SUPPLEMENTARY MATERIALS

MIL-96, a porous aluminum trimesate 3-D structure constructed from a hexagonal network of 18-rings and μ_3-oxo centered trinuclear units.

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Table A. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for MIL-96 (Al).
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Al(1)	745(1)	1490(1)	2500	12(1)
Al(2)	1693(1)	5846(1)	4166(1)	14(1)
Al(3)	0	5000	5000	12(1)
Al(4)	2676(1)	7324(1)	3345(1)	8(1)
O(1)	0	0	2500	12(1)
O(2)	1342(2)	5671(1)	4743(1)	13(1)
O(3)	2717(1)	7283(1)	4247(1)	20(1)
O(4)	1536(2)	3071(3)	2500	27(1)
O(5)	1973(3)	5986(2)	3569(1)	62(1)
O(6)	-489(2)	3831(2)	4624(1)	60(1)
O(7)	-87(2)	1645(2)	2937(1)	27(1)
O(8)	629(2)	4367(2)	4061(1)	27(1)
C(1)	-628(3)	2315(3)	3678(1)	33(1)
H(1)	33	2785	3548	40
C(2)	-1324(2)	1324(2)	3490(2)	30(1)
C(3)	-908(3)	2611(3)	4057(1)	38(1)
C(4)	-1900(2)	1900(2)	4247(2)	43(2)
H(4)	-2090	2090	4505	51
C(5)	-996(2)	996(2)	3090(1)	20(1)
C(6)	-189(3)	3678(3)	4263(1)	35(1)
OW	3333	6667	5252(3)	76(3)
O(11)	2116(4)	7884(4)	3306(3)	31(2)
O(12)	2925(4)	7075(4)	2935(3)	36(3)
O(13)	2412(5)	7588(5)	3007(4)	53(3)

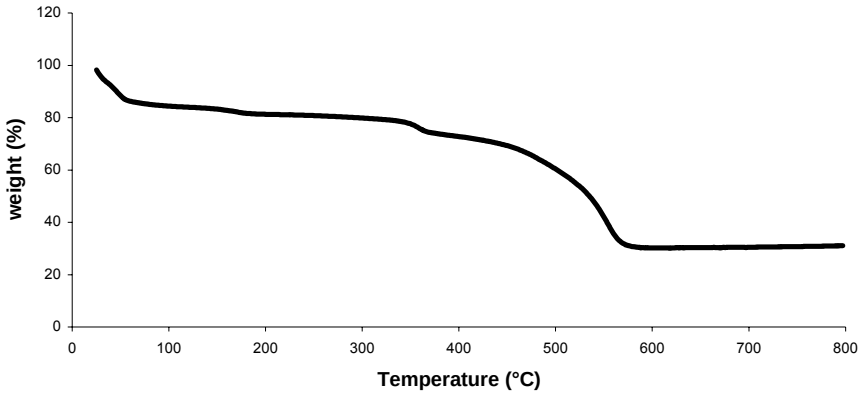

Figure a: TG curve of MIL-96 (Al) under O_2, *2°C/min*.

