

Microporous volumes from nitrogen adsorption at 77 K: when to use a different standard isotherm?

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Supporting Information

S1 Method for the preparation of the char and the activated carbons

A mixture of industrial crude glycerin (82% glycerol, from a Portuguese company) and sulfuric acid (95-97%, Sigma-Aldrich) was prepared using a volume ratio (1:0.5). The flask was stirred at room temperature until foaming ceased, typically for ~30 minutes adapting the procedure described elsewhere [1]. Then, the mixture was transferred to an autoclave (Teflon-lined, stainless-steel) and the acid carbonization was made at 180 °C for 6 h in an oven (Medline Sci. Ltd., mod. ON-02G). The acid glycerin-*char* was washed (distilled water until pH 7) and dried at 100 °C. The obtained solid was crushed to a fine powder (dimensions < 0.297 mm). The glycerin-*char* (1 g) was mixed with the adequate KOH amount dissolved ~ 10 cm³ of distilled water, followed by stirring for 2 h at ambient temperature, and then dried at 100 °C until complete water evaporation. The samples were activated at 700 °C and KOH:char weight ratios were 1:1 (for the material C2) and 2:1 for the material C1. The mixture was activated in a horizontal furnace (Thermolyne, model 21100) under N₂ flow (5 cm³ s⁻¹). The temperature was raised (10 °C min⁻¹) up to the activation temperature and kept for 1 h. After the chemical activation process, post-chemical activation was required to remove excess activating agent from the activated carbons. The glycerin-*activated carbons* were treated with HCl solution (1M), then washed with distilled water until pH 7, and dried at 100 °C to allow the evaporation of the excess water. The sample C3 was a commercial sample from Norit.

S2. Mathematical expressions for the various standard isotherms

For the universal *t-curve* the expression from Lippens and de Boer [2] was used:

$$t/\text{\AA} = \left[\frac{13.99}{0.034 - \log(p/p^0)} \right]^{0.5}$$

For the hydroxylated silica [3], the carbon [4] and the char, all used in the form of α_s -

plots, a polynomial equation of the type $\alpha_s = A_0 + A_1 (p/p^0) + A_2 (p/p^0)^2 + A_3$

$(p/p^0)^3 \dots$ was employed and the coefficients A0 to A9 are given in Table S1.

Table S1 Coefficients of the polynomial equations that relate α_s and the relative pressure (p/p^0) for the standard isotherms on the hydroxylated silica, the carbon and the char

	carbon	hydroxylated silica	char
A0	0.4964302	0.27692439	0.9646
A1	4.2880233	13.403724	-7.4791
A2	-47.262408	-204.06097	74.791
A3	338.6696	1728.6363	-291.64
A4	-1432.0171	-8338.4277	552.03
A5	3854.6654	24215.106	-504.31
A6	-6681.7747	-43107.078	178.56
A7	7192.6002	46012.132	
A8	-4345.2612	-27015.265	
A9	1119.5957	6705.4599	

S3. Pore size distributions

The pore size distributions were obtained from the nitrogen adsorption isotherms at 77 K by NLDFT (non local density functional theory) model provided by NovaWin version 10.0 software.

