SUPPORTING INFORMATION

Enhanced gas-sorption properties of a high surface area, ultramicroporous magnesium formate

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Powder X-ray diffraction

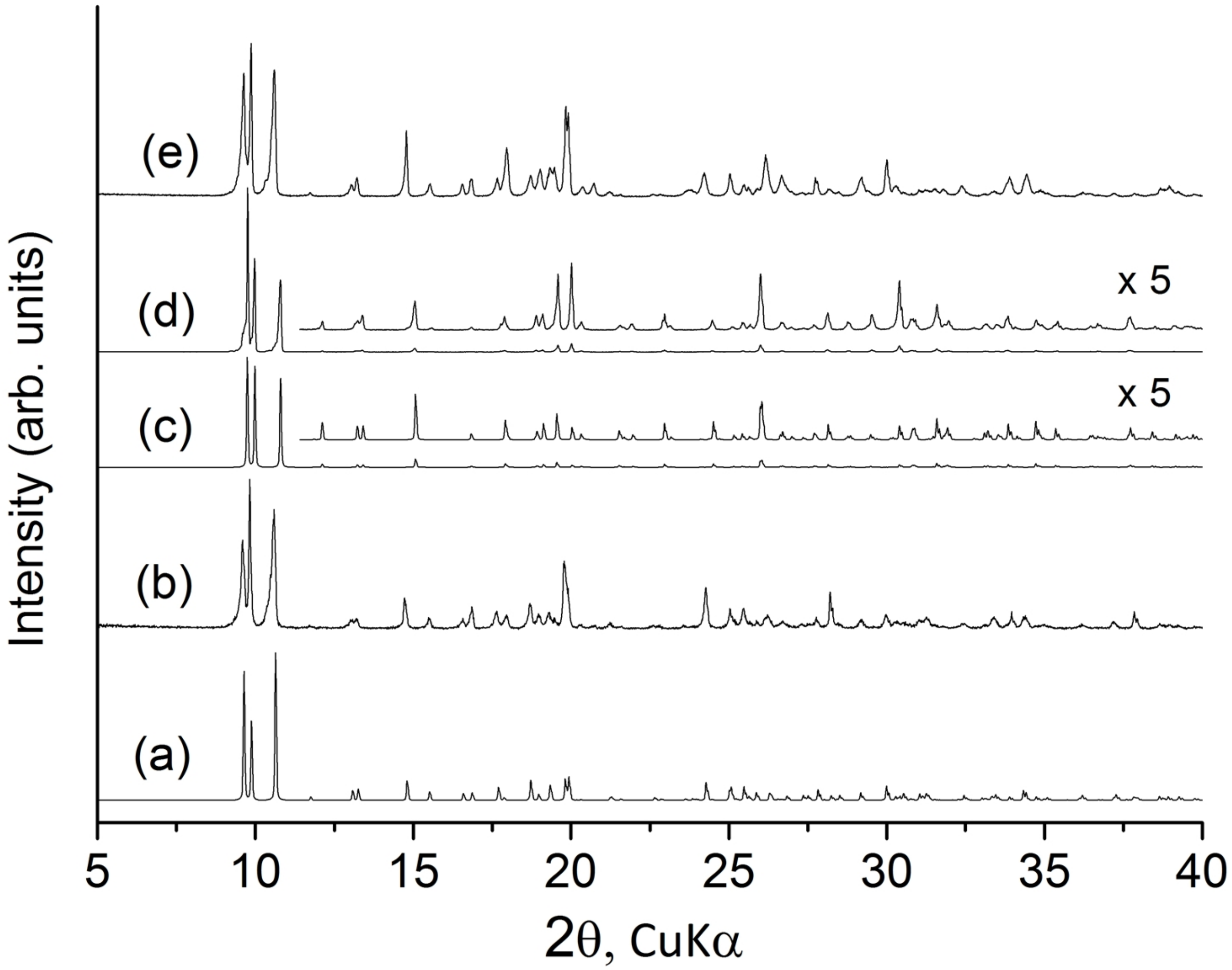

Figure S1. Calculated (a) and experimental powder X-ray diffraction pattern of the as-made material **1** (b). Calculated pxrd pattern of the evacuated solid **1’** (c) and the corresponding experimental pattern of **1’** after gas-sorption measurements, including NH_3 (d). The pxrd pattern of re-solvated solid **1’** with DMF (e). In this case the pxrd pattern was indexed using TREOR available within WinPLOTR[1] software and unit cell refinement was performed with the program CELREF.[2]

^{1}H NMR measurements

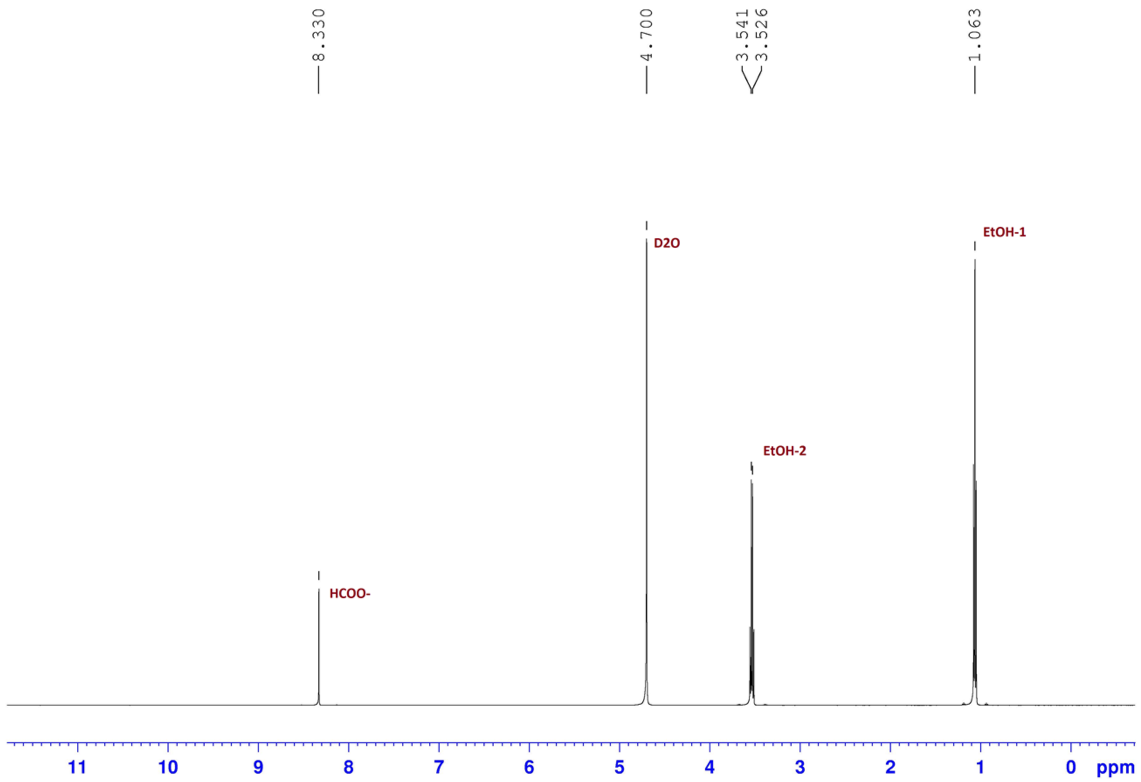

Figure S2. ^{1}H NMR spectrum of **1** after EtOH exchange and dissolving it in D_2O solution using HCl.