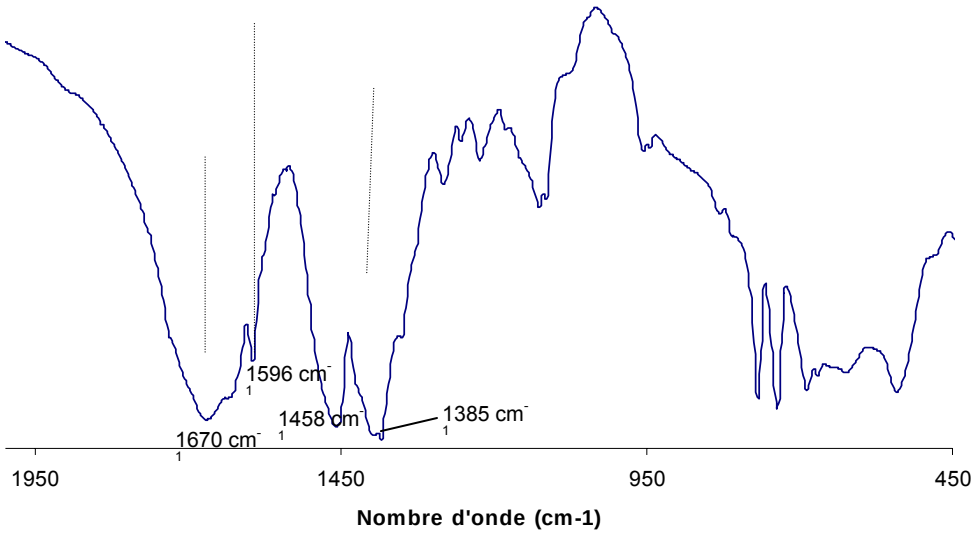

Figure b: IR spectrum of MIL-96 (Al)

IR spectroscopy. The IR spectrum was recorded on a Nicolet 550 FTIR spectrometer at room temperature in the range 400-2000 cm^{-1}, using a potassium bromide pellet. The IR spectrum of $Al_{12}O(OH)_{18}(H_2O)_3(Al_2(OH)_4)[btc]_6 \cdot 24H_2O$ shows the vibrational bands in the usual range 1400-1600 cm^{-1} for the carboxylic function. Strong absorption bands, located at 1596 and 1610 cm^{-1} and between 1458 and 1385 cm^{-1} are assigned to bound C-O group, ν_{asym} and ν_{sym}, respectively, indicating that the *btc* species is coordinated to the aluminum atoms. The absence of strong absorption bands in the area 1710-1740 cm^{-1} confirms the fully deprotonation of the *btc* moiety, in agreement with the single-crystal XRD analysis.

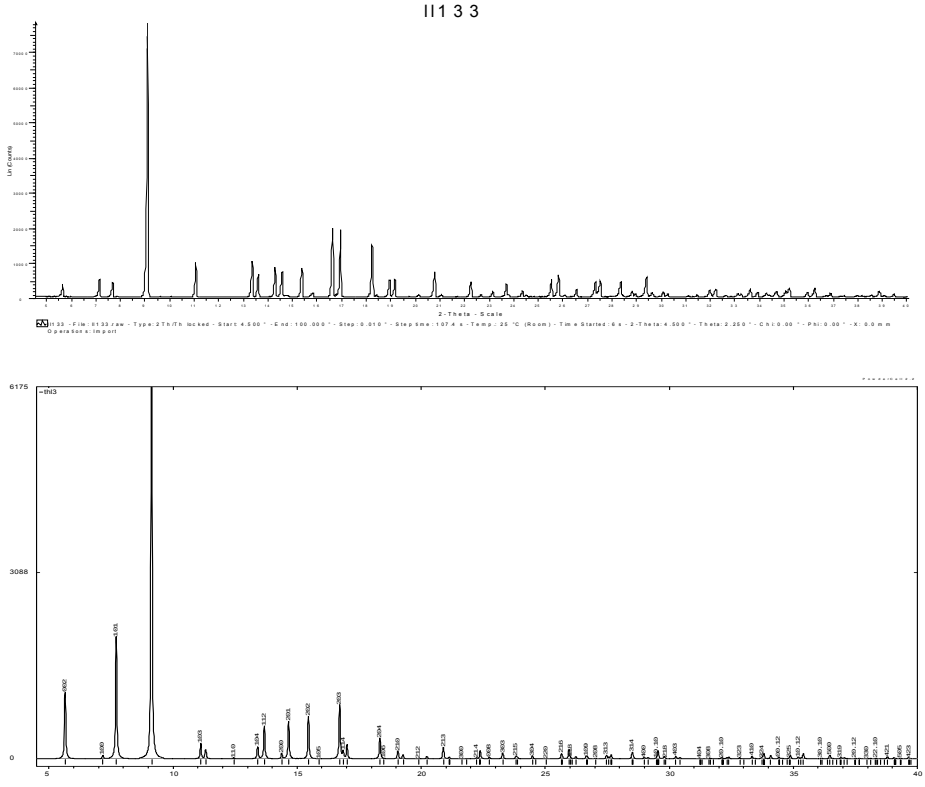

Figure c: Experimental (top) and simulated (bottom) of powder X-ray diffraction pattern (copper radiation) of MIL-96 (Al).

