Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Influence of water on the retention of methyl tertiary butyl ether by high silica ZSM-5 and Y zeolites: a multidisciplinary study on the adsorption from liquid and gas phase.

A. Martucci[a], I. Braschi[**,b], C. Bisio[c], E. Sarti[d], E. Rodeghero[a], R. Bagatin[e], L. Pasti[*,d]

a. Department of Physics and Earth Sciences Department, University of Ferrara, Via Saragat, 1, I-44123 Ferrara, Italy.
b. Department of Agricultural Sciences, University of Bologna, Viale Fanin 44 - 40127 Bologna, Italy.
c. Department of Sciences and Technological Innovation, Viale Teresa Michel 11, University of Eastern Piedmont, A. Avogadro, I-15121 Alessandria, Italy
d. Department of Chemistry and Pharmaceutical Sciences, University of Ferrara, Via L. Borsari, 46, I-44123 Ferrara, Italy
e. Research Center for Non-Conventional Energy – Istituto Eni Donegani Environmental Technologies, via Felice Maritano, 26, San Donato Milanese, I-20097 Milan, Italy

Rietveld refinements details.

The background curves were fitted by Chebyshew polynomials with 16 coefficients. The diffraction peak profiles were modelled by a pseudo-Voigt function with one Gaussian and two Lorentzian broadening coefficients and the peak intensity cut-off was set to 0.1% of the peak maximum. During the refinement of the atomic coordinates, soft-restraints were applied to the Si–O distances [Si–O = 1.605 ± 0.010 Å] with the constraint weight being progressively lowered until a minimal value. The isotropic displacement parameters were constrained in the following way: the same value for all tetrahedral cations, a second value for all framework oxygen atoms, a third one for the MTBE species and a fourth one for the residual water molecules.

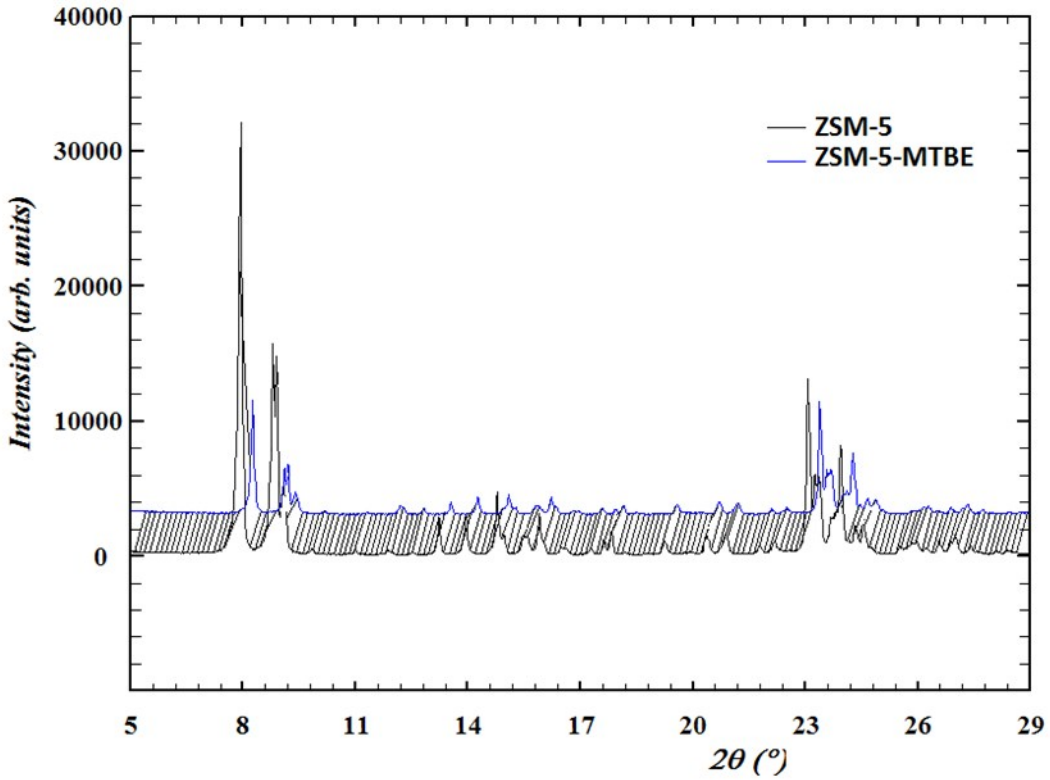

Figure 1 SI. Observed powder diffraction patterns of bare (ZSM-5, blue line) and MTBE loaded ZSM-5 (ZSM-5-MTBE, blue line), showing the differences both in the intensity and position of the diffraction peaks.

