Supplementary Information

Competitive Adsorption of VOCs from binary aqueous mixtures on zeolite

ZSM-5

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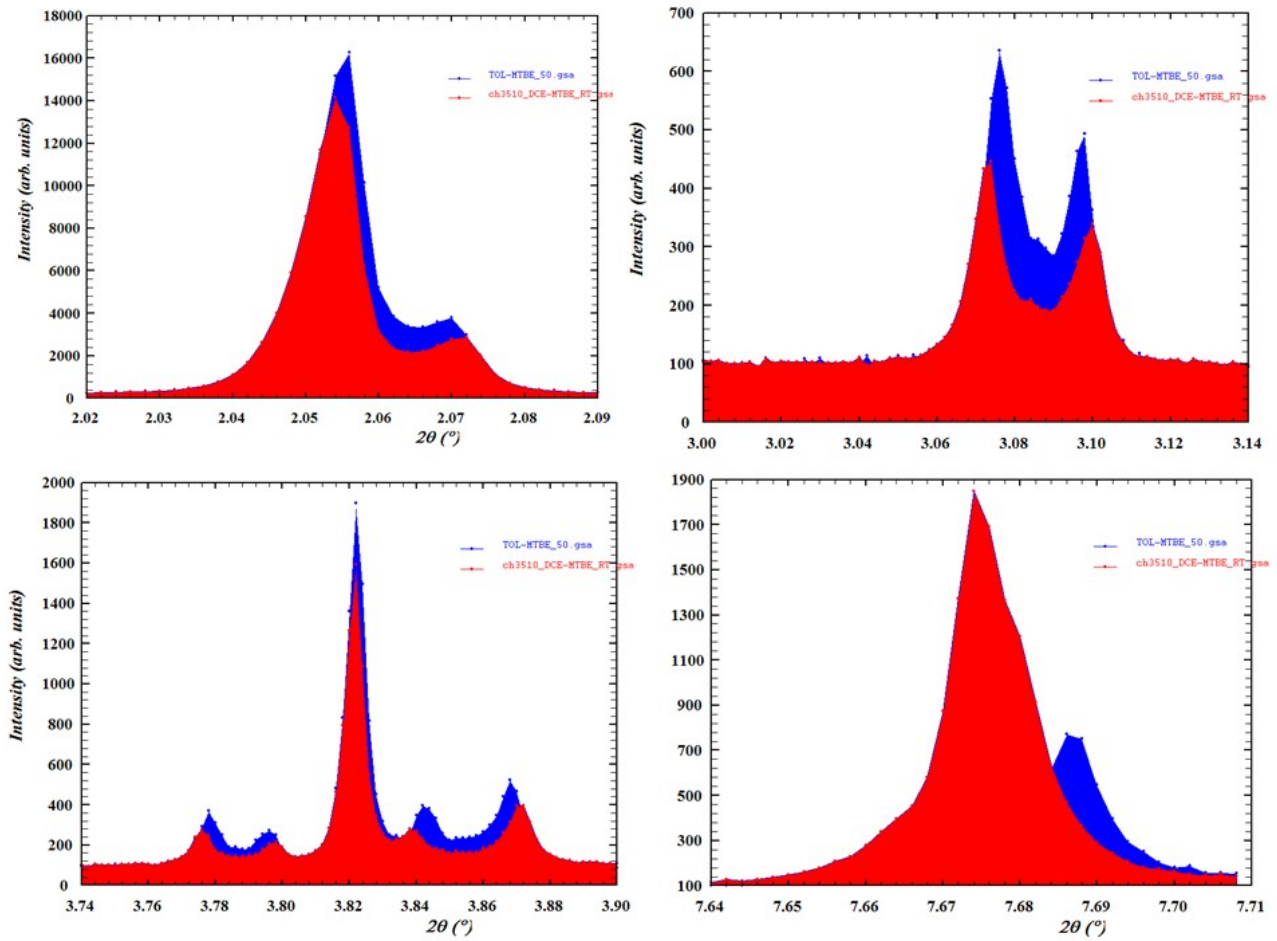
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Figure S1: ZSM-5 diffraction peak positions after binary mixture (DCE-MTBE, TOL-MTBE) adsorption in the 2.0-7.7° 2θ regions.