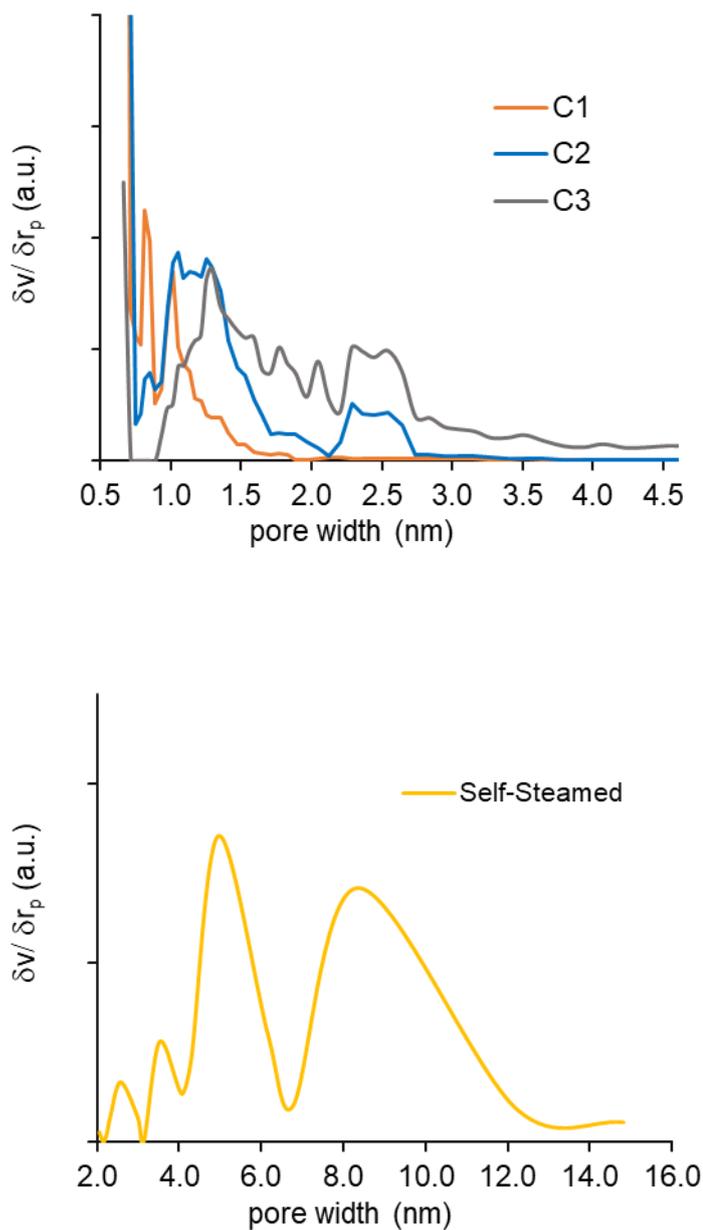
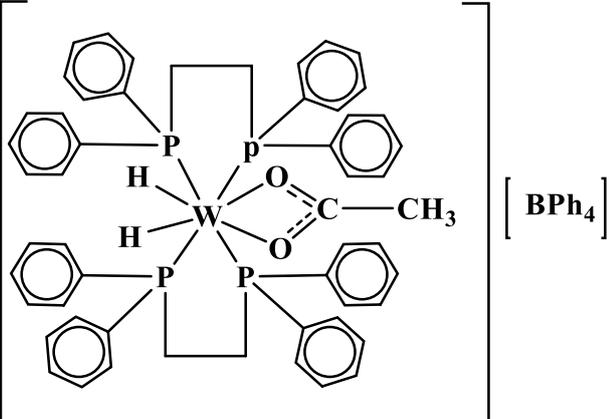
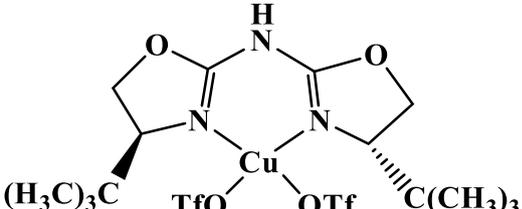
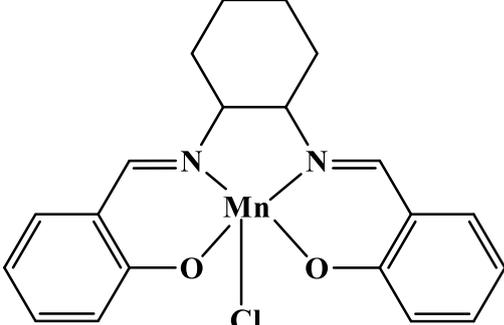
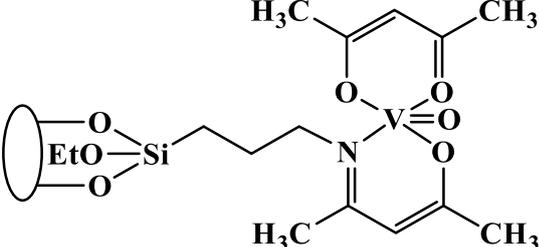


Figure S1. Pore size distributions for the carbon materials (C1, C2 and C3) and for the dealuminated Y zeolite (Self Steamed).

S4. Structures of the metallic complexes supported in different materials.

Complex	Structure	Reference
Comp1		[5]
Comp2		[6]
Comp3		[7]
Comp4		[8]

S5. Network-accessible geometric volume.

Table S2. Network-accessible geometric volume (in cm³g⁻¹) obtained with PoreBlazer [9] for the zeolites and MOFs studied in this work.

Zeolites	NaY	0.362
	Mordenite	0.241
	ETS-10	0.166
MOFs	CuBTC	0.794
	UiO-66	0.426
	MIL-53(Al)	0.527
	MIL-101	1.815

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