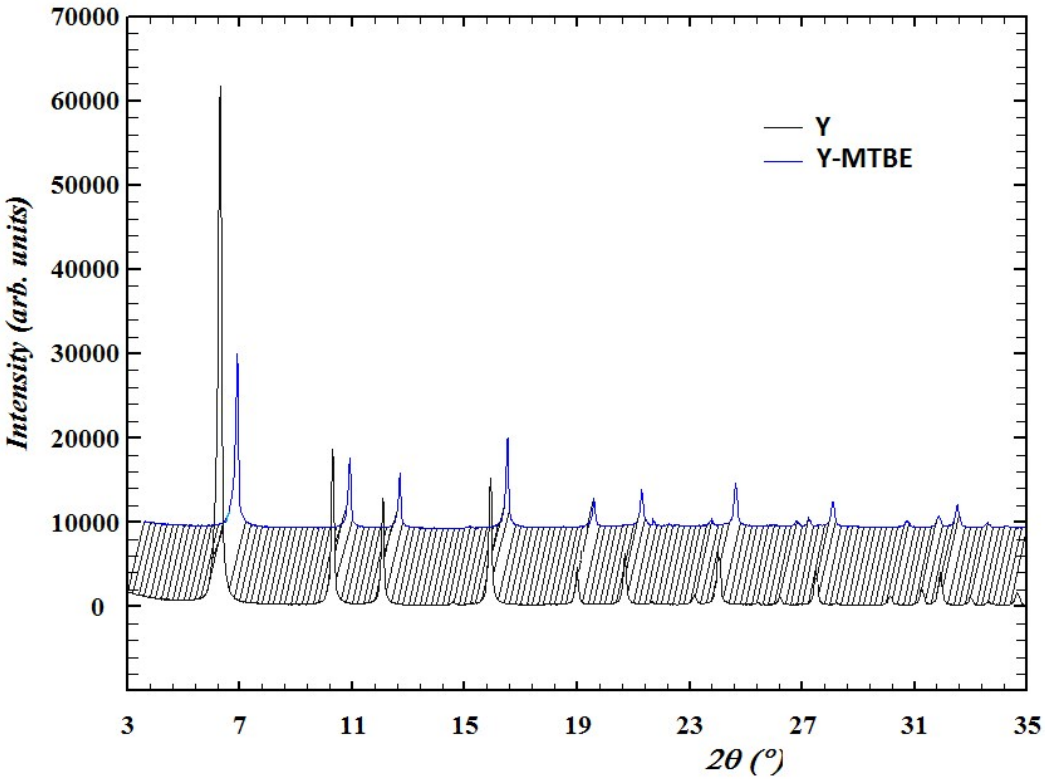

Figure 2 SI. Observed powder diffraction patterns of bare (Y, blue line) and MTBE loaded Y (Y-MTBE, blue line), showing the differences both in the intensity and position of the diffraction peaks.

Table 1 SI. Atomic coordinates, fractions and thermal parameters of ZSM-5-MTBE.