Figure S2. Thermogravimetric (TG), differential thermogravimetric (DTG) and differential thermal analysis
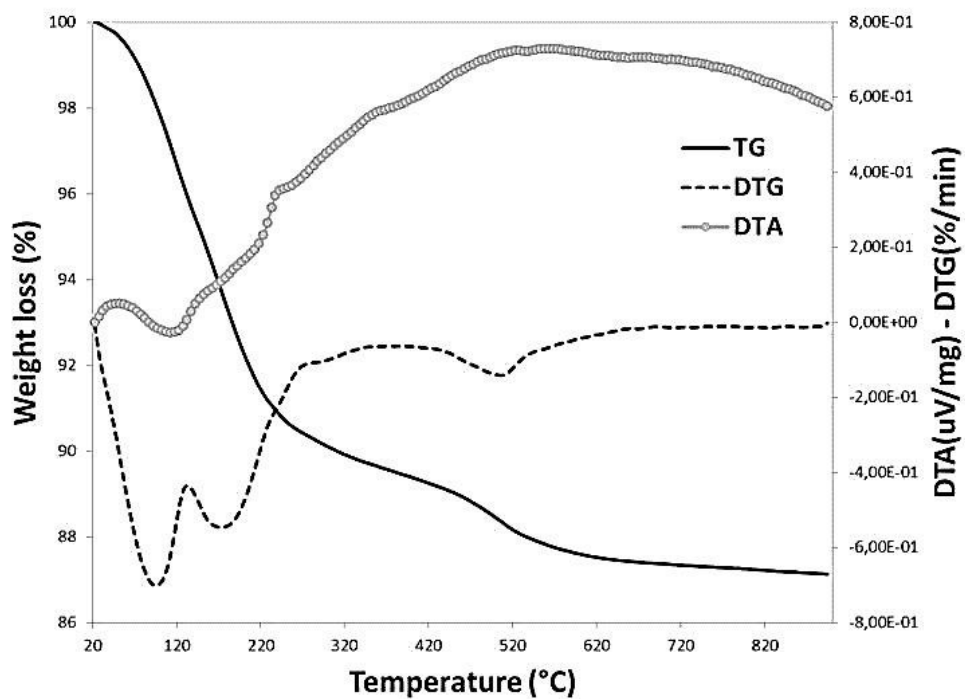
(DTA) of ZSM-5-TOL-MTBE.

Table 1SI: Physical-chemical properties of the three investigated compounds.

Compound	MW (g mol^{-1})	logKow	Solubility in water (g L^{-1})	Molecule volume (Å^3)
TOL	92.14	2.73	0.47	98.87
MTBE	88.15	1.2	26	105.60
DCE	98.95	1.48	8.7	73.30

Table 2SI: fractional atomic coordinates of ZSM-5 framework's atoms loaded with MTBE at Room Temperature (°C).

