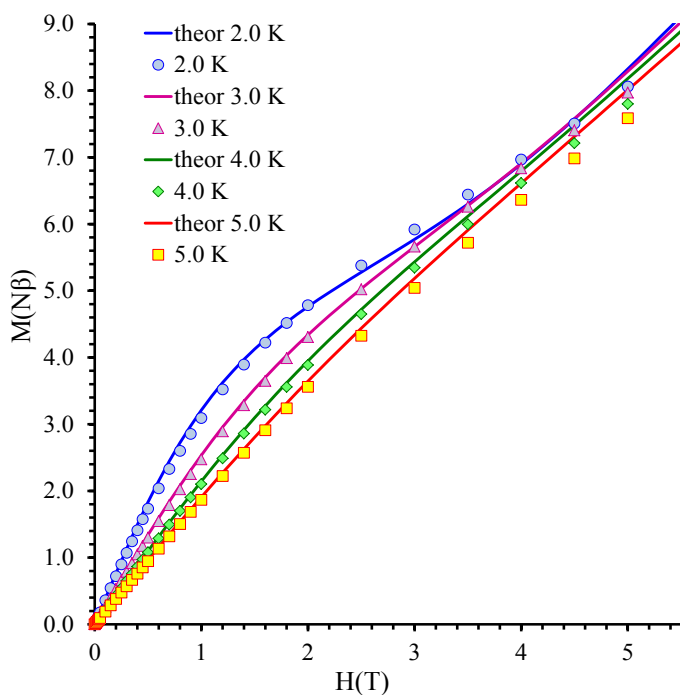
**Figure S3.** Crystal structure packing of **1** viewed along *b* axis. Non-relevant h-atoms are omitted for clarity.



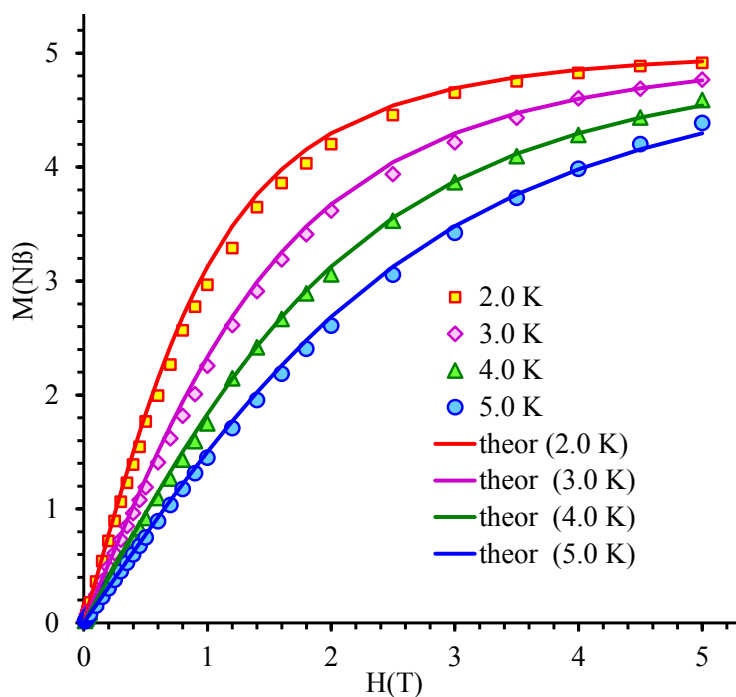
**Figure S4.** View of the crystal structure of **2** along the crystallographic axis *b*. H-atoms and solvate molecules are omitted for clarity.