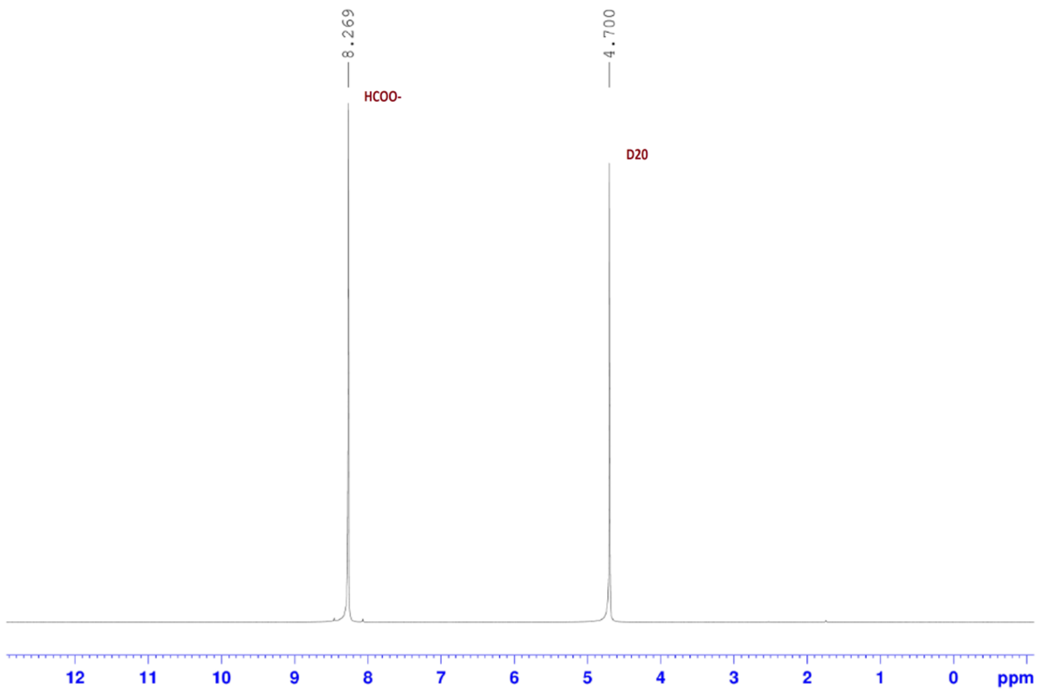

Figure S3. ^{1}H NMR spectrum of **1** after evacuating the sample at 240 ^{o}C and dissolving it in D_2O solution using HCl.

Thermal gravimetric analysis (TGA)

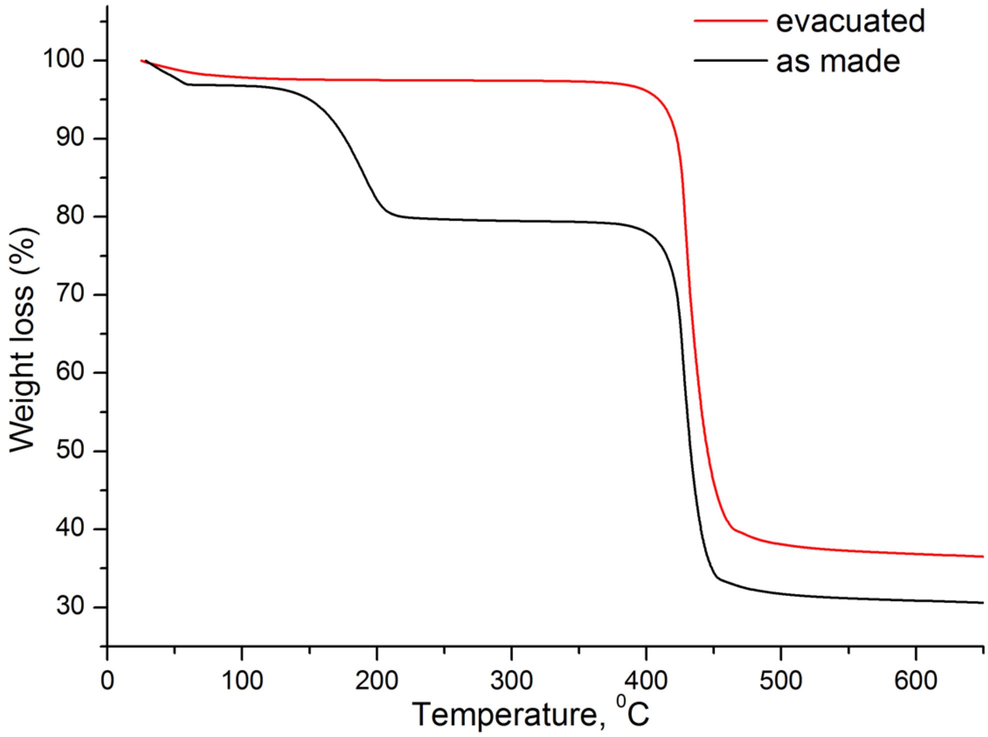

Figure S4. TGA curve for the as-made **1** and the corresponding evacuated solid **1'**, recorded under Ar flow with a heating rate of 5 deg/min.

Gas sorption measurements and analyses

Determination of BET surface area and pore size distribution using NLDFT

The apparent BET surface area in **1'** was determined using constancy criteria which requires that not only the quantity of C must be positive but also the application of BET equation should be limited to the pressure range where the term $V(1-(P/P_o))$ continuously increases as a function of P/P_o (V is the amount adsorbed in $cm^3\ g^{-1}$). This procedure is the proper method for BET surface area calculations in MOFs[3] and is recommended in a very recent standard of the International Standard Organization (ISO).[4]