	x/a	y/b	z/c	Uiso	Fraction
		ZSM-5-MTBE 30°C			
T1	0.05422(24)	0.42299(20)	-0.32853(38)	0.0042(9)	1
T2	0.03289(24)	0.31648(24)	-0.16757(38)	0.0042(9)	1
T3	0.06535(21)	0.28079(22)	0.04463(42)	0.0042(9)	1
T4	0.06465(25)	0.12496(22)	0.03471(35)	0.0042(9)	1
T5	0.02811(23)	0.07270(24)	-0.17287(40)	0.0042(9)	1
T6	0.05738(21)	0.19424(23)	-0.30775(32)	0.0042(9)	1
T7	-0.17116(22)	0.42583(22)	-0.32245(39)	0.0042(9)	1
T8	-0.12479(24)	0.31179(24)	-0.17574(39)	0.0042(9)	1
T9	-0.17543(24)	0.26949(24)	0.03311(42)	0.0042(9)	1
T10	-0.17825(23)	0.11428(23)	0.03045(44)	0.0042(9)	1
T11	-0.12891(24)	0.06690(25)	-0.17525(45)	0.0042(9)	1
T12	-0.16457(24)	0.18877(23)	-0.30996(35)	0.0042(9)	1
T13	0.44273(23)	0.42431(22)	-0.33351(34)	0.0042(9)	1
T14	0.47104(18)	0.31072(23)	-0.18160(33)	0.0042(9)	1
T15	0.43780(15)	0.27990(21)	0.03490(24)	0.0042(9)	1
T16	0.43301(25)	0.12309(21)	0.03032(36)	0.0042(9)	1
T17	0.47292(24)	0.07354(23)	-0.18408(42)	0.0042(9)	1
T18	0.44110(22)	0.18896(21)	-0.31945(37)	0.0042(9)	1
T19	0.67263(21)	0.42165(23)	-0.31214(36)	0.0042(9)	1
T20	0.63190(22)	0.31124(25)	-0.16729(33)	0.0042(9)	1
T21	0.66960(23)	0.27186(26)	0.04872(40)	0.0042(9)	1
T22	0.67089(24)	0.11689(25)	0.03547(42)	0.0042(9)	1
T23	0.63030(25)	0.07300(27)	-0.18315(42)	0.0042(9)	1
T24	0.67949(26)	0.19301(25)	-0.30059(32)	0.0042(9)	1
O1	0.06146(38)	0.37608(32)	-0.23321(54)	0.0065(18)	1
O2	0.06726(31)	0.31902(29)	-0.05965(31)	0.0065(18)	1
O3	0.05498(38)	0.20338(18)	0.02473(74)	0.0065(18)	1
O4	0.06844(32)	0.09249(41)	-0.07377(35)	0.0065(18)	1
O5	0.04798(39)	0.12189(24)	-0.26137(47)	0.0065(18)	1
O6	0.05047(35)	0.24791(29)	-0.22068(44)	0.0065(18)	1
O7	-0.15563(43)	0.37305(34)	-0.23642(59)	0.0065(18)	1
O8	-0.16183(39)	0.30522(37)	-0.07123(52)	0.0065(18)	1
O9	-0.16226(52)	0.19167(19)	0.02132(75)	0.0065(18)	1
O10	-0.17055(29)	0.07977(38)	-0.07604(41)	0.0065(18)	1
O11	-0.15305(43)	0.11786(29)	-0.25968(57)	0.0065(18)	1
O12	-0.13460(40)	0.24524(34)	-0.23883(63)	0.0065(18)	1
O13	-0.04637(20)	0.32394(34)	-0.15701(68)	0.0065(18)	1
O14	-0.05068(19)	0.07744(42)	-0.15319(75)	0.0065(18)	1
O15	0.12231(27)	0.42139(32)	-0.39012(50)	0.0065(18)	1
O16	-0.00610(31)	0.39730(35)	-0.39772(64)	0.0065(18)	1
O17	-0.13576(28)	0.40270(40)	-0.42322(52)	0.0065(18)	1
O18	0.12970(22)	0.20008(44)	-0.35745(36)	0.0065(18)	1

O19	0.00057(26)	0.20709(33)	-0.39040(42)	0.0065(18)	1
O20	-0.12807(24)	0.19087(45)	-0.41556(42)	0.0065(18)	1
O21	0.04688(41)	-0.00138(21)	-0.20486(40)	0.0065(18)	1
O22	-0.14151(37)	-0.00732(23)	-0.21337(53)	0.0065(18)	1
O23	-0.25028(17)	0.43040(38)	-0.34101(49)	0.0065(18)	1
O24	-0.24293(21)	0.20141(35)	-0.32639(24)	0.0065(18)	1
O25	-0.25142(18)	0.28204(53)	0.06530(54)	0.0065(18)	1
O26	-0.25308(18)	0.10506(50)	0.06956(52)	0.0065(18)	1
O27	0.44229(37)	0.37445(29)	-0.24093(46)	0.0065(18)	1
O28	0.45256(29)	0.31606(26)	-0.06799(25)	0.0065(18)	1
O29	0.43035(40)	0.20195(17)	0.01880(42)	0.0065(18)	1
O30	0.44315(49)	0.09043(38)	-0.07694(45)	0.0065(18)	1
O31	0.43670(39)	0.11796(22)	-0.26704(59)	0.0065(18)	1
O32	0.44854(34)	0.24521(28)	-0.23598(42)	0.0065(18)	1
O33	0.66735(28)	0.37392(35)	-0.21734(50)	0.0065(18)	1
O34	0.64609(41)	0.31062(27)	-0.04980(28)	0.0065(18)	1
O35	0.65421(49)	0.19438(21)	0.03639(79)	0.0065(18)	1
O36	0.66041(43)	0.08847(49)	-0.07489(39)	0.0065(18)	1
O37	0.66624(43)	0.11901(27)	-0.26347(52)	0.0065(18)	1
O38	0.66036(41)	0.24441(33)	-0.21484(38)	0.0065(18)	1
O39	0.55290(16)	0.31543(44)	-0.18834(62)	0.0065(18)	1
O40	0.55165(21)	0.08823(35)	-0.18408(87)	0.0065(18)	1
O41	0.37281(25)	0.41915(38)	-0.39216(48)	0.0065(18)	1
O42	0.50237(30)	0.40541(40)	-0.40683(50)	0.0065(18)	1
O43	0.63233(29)	0.39012(36)	-0.40436(43)	0.0065(18)	1
O44	0.37444(27)	0.20140(39)	-0.38382(62)	0.0065(18)	1
O45	0.50498(26)	0.19123(36)	-0.39040(48)	0.0065(18)	1
O46	0.63497(18)	0.20763(40)	-0.39774(31)	0.0065(18)	1
O47	0.46054(32)	-0.00312(17)	-0.20787(47)	0.0065(18)	1
O48	0.64278(38)	-0.00319(23)	-0.20991(57)	0.0065(18)	1