	x/a	y/b	z/c	Ui/Ue*100	Fraction
T1	0.05485(26)	0.42432(31)	-0.3276(6)	0.14(1)	1.00
T2	0.03485(30)	0.31865(38)	-0.1673(6)	0.14(1)	1.00
T3	0.06516(35)	0.28024(23)	0.0455(7)	0.14(1)	1.00
T4	0.06455(27)	0.12526(22)	0.0376(6)	0.14(1)	1.00
T5	0.02996(24)	0.07265(29)	-0.1719(7)	0.14(1)	1.00
T6	0.06110(33)	0.19554(34)	-0.3046(6)	0.14(1)	1.00
T7	-0.17119(25)	0.42693(27)	-0.3237(6)	0.14(1)	1.00
T8	-0.12353(26)	0.31133(31)	-0.1799(6)	0.14(1)	1.00
T9	-0.17488(27)	0.26983(22)	0.0293(6)	0.14(1)	1.00
T10	-0.17781(22)	0.11384(24)	0.0313(7)	0.14(1)	1.00
T11	-0.12786(23)	0.06556(31)	-0.1749(7)	0.14(1)	1.00
T12	-0.16412(27)	0.18672(30)	-0.3108(6)	0.14(1)	1.00
T13	0.44295(27)	0.42349(29)	-0.3283(6)	0.14(1)	1.00
T14	0.47469(28)	0.31202(36)	-0.1810(5)	0.14(1)	1.00
T15	0.44046(32)	0.28009(25)	0.0416(6)	0.14(1)	1.00
T16	0.43268(29)	0.12310(28)	0.0344(6)	0.14(1)	1.00
T17	0.47275(25)	0.07612(37)	-0.1836(7)	0.14(1)	1.00
T18	0.44035(27)	0.19127(29)	-0.3180(8)	0.14(1)	1.00
T19	0.67261(23)	0.42120(29)	-0.3117(5)	0.14(1)	1.00
T20	0.63309(27)	0.31026(37)	-0.1686(6)	0.14(1)	1.00
T21	0.67142(23)	0.27247(24)	0.0470(5)	0.14(1)	1.00
T22	0.67166(26)	0.11650(26)	0.0330(6)	0.14(1)	1.00
T23	0.63050(26)	0.07350(38)	-0.1864(6)	0.14(1)	1.00
T24	0.68116(29)	0.19340(36)	-0.3030(7)	0.14(1)	1.00
O1	0.06334(54)	0.37966(55)	-0.2299(9)	0.28(1)	1.00
O2	0.06509(65)	0.32098(36)	-0.0566(7)	0.28(1)	1.00
O3	0.05456(46)	0.20323(18)	0.0224(10	0.28(1)	1.00
O4	0.06687(45)	0.08974(58)	-0.0688(8)	0.28(1)	1.00
O5	0.05315(54)	0.12381(40)	-0.2557(10	0.28(1)	1.00
O6	0.05612(70)	0.25079(50)	-0.2196(6)	0.28(1)	1.00
O7	-0.15476(60)	0.37207(53)	-0.2411(10	0.28(1)	1.00
O8	-0.15946(70)	0.30563(45)	-0.0743(6)	0.28(1)	1.00
O9	-0.16576(43)	0.19157(19)	0.0169(11	0.28(1)	1.00
O10	-0.16620(43)	0.07643(40)	-0.0722(7)	0.28(1)	1.00
O11	-0.15587(46)	0.11678(43)	-0.2561(10	0.28(1)	1.00
O12	-0.13446(57)	0.24415(51)	-0.2411(9)	0.28(1)	1.00
O13	-0.04502(25)	0.32337(47)	-0.1630(14	0.28(1)	1.00
O14	-0.04937(19)	0.07777(54)	-0.1580(12	0.28(1)	1.00
O15	0.12130(24)	0.41961(39)	-0.3927(7)	0.28(1)	1.00
O16	-0.00770(26)	0.39853(67)	-0.3920(10	0.28(1)	1.00
O17	-0.13638(29)	0.40681(46)	-0.4262(8)	0.28(1)	1.00