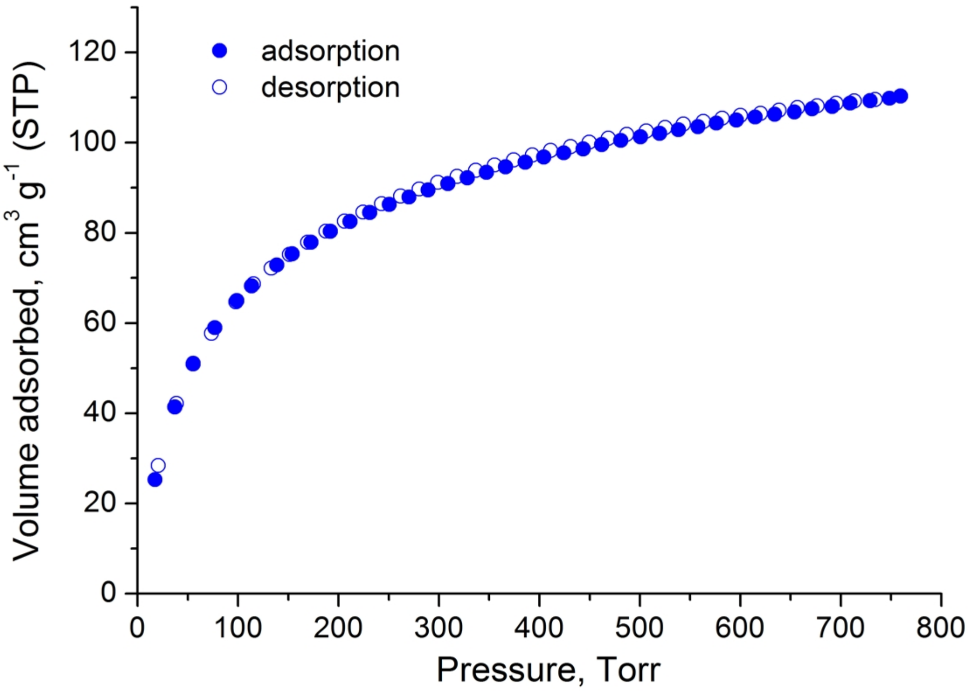

Figure S5. Hydrogen sorption isotherm of **1’** recorded at 77 K.

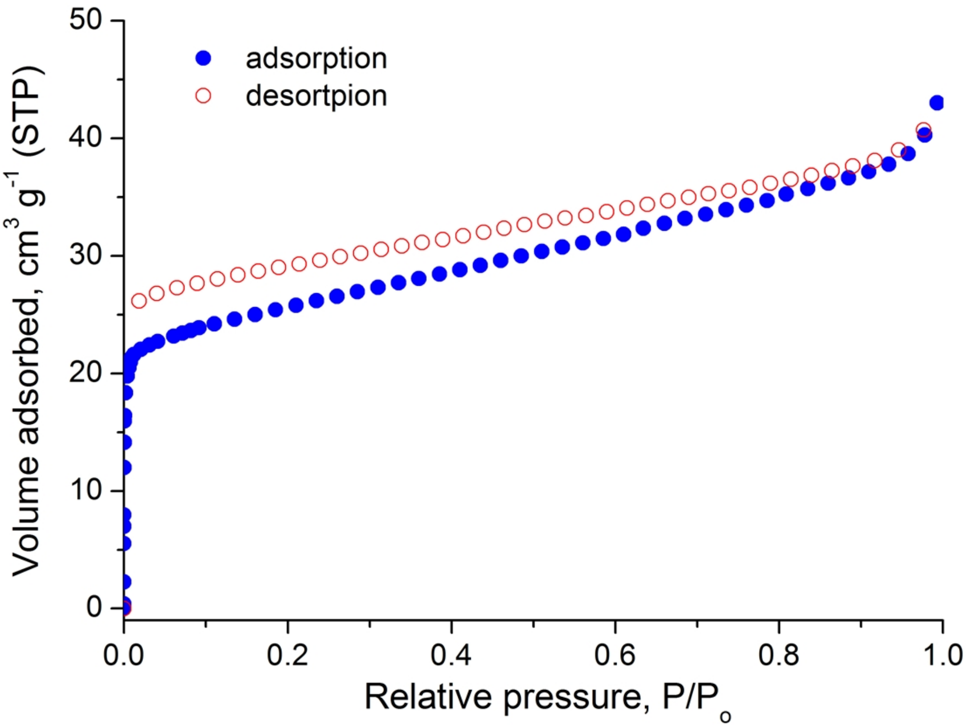

Figure S6. Argon sorption isotherm of **1’** recorded at 87 K, immediately after the hydrogen sorption at 77 K shown above.

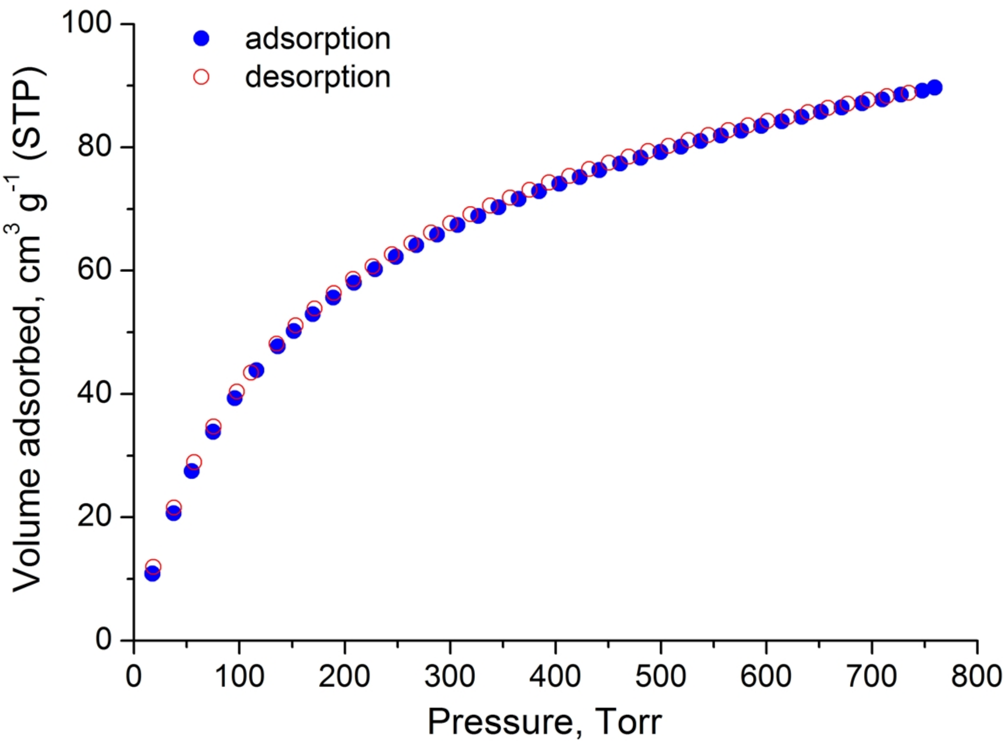

Figure S7. Hydrogen sorption isotherm of **1’** recorded at 87 K.