Table 3SI: fractional atomic coordinates of ZSM-5 framework's atoms loaded with MTBE and DCE mixture at Room Temperature (°C)

	ZSM-5-DCE-MTBE -30°C				
	x/a	y/b	z/c	Uiso	Fraction
T1	0.05462(19)	0.42182(19)	-0.32417(32)	0.006(7)	1
T2	0.03358(21)	0.31680(21)	-0.16631(32)	0.006(7)	1
T3	0.06290(21)	0.27997(19)	0.05014(34)	0.006(7)	1
T4	0.06256(20)	0.12432(18)	0.03536(32)	0.006(7)	1
T5	0.02814(18)	0.07568(22)	-0.17463(33)	0.006(7)	1
T6	0.05838(21)	0.19612(19)	-0.31093(35)	0.006(1)	1
T7	-0.17182(17)	0.42669(18)	-0.32289(33)	0.006(1)	1
T8	-0.12432(19)	0.31186(19)	-0.17895(32)	0.006(1)	1
T9	-0.17488(18)	0.27098(20)	0.03161(34)	0.006(1)	1
T10	-0.17767(17)	0.11601(20)	0.03348(38)	0.006(1)	1
T11	-0.12918(19)	0.06854(22)	-0.17399(36)	0.006(1)	1
T12	-0.16394(19)	0.18849(19)	-0.31393(34)	0.006(1)	1
T13	0.44311(20)	0.42731(20)	-0.33397(33)	0.006(1)	1
T14	0.47426(19)	0.31154(23)	-0.18726(34)	0.006(1)	1
T15	0.43981(21)	0.27906(18)	0.03298(35)	0.006(1)	1
T16	0.43396(21)	0.12298(19)	0.03431(30)	0.006(1)	1
T17	0.47423(19)	0.07325(21)	-0.18088(35)	0.006(1)	1
T18	0.43869(20)	0.18764(18)	-0.31803(40)	0.006(1)	1
T19	0.67165(17)	0.42225(19)	-0.31369(31)	0.006(1)	1
T20	0.63285(18)	0.31079(21)	-0.16849(32)	0.006(1)	1
T21	0.66961(19)	0.27306(21)	0.04659(33)	0.006(1)	1
T22	0.67028(18)	0.11838(20)	0.03575(35)	0.006(1)	1
T23	0.63168(20)	0.07382(22)	-0.18358(33)	0.006(1)	1
T24	0.68193(19)	0.19456(21)	-0.30117(34)	0.006(1)	1
O1	0.06357(30)	0.37897(27)	-0.22484(44)	0.012(1)	1
O2	0.06548(32)	0.31485(35)	-0.05671(29)	0.012(1)	1
O3	0.04929(32)	0.20250(15)	0.03525(73)	0.012(1)	1
O4	0.06832(26)	0.09826(44)	-0.07677(36)	0.012(1)	1
O5	0.04586(34)	0.12422(20)	-0.26487(45)	0.012(1)	1
O6	0.05209(42)	0.25037(26)	-0.22484(49)	0.012(1)	1
O7	-0.15505(36)	0.37405(29)	-0.23727(52)	0.012(1)	1
O8	-0.16146(37)	0.30364(32)	-0.07484(39)	0.012(1)	1
O9	-0.16003(42)	0.19320(17)	0.02626(69)	0.012(1)	1
O10	-0.16907(24)	0.08228(38)	-0.07342(37)	0.012(1)	1
O11	-0.15419(34)	0.11894(25)	-0.25855(49)	0.012(1)	1
O12	-0.13503(37)	0.24645(30)	-0.24445(57)	0.012(1)	1
O13	-0.04598(17)	0.32356(31)	-0.15952(70)	0.012(1)	1
O14	-0.05059(14)	0.07861(34)	-0.15426(59)	0.012(1)	1
O15	0.12190(21)	0.41832(30)	-0.38771(41)	0.012(1)	1
O16	-0.00646(24)	0.39279(36)	-0.38878(50)	0.012(1)	1
O17	-0.13482(23)	0.40570(33)	-0.42320(44)	0.012(1)	1

