Electronic Supplementary Material (ESI) for New Journal of Chemistry.

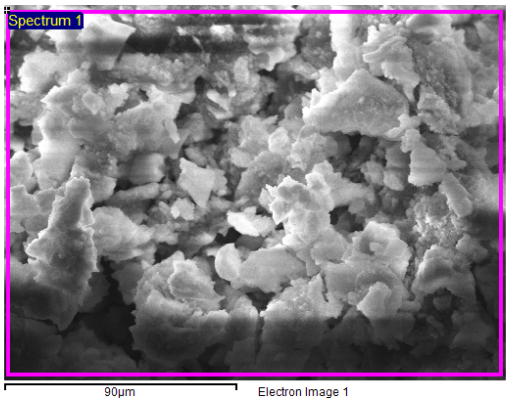
SUPPLEMENTARY SECTION

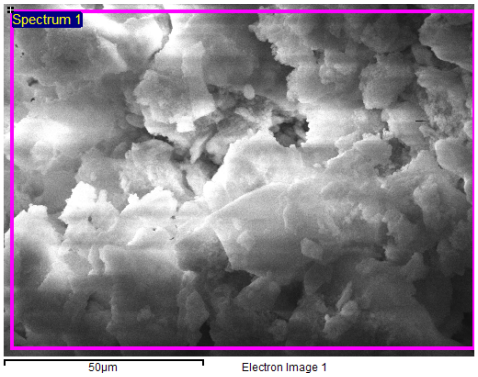
Spectrum processing :
Peak possibly omitted : 0.258 keV

Processing option : All elements analyzed (Normalised)
Number of iterations = 4

Standard :
O SiO2 1-Jun-1999 12:00 AM
Si SiO2 1-Jun-1999 12:00 AM

Element	Weight%	Atomic%
O K	55.71	68.83
Si K	44.29	31.17
Totals	100.00	





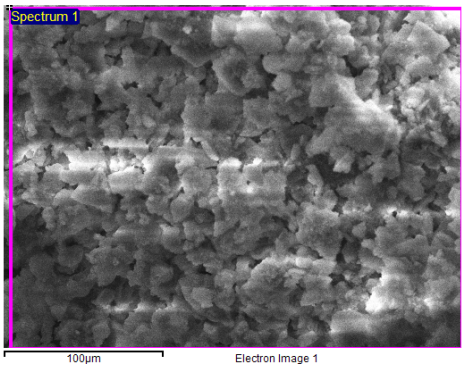


Figure S1. Output of SEM analysis on AHP-MCM41@ and images of different area of the sample.

Spectrum processing :
Peak possibly omitted : 0.259 keV

Processing option : All elements analyzed (Normalised)
Number of iterations = 4

Standard :
O SiO2 1-Jun-1999 12:00 AM
Si SiO2 1-Jun-1999 12:00 AM
Fe Fe 1-Jun-1999 12:00 AM

Element	Weight%	Atomic%
O K	52.94	66.70
Si K	45.75	32.83
Fe K	1.30	0.47
Totals	100.00	

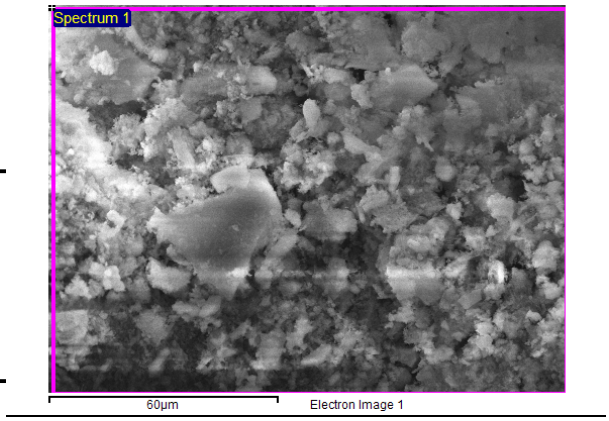


Figure S2. The output of SEM analysis on AHP-MCM41@ on a sample previously saturated with iron(III) (form solution at pH=2) and an image of one of them.