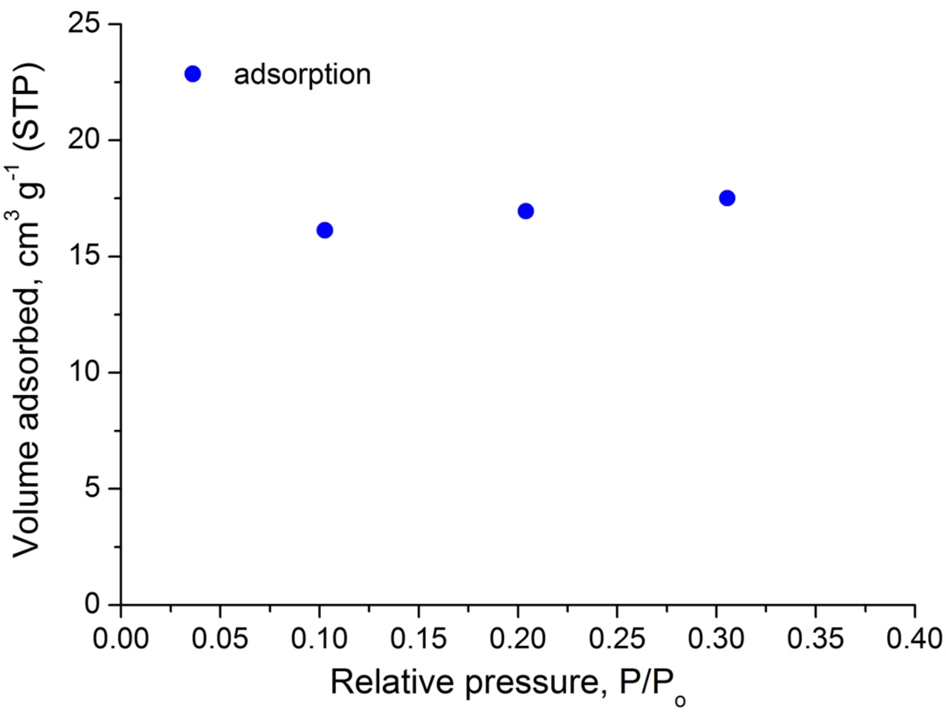

Figure S8. Three (3) point BET, N_2 sorption measurement at 77 K of **1’** after the hydrogen sorption at 87 K shown above.

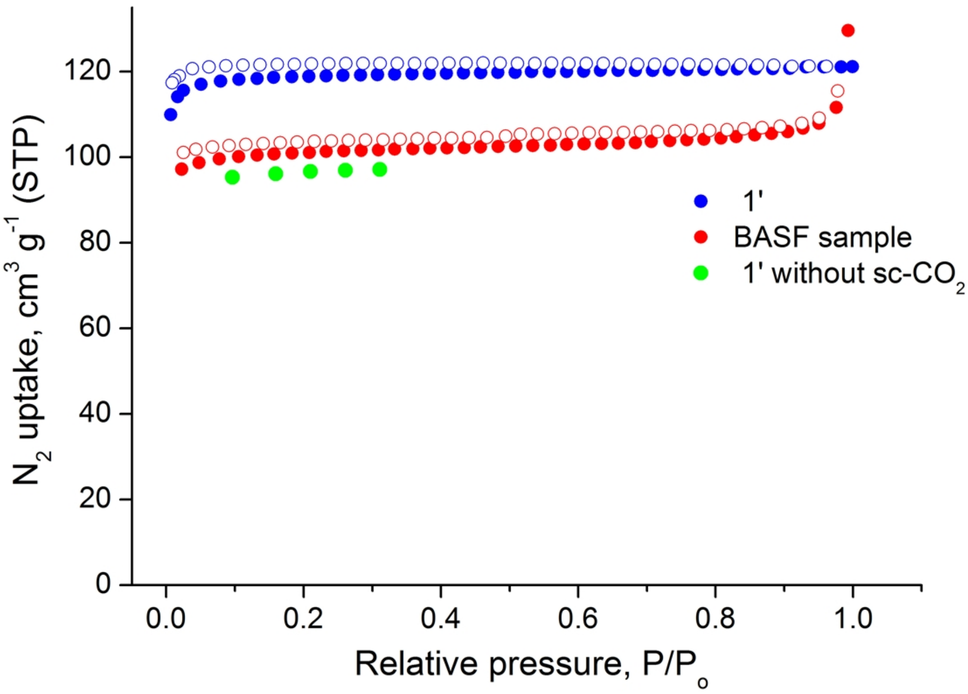

Figure S9. Nitrogen sorption isotherm at 77 K of **1'**, the BASF magnesium formate sample and **1'** prepared by heating an EtOH exchanged **1** to 240 °C overnight (5 point BET measurement).

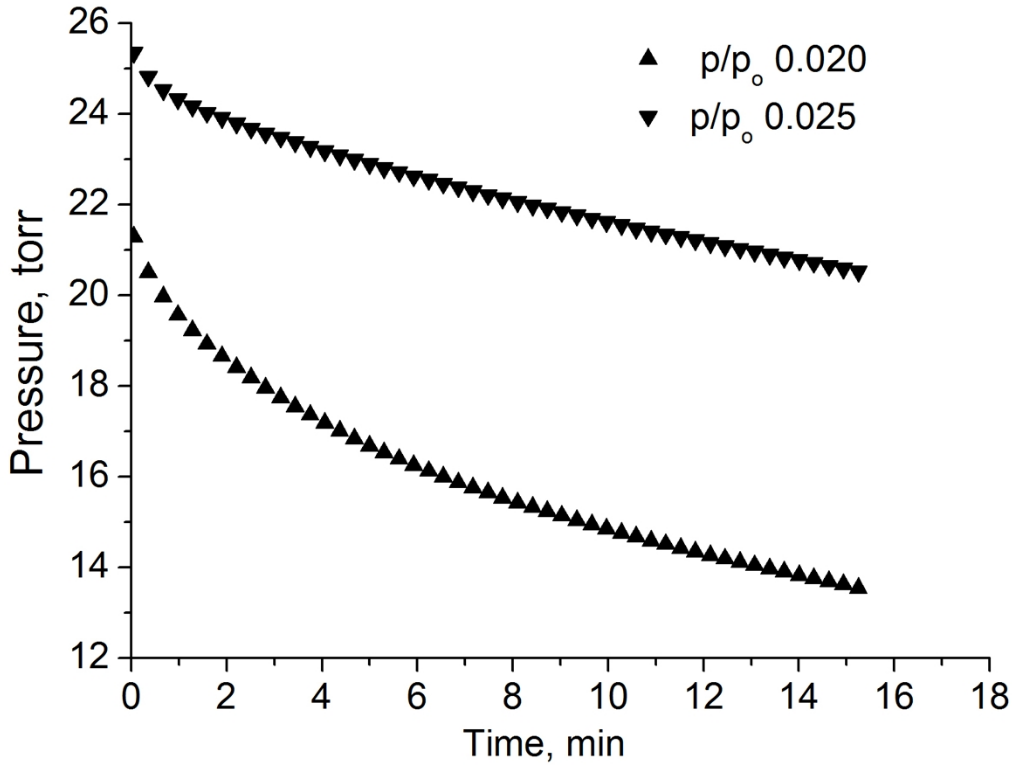

Figure S10. Nitrogen kinetic adsorption data of **1'** at 77 K for the indicated equilibrium points.