O18	0.13177(19)	0.19907(38)	-0.35761(30)	0.012(1)	1
O19	0.00393(23)	0.21012(30)	-0.39649(53)	0.012(1)	1
O20	-0.12433(25)	0.18774(37)	-0.41682(36)	0.012(1)	1
O21	0.04921(34)	0.00192(20)	-0.20446(37)	0.012(1)	1
O22	-0.14259(33)	-0.00573(20)	-0.21046(43)	0.012(1)	1
O23	-0.25099(13)	0.42853(36)	-0.34221(44)	0.012(1)	1
O24	-0.24183(16)	0.20094(32)	-0.33578(56)	0.012(1)	1
O25	-0.25135(15)	0.28285(43)	0.06134(48)	0.012(1)	1
O26	-0.25339(13)	0.10761(42)	0.06945(46)	0.012(1)	1
O27	0.44857(37)	0.37736(26)	-0.24185(47)	0.012(1)	1
O28	0.45227(40)	0.31265(31)	-0.07304(36)	0.012(1)	1
O29	0.42720(32)	0.20132(16)	0.01904(62)	0.012(1)	1
O30	0.44949(40)	0.08892(38)	-0.07047(40)	0.012(1)	1
O31	0.43466(27)	0.11913(23)	-0.25858(57)	0.012(1)	1
O32	0.44255(32)	0.24795(27)	-0.24090(62)	0.012(1)	1
O33	0.66423(34)	0.37579(29)	-0.21788(41)	0.012(1)	1
O34	0.64481(33)	0.31237(28)	-0.05051(28)	0.012(1)	1
O35	0.65343(40)	0.19587(17)	0.03391(68)	0.012(1)	1
O36	0.65915(36)	0.08833(39)	-0.07342(32)	0.012(1)	1
O37	0.66883(30)	0.12111(24)	-0.26109(45)	0.012(1)	1
O38	0.66833(41)	0.24654(30)	-0.21375(44)	0.012(1)	1
O39	0.55429(16)	0.30793(47)	-0.19265(57)	0.012(1)	1
O40	0.55286(17)	0.08771(29)	-0.18824(66)	0.012(1)	1
O41	0.37183(19)	0.41868(32)	-0.38797(43)	0.012(1)	1
O42	0.50143(23)	0.41202(34)	-0.41144(51)	0.012(1)	1
O43	0.63065(23)	0.39101(30)	-0.40527(37)	0.012(1)	1
O44	0.37331(27)	0.19559(36)	-0.38694(53)	0.012(1)	1
O45	0.50399(26)	0.18802(38)	-0.38606(45)	0.012(1)	1
O46	0.63295(21)	0.20963(34)	-0.39318(38)	0.012(1)	1
O47	0.46035(30)	-0.00299(18)	-0.20561(40)	0.012(1)	1
O48	0.64615(33)	-0.00177(20)	-0.21152(44)	0.012(1)	1

Table 4SI: fractional atomic coordinates of ZSM-5 framework's atoms loaded with MTBE and TOL mixture at Room Temperature (°C)