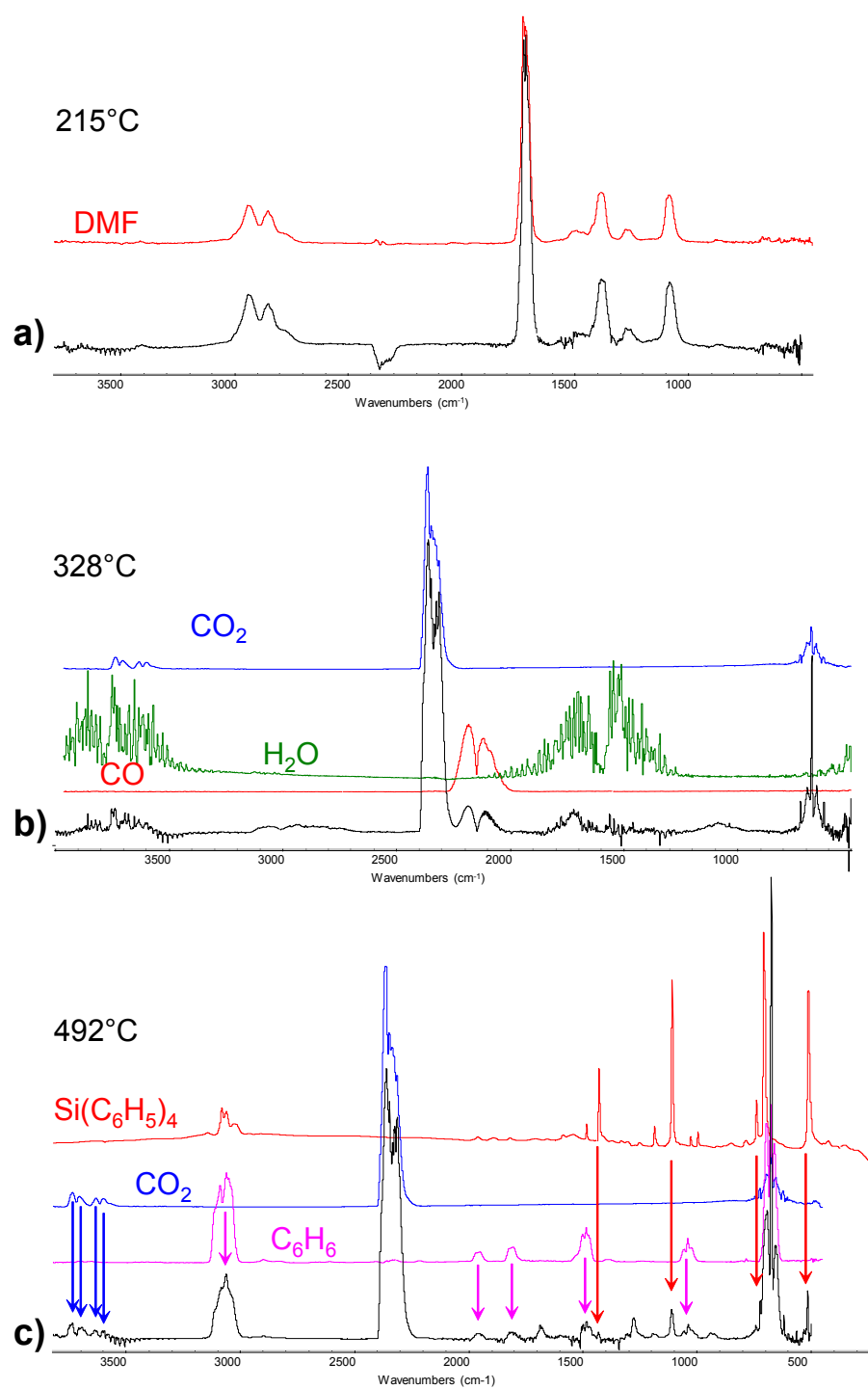
**Figure S5.**  $\chi T$  versus  $T$  plots in logarithmic scale for **1** and **2**. The solid lines correspond to the simulation according the Hamiltonians (eq. 1 and 2) with parameters described in the main text.



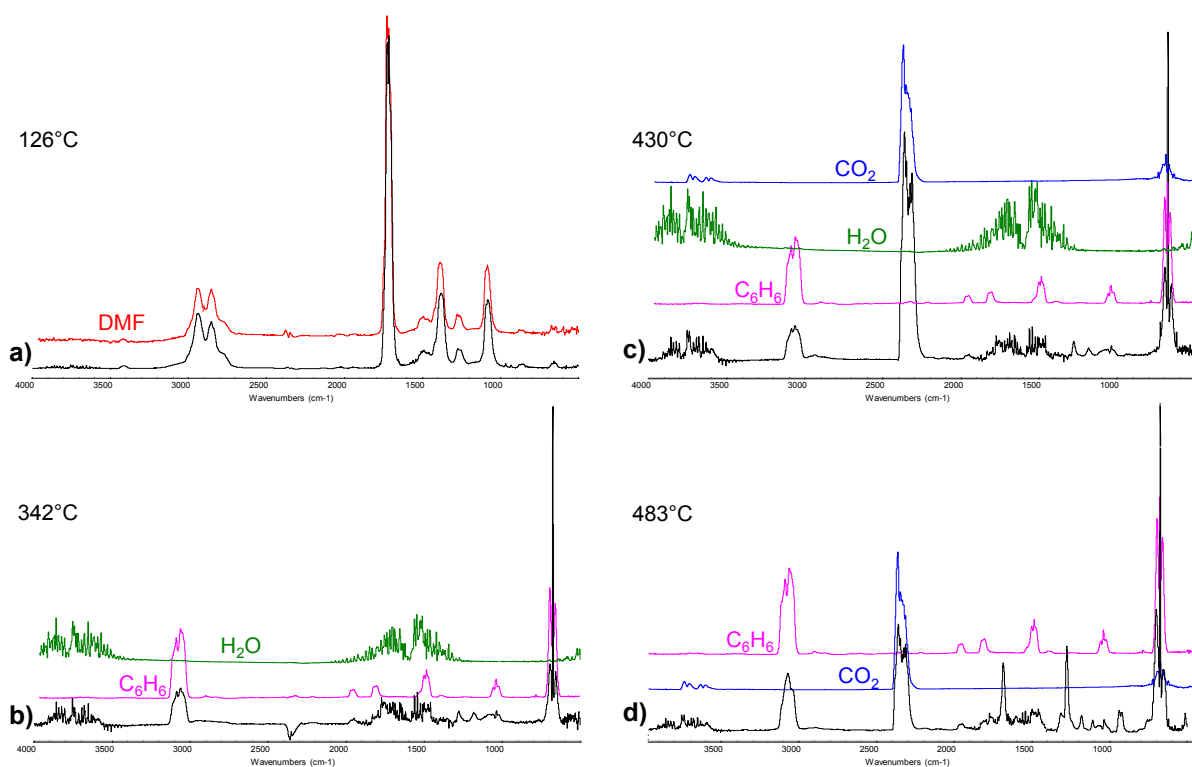
**Figure S6.** Field dependence of magnetization for **1** at 2.0, 3.0, 4.0 and 5.0 K. The solid lines correspond to the simulation according to the Hamiltonians given in eq. (1 main text ) with  $J_a = -0.65 \text{ cm}^{-1}$ ;  $J_b = -1.3 \text{ cm}^{-1}$ ;  $g = 1.98$ .