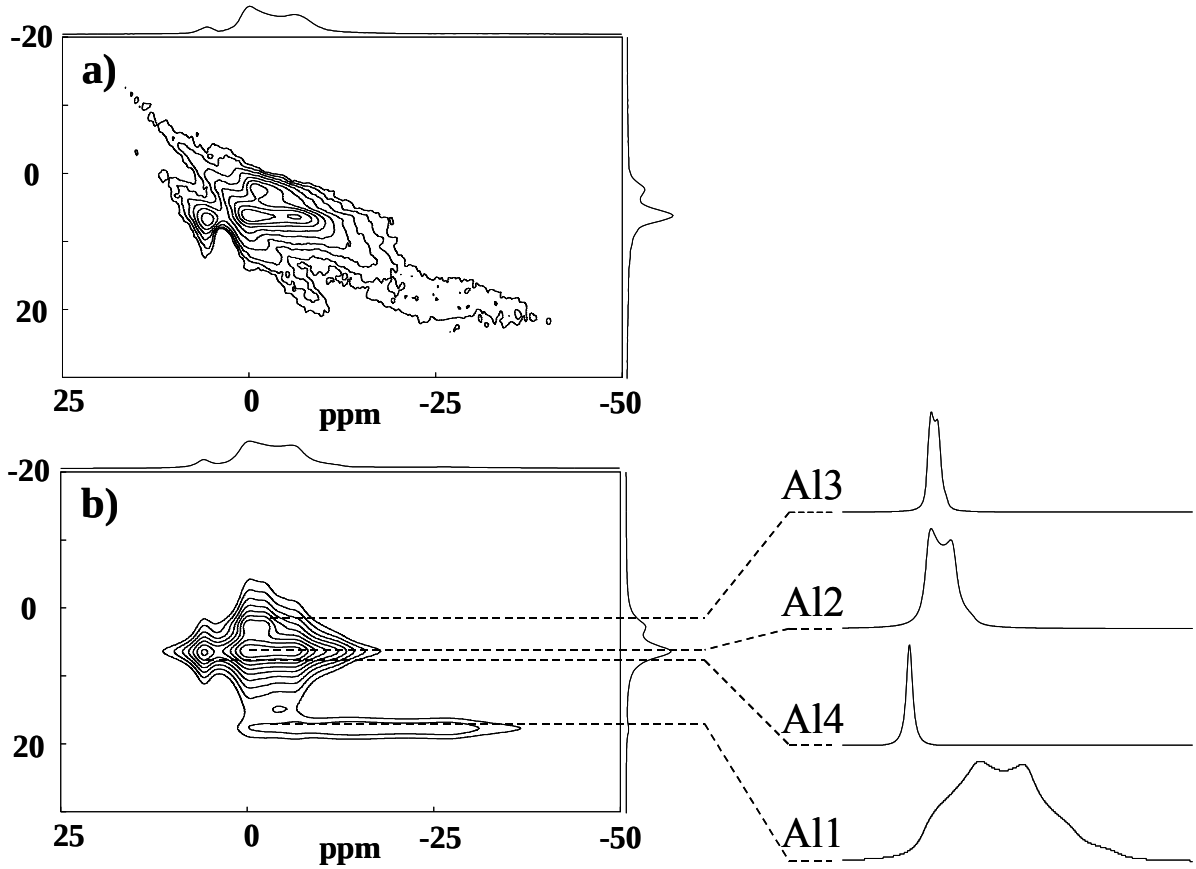

Figure d: Experimental (a) and simulated (b) 2D ^{27}Al 3QMAS-FAM-II NMR spectrum of $Al_{12}O(OH)_{18}(H_2O)_3(Al_2(OH)_4)[btc]_6 \cdot 24H_2O$ (MIL-96). The four components used in the simulation are shown in the right side of calculated spectrum.