		ZSM-5-MTBE-TOL -30°C			
	x/a	y/b	z/c	Uiso	Fraction
T1	0.05368(24)	0.42216(21)	-0.32790(39)	0.003(1)	1
T2	0.03334(26)	0.31657(25)	-0.16674(38)	0.003(1)	1
T3	0.06515(22)	0.28088(24)	0.04645(44)	0.003(1)	1
T4	0.06344(22)	0.12511(24)	0.03500(37)	0.003(1)	1
T5	0.02850(23)	0.07306(26)	-0.17391(39)	0.003(1)	1
T6	0.05741(21)	0.19488(25)	-0.30799(32)	0.003(1)	1
T7	-0.17122(23)	0.42565(22)	-0.32420(39)	0.003(1)	1
T8	-0.12417(25)	0.31132(25)	-0.17770(40)	0.003(1)	1
T9	-0.17593(24)	0.27046(25)	0.03146(40)	0.003(1)	1
T10	-0.17898(23)	0.11443(22)	0.03097(34)	0.003(1)	1
T11	-0.12905(24)	0.06660(24)	-0.17554(37)	0.003(1)	1
T12	-0.16406(24)	0.18832(24)	-0.31122(37)	0.003(1)	1
T13	0.44213(22)	0.42439(23)	-0.33275(35)	0.003(1)	1
T14	0.47133(18)	0.31004(24)	-0.18197(34)	0.003(1)	1
T15	0.43779(16)	0.27995(22)	0.03492(26)	0.003(1)	1
T16	0.43281(25)	0.12352(22)	0.03065(38)	0.003(1)	1
T17	0.47316(25)	0.07360(24)	-0.18441(40)	0.003(1)	1
T18	0.44054(23)	0.18840(22)	-0.31947(39)	0.003(1)	1
T19	0.67239(21)	0.42101(24)	-0.31272(38)	0.003(1)	1
T20	0.63199(23)	0.31032(25)	-0.16755(35)	0.003(1)	1
T21	0.66988(25)	0.27305(27)	0.04793(42)	0.003(1)	1
T22	0.67036(21)	0.11739(24)	0.03381(41)	0.003(1)	1
T23	0.63057(26)	0.07311(27)	-0.18546(37)	0.003(1)	1
T24	0.68043(26)	0.19322(25)	-0.30066(34)	0.003(1)	1
O1	0.06233(39)	0.37651(33)	-0.23136(56)	0.005(1)	1
O2	0.06708(33)	0.31866(31)	-0.05823(32)	0.005(1)	1
O3	0.05312(39)	0.20357(19)	0.02716(76)	0.005(1)	1
O4	0.06768(32)	0.09398(42)	-0.07435(36)	0.005(1)	1
O5	0.04793(41)	0.12223(24)	-0.26256(46)	0.005(1)	1
O6	0.05116(37)	0.24815(30)	-0.22018(45)	0.005(1)	1
O7	-0.15472(44)	0.37221(34)	-0.23950(55)	0.005(1)	1
O8	-0.16216(38)	0.30449(33)	-0.07408(50)	0.005(1)	1
O9	-0.16508(39)	0.19211(19)	0.02194(61)	0.005(1)	1
O10	-0.16901(29)	0.07971(39)	-0.07495(32)	0.005(1)	1
O11	-0.15393(43)	0.11758(28)	-0.25945(49)	0.005(1)	1
O12	-0.13280(37)	0.24465(33)	-0.24096(60)	0.005(1)	1
O13	-0.04599(21)	0.32405(35)	-0.15719(69)	0.005(1)	1
O14	-0.05049(19)	0.07672(42)	-0.15553(70)	0.005(1)	1
O15	0.12074(25)	0.41955(36)	-0.39180(52)	0.005(1)	1
O16	-0.00752(29)	0.39548(37)	-0.39430(65)	0.005(1)	1