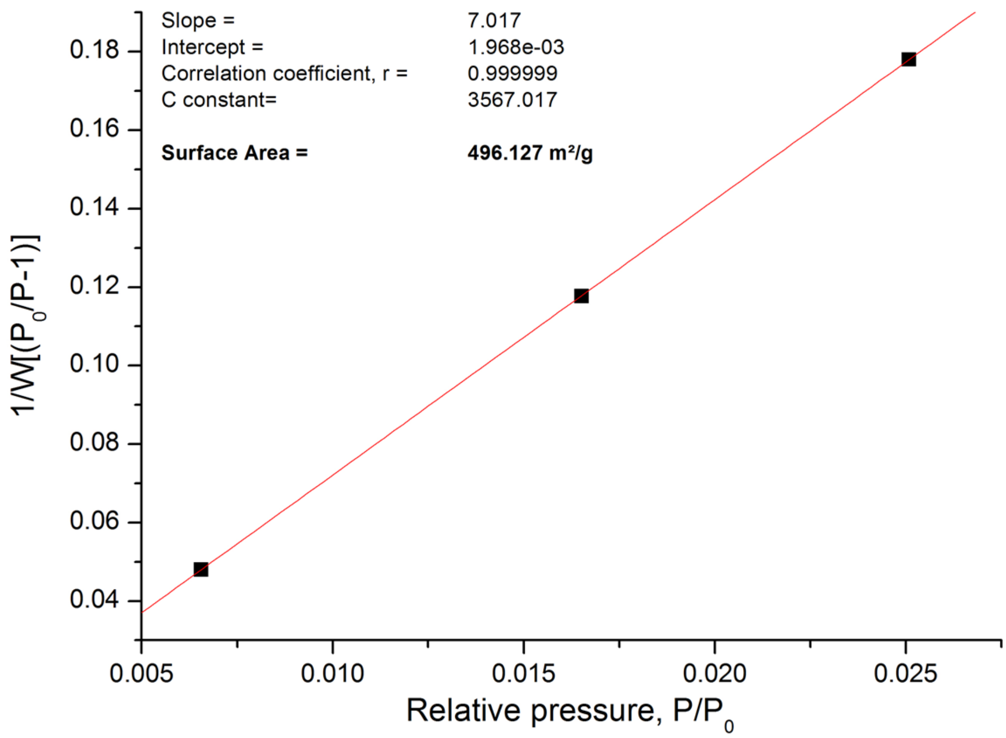

Figure S11. BET plot for **1'** from N_2 adsorption isotherm.

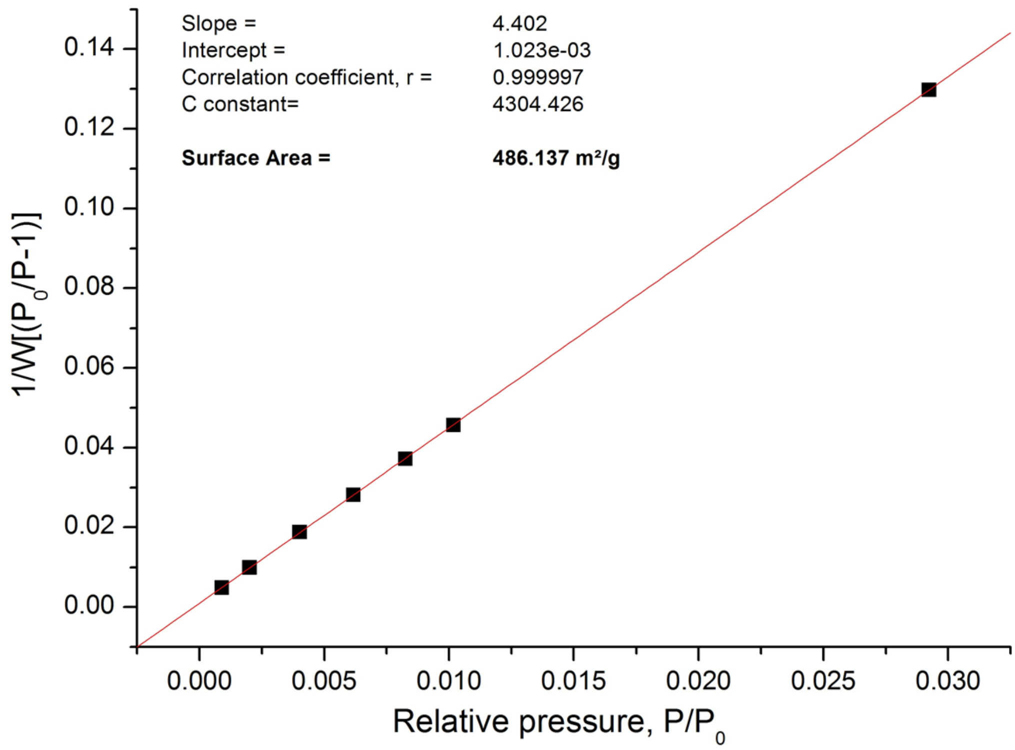

Figure S12. BET plot for **1'** from Ar adsorption isotherm.

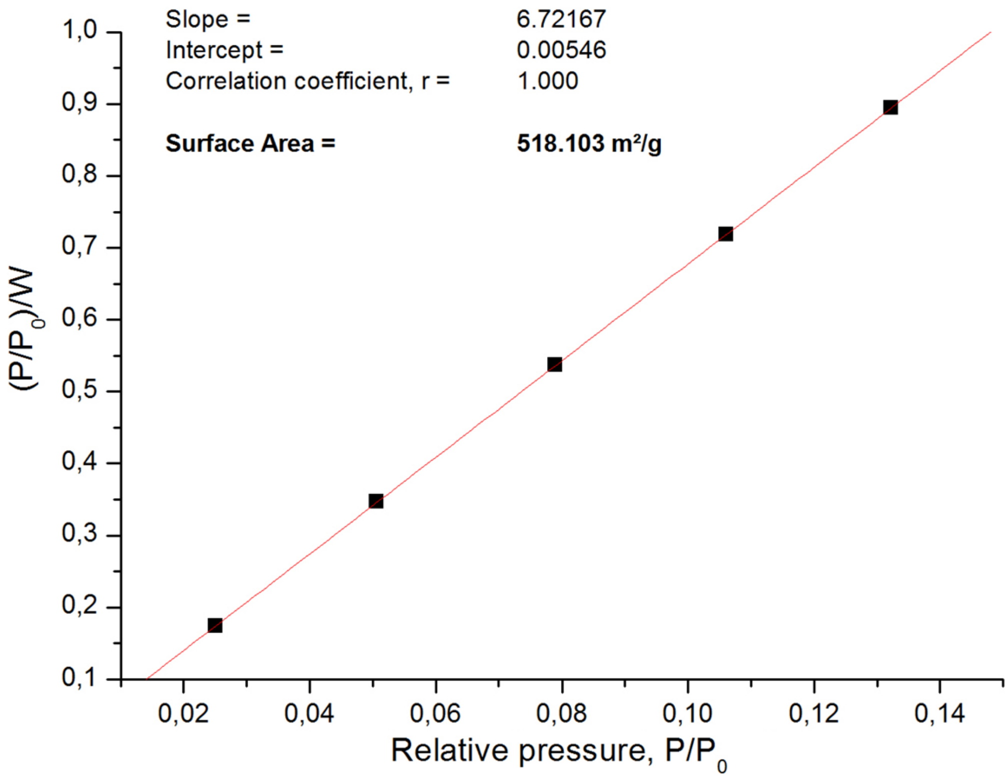

Figure S13. Langmuir plot for **1’** from N_2 adsorption isotherm.