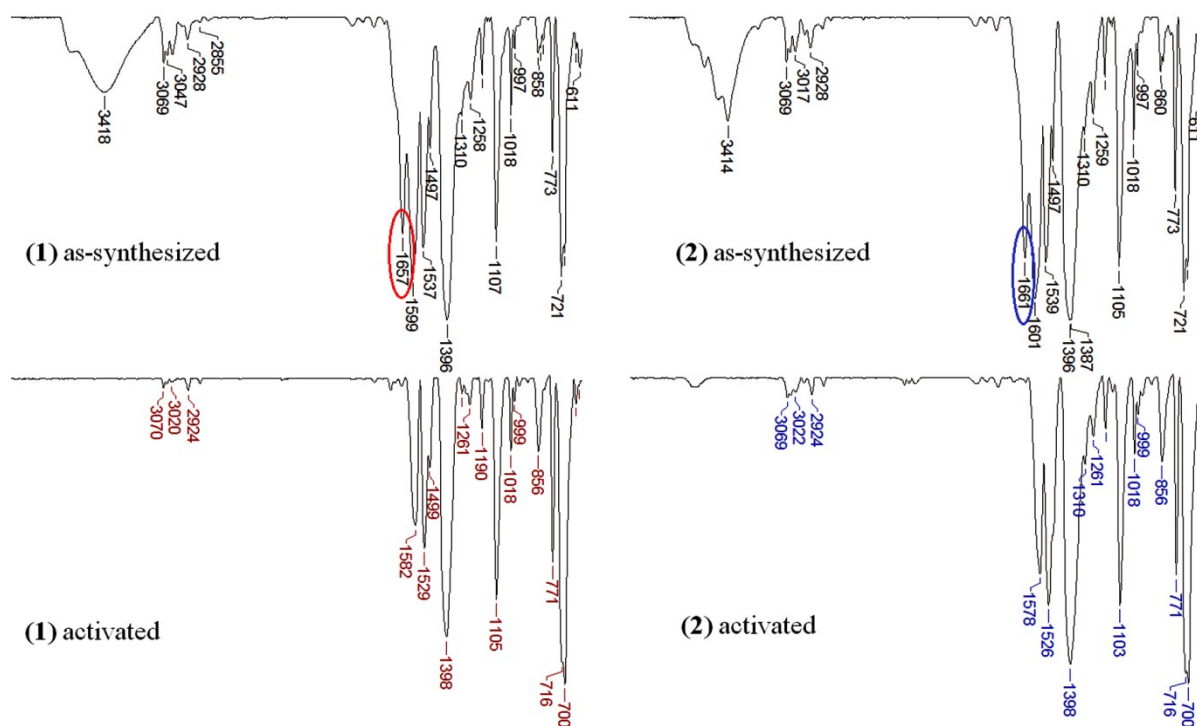
**Figure S7.** Simultaneous field dependence of magnetization for **2** at temperature indicated in legend. The solid lines correspond to simulation according the Brillouin function with  $S=5/2$ ;  $g = 2.0$



**Figure S8.** FTIR spectra of the gases evolved during the heating of **2** and comparison with model compounds spectra.



**Figure S9.** Selected FTIR spectra of the gases evolved during the heating of **1** at indicated temperature.



**Figure S10.** IR spectra of compounds **1** and **2** before and after heating activation.

**Table S1.** Theoretically estimated void volume values of the crystalline compounds accessible to different guests molecules after removal of disordered crystallization solvents by activation process

<b>Guest compound (R, Å)</b>	<b>Contact surface area</b>				<b>Solvent accessible surface</b>			
	<b>% of unit cell volume</b>		<b>Void volume (Å<sup>3</sup>)</b>		<b>% of unit cell volume</b>		<b>Void volume (Å<sup>3</sup>)</b>	
	<b>1</b>	<b>2</b>	<b>1</b>	<b>2</b>	<b>1</b>	<b>2</b>	<b>1</b>	<b>2</b>
<b>Compound</b>								
N <sub>2</sub> (0.750)	35.7	36.4	1275.17	4654.59	18.0	19.5	642.67	2497.89
Ar (0.940)	31.1	31.8	1110.83	4063.19	12.8	14.6	457.43	1868.18
CO <sub>2</sub> (1.935)	17.9	19.2	640.97	2454.79	1.6	1.9	57.04	243.03