O17	-0.13617(27)	0.40420(39)	-0.42600(48)	0.005(1)	1
O18	0.12970(22)	0.20031(46)	-0.35769(38)	0.005(1)	1
O19	0.00052(26)	0.20846(34)	-0.39002(43)	0.005(1)	1
O20	-0.12762(25)	0.18888(41)	-0.41676(42)	0.005(1)	1
O21	0.04865(37)	-0.00091(22)	-0.20480(42)	0.005(1)	1
O22	-0.14228(39)	-0.00759(21)	-0.21338(52)	0.005(1)	1
O23	-0.25055(17)	0.42913(40)	-0.34213(48)	0.005(1)	1
O24	-0.24219(20)	0.20229(33)	-0.32741(26)	0.005(1)	1
O25	-0.25141(20)	0.28532(44)	0.06417(56)	0.005(1)	1
O26	-0.25406(17)	0.10265(28)	0.06769(28)	0.005(1)	1
O27	0.44365(37)	0.37485(30)	-0.23985(47)	0.005(1)	1
O28	0.45393(29)	0.31534(27)	-0.06809(26)	0.005(1)	1
O29	0.42823(39)	0.20220(18)	0.01903(42)	0.005(1)	1
O30	0.44620(49)	0.09111(41)	-0.07592(48)	0.005(1)	1
O31	0.43502(33)	0.11779(24)	-0.26589(65)	0.005(1)	1
O32	0.44674(35)	0.24536(30)	-0.23680(43)	0.005(1)	1
O33	0.66694(29)	0.37309(31)	-0.21820(48)	0.005(1)	1
O34	0.64498(42)	0.31145(28)	-0.04993(29)	0.005(1)	1
O35	0.65645(37)	0.19527(21)	0.03533(82)	0.005(1)	1
O36	0.65889(37)	0.08964(51)	-0.07658(38)	0.005(1)	1
O37	0.66762(42)	0.11866(25)	-0.26535(54)	0.005(1)	1
O38	0.66190(39)	0.24345(31)	-0.21300(37)	0.005(1)	1
O39	0.55314(16)	0.31296(44)	-0.19040(63)	0.005(1)	1
O40	0.55188(21)	0.08805(37)	-0.18923(68)	0.005(1)	1
O41	0.37150(14)	0.41753(28)	-0.38924(29)	0.005(1)	1
O42	0.50130(21)	0.40645(41)	-0.40748(52)	0.005(1)	1
O43	0.63130(24)	0.39013(37)	-0.40462(44)	0.005(1)	1
O44	0.37512(27)	0.20059(40)	-0.38686(58)	0.005(1)	1
O45	0.50568(26)	0.18985(35)	-0.38797(50)	0.005(1)	1
O46	0.63524(18)	0.20879(40)	-0.39676(32)	0.005(1)	1
O47	0.46021(33)	-0.00329(17)	-0.20654(50)	0.005(1)	1
O48	0.64387(38)	-0.00331(22)	-0.20994(61)	0.005(1)	1

Table 5SI: extraframework coordinates of ZSM-5 loaded with DCE, TOL and MTBE as single molecules and mixture of them at Room Temperature (°C)

ZSM-5-DCE-30 (*)					
	x/a	y/b	z/c	UISO	Fraction
DCE1 site					
C1	0.772(1)	0.468(8)	0.060(5)	0.11(2)	0.85(1)
C11	0.686(1)	0.470(3)	0.069(2)	0.11(2)	0.85(1)
Cl2	0.893(1)	0.484(2)	-0.029(2)	0.11(2)	0.85(1)
C2	0.807(1)	0.487(8)	-0.020(5)	0.11(2)	0.85(1)
DCE2 site					
C3	0.748(8)	0.796(1)	0.170(2)	0.15(2)	0.76(1)
Cl3	0.739(2)	0.720(1)	0.115(2)	0.15(2)	0.76(1)
C4	0.747(9)	0.855(1)	0.121(2)	0.15(2)	0.76(1)
Cl4	0.75(3)	0.931(1)	0.177(2)	0.15(2)	0.76(1)
(*) Martucci et al. 2015					

ZSM-5-TOL-30 (**)					
	x/a	y/b	z/c	UISO	Fraction
TOL1 site					
C1	0.7491(36)	0.5795(28)	0.0559(75)	16.1(17)	0.86(1)
C2	0.3020(27)	0.4599(39)	-0.0152(83)	16.1(17)	0.86(1)
C3	0.8113(31)	0.5512(26)	0.0733(53)	16.1(17)	0.86(1)
C4	0.8270(23)	0.4906(22)	0.0315(41)	16.1(17)	0.86(1)
C5	0.7170(30)	0.4849(40)	-0.0412(70)	16.1(17)	0.86(1)
C6	0.2213(34)	0.5441(26)	0.0213(56)	16.1(17)	0.86(1)
C7	0.8884(28)	0.4625(46)	0.0496(41)	16.1(17)	0.86(1)
TOL2 site					
C8	0.2339(16)	0.1859(21)	0.8186(28)	21.8(24)	0.64(1)
C9	0.2339(16)	0.1270(21)	0.7645(28)	21.8(24)	0.64(1)
C10	0.2339(16)	0.1219(21)	0.9693(28)	21.8(24)	0.64(1)
C11	0.2339(16)	0.1829(21)	0.9209(28)	21.8(24)	0.64(1)
C12	0.2339(16)	0.0660(21)	0.9150(28)	21.8(24)	0.64(1)
C13	0.2339(16)	0.0660(21)	0.8131(28)	21.8(24)	0.64(1)
C14	0.2339(16)	0.0098(21)	0.7604(28)	21.8(24)	0.64(1)
(**) Rodeghero et al. 2015					