O18	0.13225(30)	0.20067(63)	-0.3578(6)	0.28(1)	1.00
O19	0.00281(36)	0.20699(58)	-0.3853(8)	0.28(1)	1.00
O20	-0.12480(43)	0.18536(56)	-0.4139(6)	0.28(1)	1.00
O21	0.04914(59)	-0.00092(30)	-0.2053(4)	0.28(1)	1.00
O22	-0.13985(42)	-0.00852(32)	-0.2134(6)	0.28(1)	1.00
O23	-0.25050(19)	0.43143(43)	-0.3405(6)	0.28(1)	1.00
O24	-0.24175(24)	0.20067(57)	-0.3323(10	0.28(1)	1.00
O25	-0.25010(21)	0.28579(44)	0.0616(7)	0.28(1)	1.00
O26	-0.25291(17)	0.10150(47)	0.0673(9)	0.28(1)	1.00
O27	0.44397(47)	0.37698(45)	-0.2319(10	0.28(1)	1.00
O28	0.45584(65)	0.31080(52)	-0.0656(6)	0.28(1)	1.00
O29	0.42788(39)	0.20216(25)	0.0312(12	0.28(1)	1.00
O30	0.44687(64)	0.09561(68)	-0.0751(8)	0.28(1)	1.00
O31	0.43517(45)	0.12041(38)	-0.2655(11	0.28(1)	1.00
O32	0.44467(45)	0.24768(47)	-0.2346(9)	0.28(1)	1.00
O33	0.66809(35)	0.37384(57)	-0.2165(8)	0.28(1)	1.00
O34	0.64524(43)	0.31013(47)	-0.0507(6)	0.28(1)	1.00
O35	0.65861(44)	0.19464(21)	0.0352(11	0.28(1)	1.00
O36	0.65966(59)	0.08921(63)	-0.0776(6)	0.28(1)	1.00
O37	0.66721(44)	0.11938(43)	-0.2662(8)	0.28(1)	1.00
O38	0.66425(68)	0.24440(56)	-0.2156(8)	0.28(1)	1.00
O39	0.55439(25)	0.31252(61)	-0.1919(9)	0.28(1)	1.00
O40	0.55179(22)	0.08849(46)	-0.1893(12	0.28(1)	1.00
O41	0.37342(24)	0.41421(52)	-0.3868(8)	0.28(1)	1.00
O42	0.50343(27)	0.40376(58)	-0.3997(9)	0.28(1)	1.00
O43	0.63324(28)	0.38812(37)	-0.4034(7)	0.28(1)	1.00
O44	0.37565(32)	0.20353(22)	-0.3867(9)	0.28(1)	1.00
O45	0.50597(30)	0.19374(58)	-0.3853(9)	0.28(1)	1.00
O46	0.63532(29)	0.20936(41)	-0.3982(7)	0.28(1)	1.00
O47	0.45735(46)	-0.00039(34)	-0.2044(6)	0.28(1)	1.00
O48	0.64327(39)	-0.00273(36)	-0.2125(7)	0.28(1)	1.00
C2b	0.7173(56)	0.5043(87)	0.206(4)	10.35(7)	1.00(1)
C1b	0.7391(30)	0.5103(27)	0.104(4)	10.35(7)	1.00(1)
C4b	0.2389(81)	0.4223(45)	-0.085(11)	10.35(7)	1.00(1)
O1b	0.68383(32)	0.49424(58)	0.0368(54)	10.35(7)	1.00(1)
C3b	0.7942(56)	0.4650(77)	0.086(11)	10.35(7)	1.00(1)
C5b	0.6541(51)	0.5215(82)	-0.049(8)	10.35(7)	1.00(1)
C1a	0.7703(92)	0.7131(72)	0.106(10)	11.32(6)	0.50(1)
C2a	0.7731(57)	0.6754(65)	0.198(19)	11.32(6)	0.50(1)
c3a	0.8128(71)	0.6819(86)	0.032(25)	11.32(6)	0.50(1)
C4a	0.7936(73)	0.7801(10)	0.124(29)	11.32(6)	0.50(1)
O5a	0.7018(85)	0.7150(82)	0.0687(18)	11.32(6)	0.50(1)
C6a	0.6566(57)	0.7030(54)	0.146(26)	11.32(6)	0.50(1)
w	0.7885(33)	0.3762(24)	0.1888(25)	7.57(3)	0.98(8)

Table 2 SI. Atomic coordinates, fractions and thermal parameters of Y-MTBE.

	x/a	y/b	z/c	Ui/Ue*100	Fraction
T1	-0.0521(4)	0.1279(6)	0.0350(5)	0.67(1)	1.00
T2	-0.0575(4)	0.0370(5)	0.1244(6)	0.67(1)	1.00
O1	-0.1100(6)	0.0008(9)	0.1054(8)	0.85(1)	1.00
O2	-0.0038(4)	0.0011(5)	0.1406(5)	0.85(1)	1.00
O3	-0.0363(5)	0.0772(6)	0.0754(5)	0.85(1)	1.00
O4	-0.0742(4)	0.0690(5)	0.1808(6)	0.85(1)	1.00
C1	0.500000	0.000000	0.000000	6.25(1)	0.388(8)
C3	0.4792(3)	0.0958(2)	0.0496(3)	6.25(1)	0.388(8)
C2/O2	0.4771(7)	0.0579(4)	0.0051(3)	6.25(1)	0.388(8)
W	0.0667(6)	0.6427(3)	-0.02737(3)	5.48(2)	0.428(5)