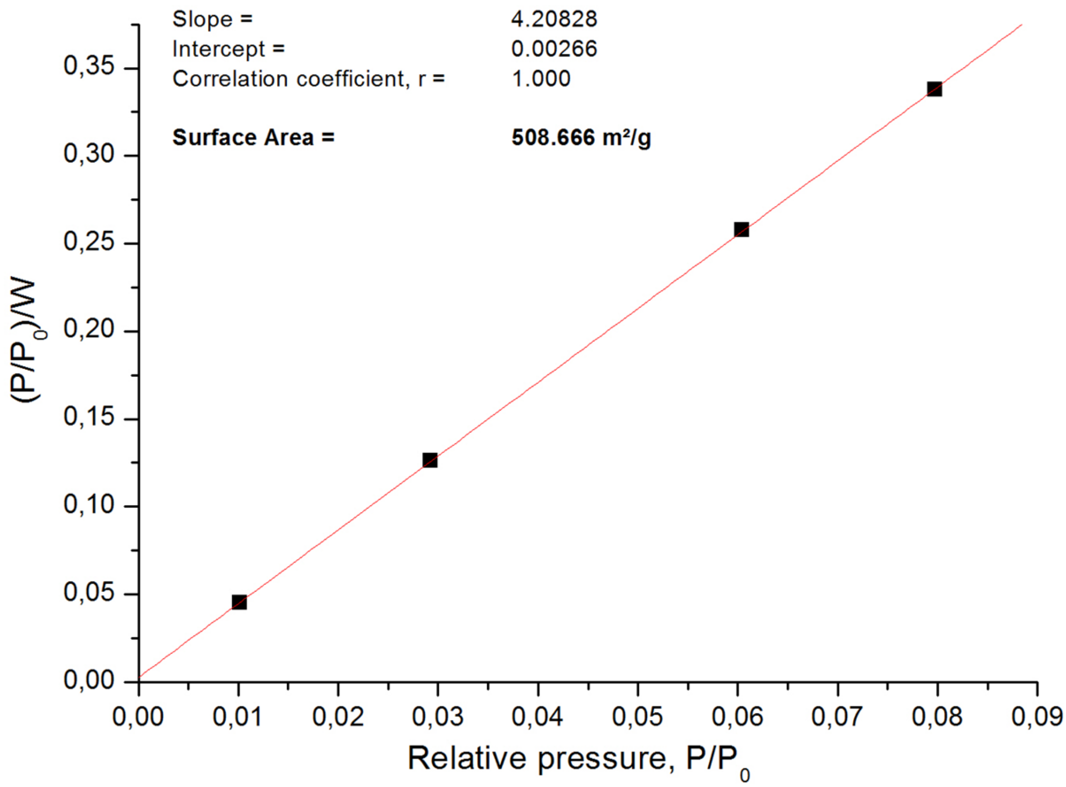

Figure S14. Langmuir plot for **1’** from Ar adsorption isotherm.

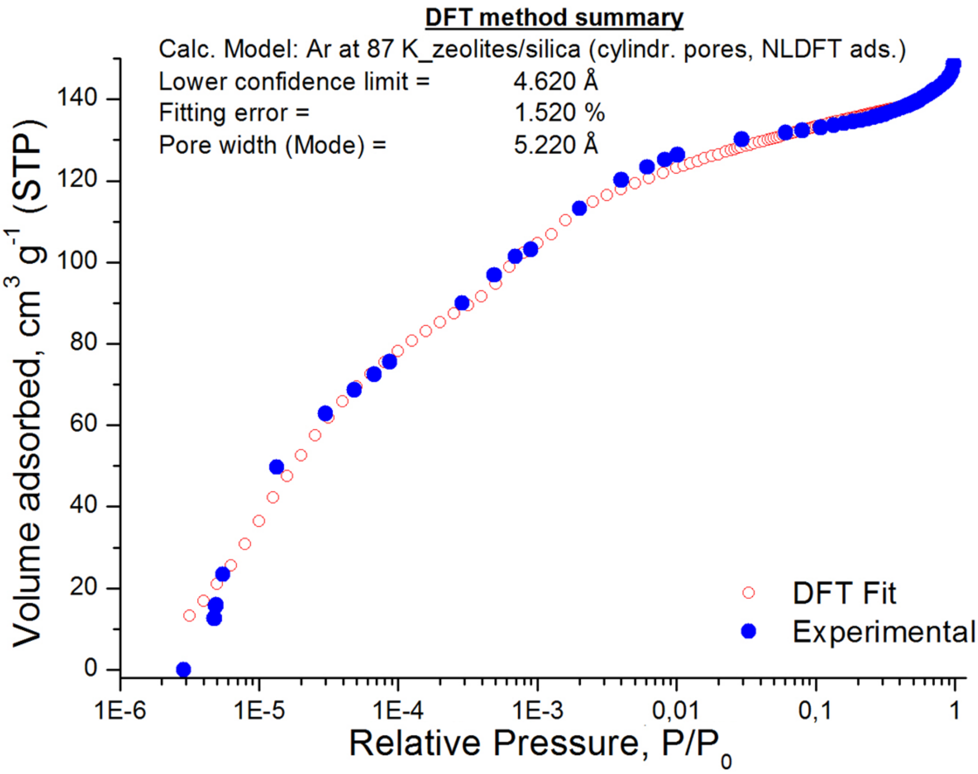

Figure S15. Argon adsorption isotherm of **1’** recorded at 87 K and the corresponding NLDFT fitting.

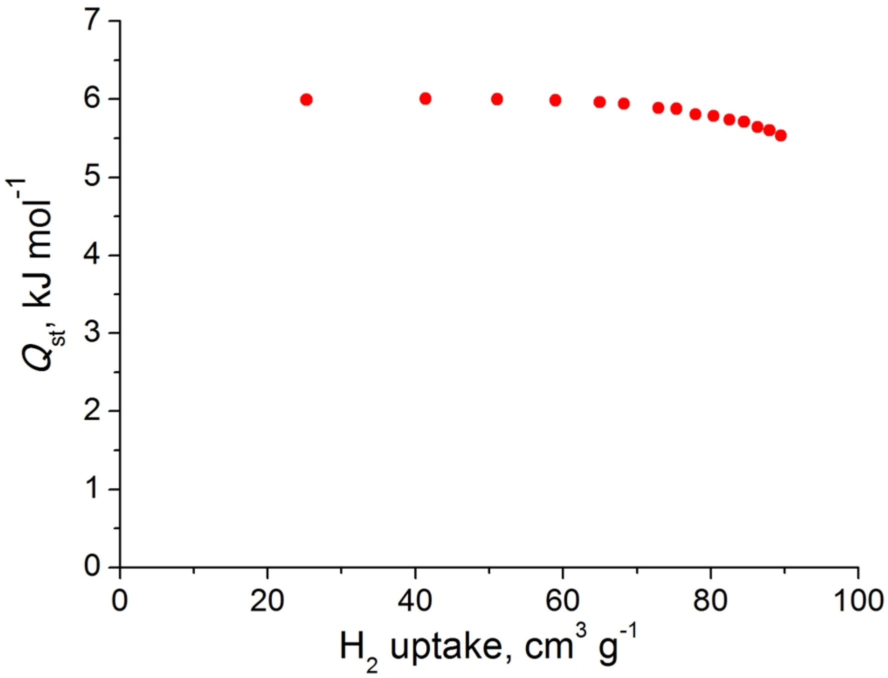

Figure S16. H_2 isosteric heat of adsorption in **1’** as a function of surface coverage.