ZSM-5-MTBE-30 (***)					
	x/a	y/b	z/c	UISO	Fraction
MTBE1 site					
C1M	0.7413 (1)	0.5649(1)	0.1387 (1)	0.195(23)	1.00(1)
C2M	0.7567(1)	0.4946 (1)	0.1307 (1)	0.195(23)	1.00(1))
C3M	0.1765 (1)	0.5163 (1)	-0.0915 (1)	0.195(23)	1.00(1)
OMM-M	0.7051 (1)	0.4680(1)	0.0647 (1)	0.195(23)	1.00(1)
C4M	0.7473 (1)	0.4604 (1)	0.2250(1)	0.195(23)	1.00(1)
C5M	0.6839 (1)	0.5074 (1)	-0.0157(5)	0.195(23)	1.00(1)
MTBE2 site					
C1aM	0.7425(1)	0.7197 (1)	0.0723(1)	0.123(4)	0.92(1)
C2aM	0.7471(1)	0.6937 (1)	0.1733 (1)	0.123(4)	0.92(1)
c3a	0.7692(1)	0.6740 (1)	0.0002 (1)	0.123(4)	0.92(1)
C4aM	0.7734(1)	0.7850(1)	0.06569(1)	0.123(4)	0.92(1)

	x/a	y/b	z/c	UISO	Fraction
O5aM	0.6695(1)	0.7210(1)	0.0520(1)	0.123(4)	0.92(1)
C6aM	0.6211(1)	0.75641(1)	0.1131(1)	0.123(4)	0.92(1)

(***) In this work

		ZSM-5- DCE-MTBE -30°C			
	x/a	y/b	z/c	UISO	Fraction
		MTBE1 site			
C1	0.7392 (4)	0.5740(2)	0.0598(1)	0.071(1)	0.81(1)
C2	0.7310(3)	0.5042(2)	0.0837(1)	0.071(1)	0.81(1)
C3	0.2188 (3)	0.5365(3)	-0.035(8)	0.071(1)	0.81(1)
OMM	0.6636(3)	0.4878(3)	0.0496(1)	0.071(1)	0.81(1)
C4	0.7303(6)	0.4931(5)	0.1907(1)	0.071(1)	0.81(1)
C5	0.6406(4)	0.5172(5)	-0.038(7)	0.071(1)	0.81(1)
		DCE2 site			
DCE-Cl	0.7455(20)	0.6895(7)	0.1577(18)	0.087(1)	0.68(1)
DCE-C1	0.7618(16)	0.7682(9)	0.1168(18)	0.087(1)	0.68(1)
DCE-C2	0.7418(16)	0.8225(7)	0.1657(14)	0.087(1)	0.68(1)
DCE-Cl2	0.7583(16)	0.9012(9)	0.1252(21)	0.087(1)	0.68(1)
		ZSM-5- TOL-MTBE -30°C			
	x/a	y/b	z/c	UISO	Fraction
		TOL1 site			
M7	0.7776(1)	0.8978(1)	0.1843(5)	0.160(1)	0.94(1)
M1	0.2175(1)	0.0447(3)	0.6601(3)	0.160(1)	0.94(1)
M2	0.2175(1)	-0.0140(3)	0.6078(3)	0.160(1)	0.94(1)
M3	0.2175(1)	-0.0162(3)	0.8130(3)	0.160(1)	0.94(1)
M4	0.2175(1)	0.0447(3)	0.76319(3)	0.160(1)	0.94(1)
M5	0.2175(1)	-0.0744(3)	0.76319(3)	0.160(1)	0.94(1)
M6	0.2175(1)	-0.0744(3)	0.6578(3)	0.160(1)	0.94(1)
		MTBE2 site			
C1a	0.7434(2)	0.7227(2)	0.7227(3)	0.088(5)	0.84(10)
C2a	0.7227(3)	0.7057(6)	0.1696(3)	0.088(5)	0.84(10)
c3a	0.7701(2)	0.6727(4)	-0.0002(3)	0.088(5)	0.84(10)
C4a	0.7696(3)	0.7696(2)	0.0437(8)	0.088(5)	0.84(10)
O5a	0.6698(3)	0.7186(1)	0.0512(1)	0.088(5)	0.84(10)
C6a	0.6221(1)	0.6221(2)	0.1129(2)	0.088(5)	0.84(10)