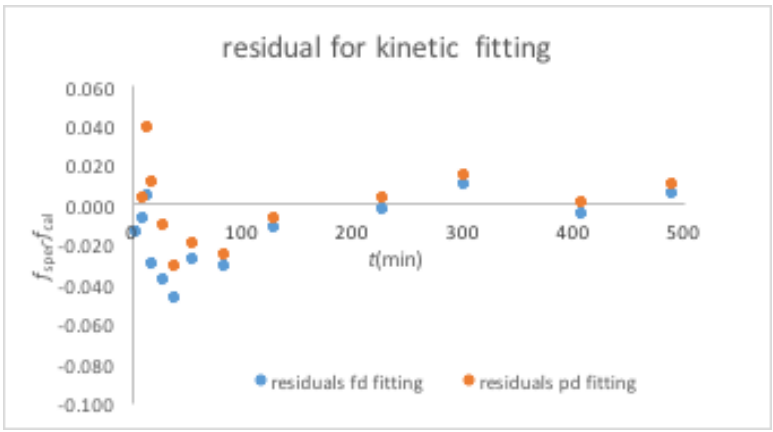


Figure 3S- Residuals (f_{sper}-f_{calc}) of the two fitting models as a function of time for the experimental points of figure 2.

Table 1S Reference values* employed for α_M calculation. See text for details.

	Log β	*p*	*n*	*m*
$FeOH^{2+}$	-2.19	-1	0	1
$Fe(OH)_2^{+}$	-5.67	-2	0	1
$Fe(OH)_3$	-12.56	-3	0	1
$Fe_2(OH)_2^{4+}$	-2.95	-2	0	2
$Fe_3(OH)_4^{5+}$	-6.3	-4	0	3
$Fe(OH)_3$(am)	-4.891	-3	0	1
$HEDTA^{3-}$	10.948	1	1	0
H_2EDTA^{2-}	17.221	2	1	0
H_3EDTA^{-}	20.359	3	1	0
H_4EDTA	22.583	4	1	0
H_5EDTA^{+}	24.083	5	1	0
H_6EDTA^{2+}	23.859	6	1	0
$Fe(EDTA)^{-}$	27.8	0	1	1
$Fe(EDTA)(OH)^{2-}$	19.97	-1	1	1
Fe(HEDTA)	29.3	1	1	1
$Fe_2(EDTA)_2(OH)_2^{4}$	41.8	-2	2	2

* For iron(III) hydrolysis, the selected values were found from Leslie Pettit and Gwyneth Pettit, SC-Database, Academic Software, extrapolating the most reliable literature values at I = 0. EDTA protonation and complexation constants are from Arthur E. Martell, Robert M. Smith - 1989 - Stability Constants, Chemical Society (London)

Complexation and protonation constant of the monomeric unit in solution

Experimental

Complex formation equilibria of AHP with Fe(III) were revisited[1S] since the published results were partial. Titrations were done in a thermostated glass cell, equipped with a magnetic stirrer, a DL 53 titrator, Mettler Toledo, with a combined DG 115-SC. Fe(III) complex formation constants were determined potentiometrically. Solutions were titrated with 0.1 M KOH at 25.0 °C, and 0.1 M KNO_3 ionic strength. The electrode was daily calibrated for hydrogen ion concentration by titrating HNO_3 with KOH in the above experimental conditions and the results were analysed with Gran procedure. [2S] The complex formation constants were studied using constant ligand concentration and 1:1, 1:2 and 1:3 metal/ligand molar ratios. Potentiometric data were processed with Hyperquad [3S] program. The reported log β values are referred to the overall equilibria: $m\mathrm{M} + p\mathrm{H} + n\mathrm{L} \leftrightharpoons \mathrm{MH}_p\mathrm{L}_n$ (the charges are omitted), where *m* might also be 0, in the case of protonation equilibria, and *p* can be negative.

Table 2S Set of log β values to compare with those identified in the solid phase

	log β_{mnp}	*p*	*n*	*m*	*ref*
HL	10.07	1	1	0	23
H_2L	19.16	2	1	0	23
H_3L	22.36	3	1	0	23

	log β_{mnp}	*p*	*n*	*m*	*ref*
FeHL	26.42	1	1	1	This paper
FeH_2L_2	47.31	2	2	1	This paper
FeL_3	38.79	0	3	1	This paper
FeH_3L_3	65.06	3	3	1	This paper
FeH_2L_3	57.43	2	3	1	This paper

[1S] R. Grazina, Ph.D. Thesis, Technical University of Lisbon (IST), Lisbon, Portugal, 2006
[2S] G. Gran, Analyst, 77 (1952) 661–671
[3S] P. Gans, A. Sabatini and A. Vacca, Talanta, 43 (1996) 1739–1753