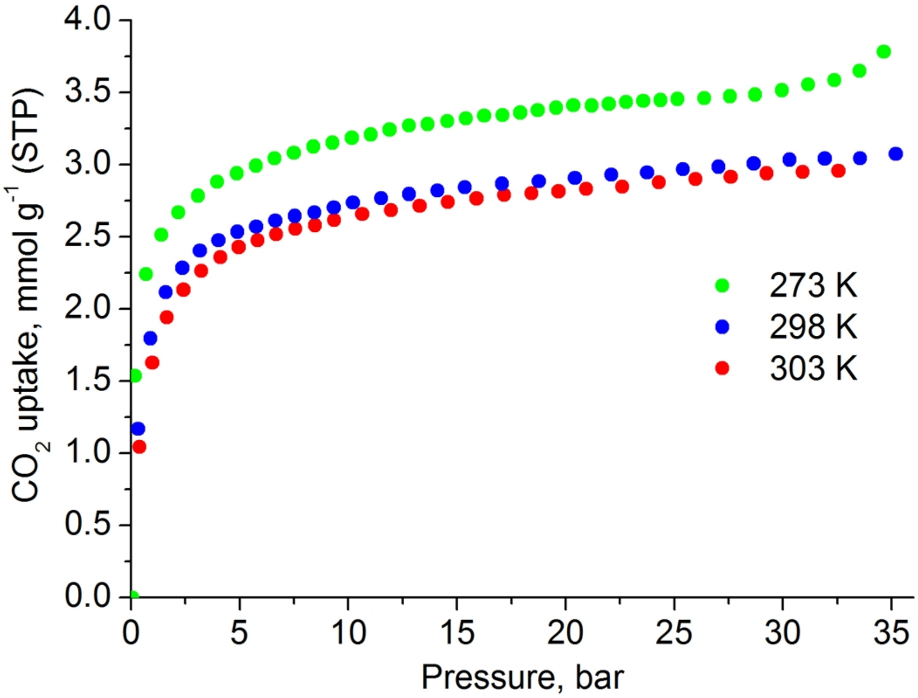

Figure S17. High pressure CO_2 adsorption isotherms of **1’** at the indicated temperatures.

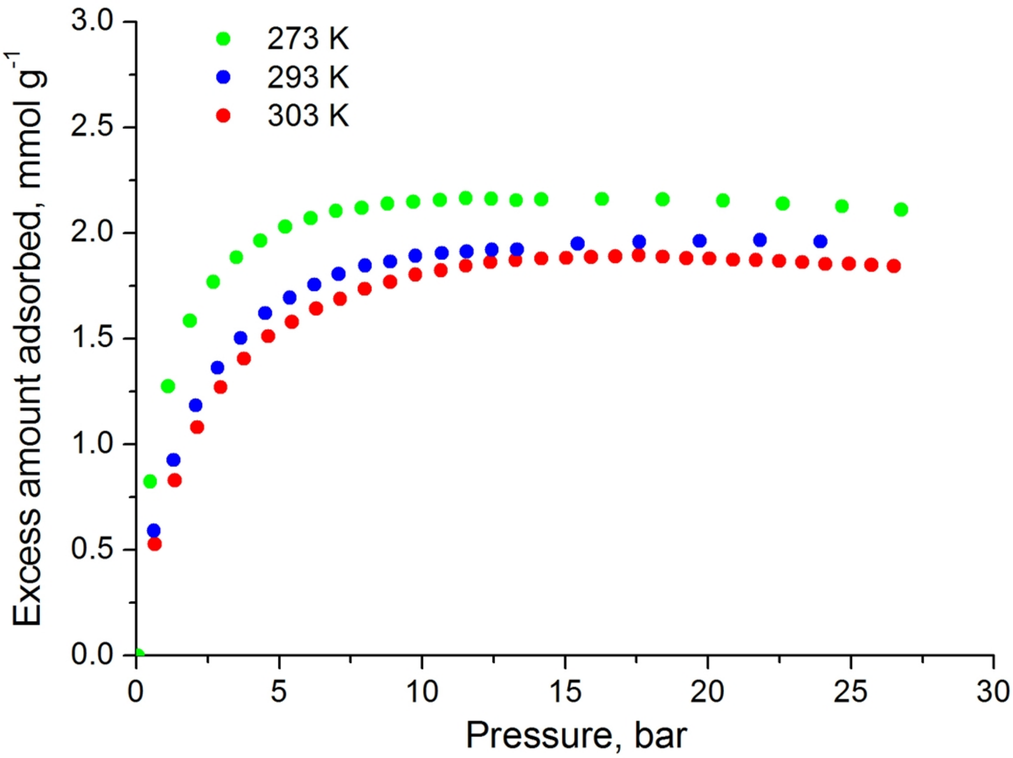

Figure S18. High pressure excess CH_4 adsorption isotherms of **1’** at the indicated temperatures.

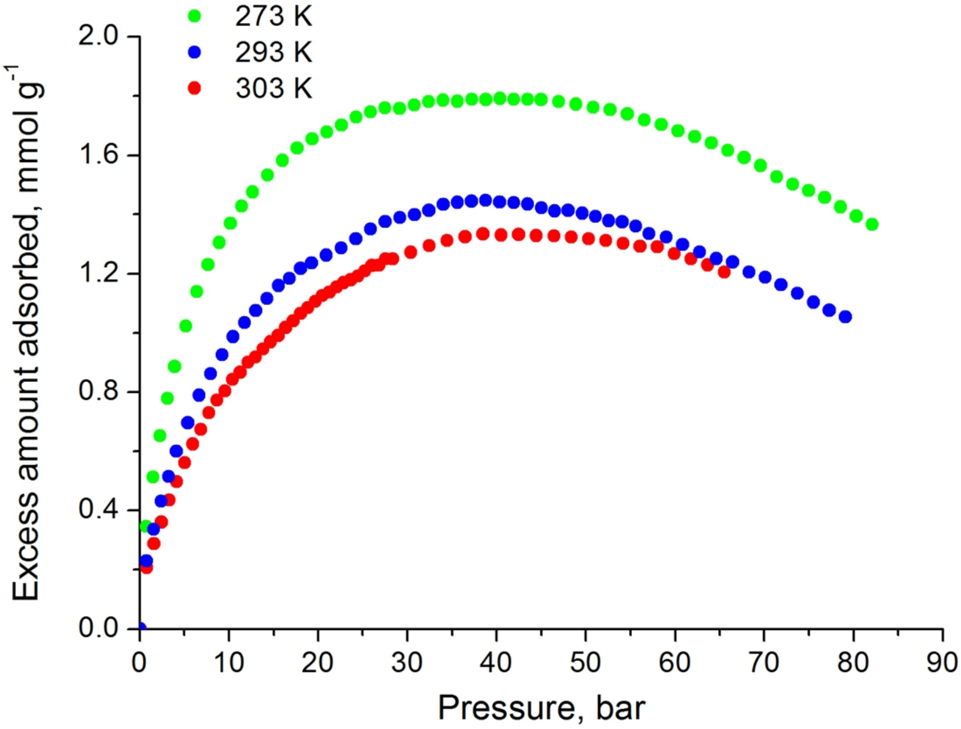

Figure S19. High pressure excess N_2 adsorption isotherms of **1’** at the indicated temperatures.

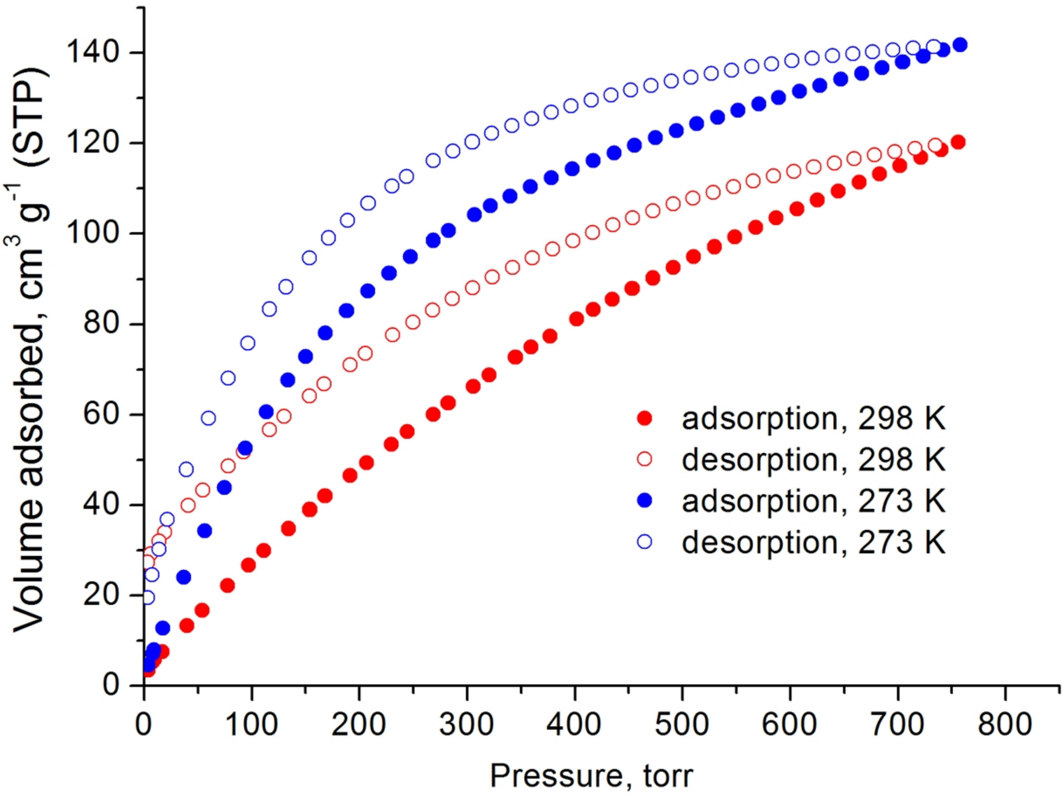

Figure S20. Ammonia sorption isotherms of **1’** at 298 K and 273 K up to 1 bar. Before each measurement the sample was reactivated at 240 °C overnight.

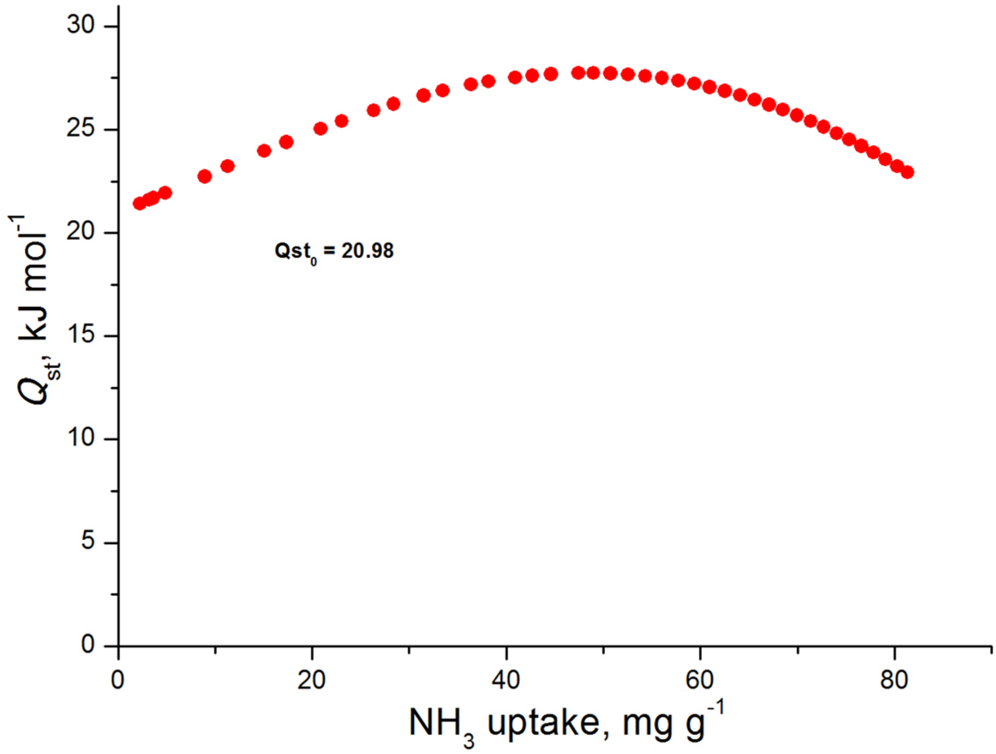

Figure S21. NH_3 isosteric heat of adsorption in **1'** as a function of surface coverage.

References

[1] Roisnel, T. and Rodríguez-Carvajal, J., "WinPLOTR: a windows tool for powder diffraction pattern analysis," *Materials Science Forum*, **2001,** *378–381*, 118–123.

[2] LMGP-Suite Suite of Programs for the interpretation of X-ray Experiments, by Jean laugier and Bernard Bochu, ENSP/Laboratoire des Matériaux et du Génie Physique, BP 46. 38042 Saint Martin d'Hères, France. WWW: *http://www.inpg.fr/LMGP and* [http://www.ccp14.ac.uk/tutorial/lmgp/.](http://www.ccp14.ac.uk/tutorial/lmgp/)

[3] J. Moellmer, E. B. Celer, R. Luebke, A. J. Cairns, R. Staudt, M. Eddaoudi, M. Thommes, *Micropor. Mesopor. Mater,* 2010, **129**, 345.

[4] ISO-FDIS 9277:2010.