

SUPPLEMENTAL INFORMATION

Temperature induced monoclinic to orthorhombic phase transition in protonated ZSM-5 zeolites with different Si/Al ratios: An in-situ synchrotron X-ray powder diffraction study

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Framework atomic coordinates, site atomic fraction (site occupancy), and atomic displacement parameters (ADPs) at room-temperature (*RT*) for samples ZSM-5c_15, ZSM-5c_20, ZSM-5c_37 and ZSM-5c_69 are reported in Tables SI1–SI4.

Framework atomic coordinates, site atomic fraction (site occupancy), and atomic displacement parameters (ADPs) at selected temperatures of 200, 400, 600 and 800 °C for sample ZSM-5c_15 are given in Tables SI5–SI8, for sample ZSM-5c_20 in Tables SI9–SI12, for sample ZSM-5c_37 in Tables SI13–SI16, and for ZSM-5c_69 in Tables SI17–SI20.

T-O bond distances and T-O-T angles at *RT* for sample ZSM-5c_15 are given in Table SI21, while those for samples ZSM-5c_20, ZSM-5c_37, and ZSM-5c_69 are given in Table SI22.

T-O bond distances and T-O-T angles at 200, 400, 600 and 800 °C for samples ZSM-5c_15, ZSM-5c_20, ZSM-5c_37, and ZSM-5c_69 are given in Tables SI23–SI26.

Table S1

ZSM-5c 15, room temperature

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.4240(1)	0.05658(8)	-0.3330(4)	1.0	0.40(2)
T2	0.3128(1)	0.02987(8)	-0.1804(4)	1.0	0.40(2)
T3	0.2815(1)	0.05902(8)	0.0377(4)	1.0	0.40(2)
T4	0.1244(1)	0.06556(8)	0.0309(4)	1.0	0.40(2)
T5	0.0722(1)	0.02759(8)	-0.1781(4)	1.0	0.40(2)
T6	0.1904(1)	0.06149(8)	-0.3132(4)	1.0	0.40(2)
T7	0.4242(1)	-0.17245(8)	-0.3172(4)	1.0	0.40(2)
T8	0.3107(1)	-0.12937(8)	-0.1761(4)	1.0	0.40(2)
T9	0.2719(1)	-0.17118(8)	0.0406(4)	1.0	0.40(2)
T10	0.11692(1)	-0.17428(8)	0.0346(4)	1.0	0.40(2)
T11	0.07135(1)	-0.12930(8)	-0.1780(4)	1.0	0.40(2)
T12	0.1890(1)	-0.17267(8)	-0.3123(4)	1.0	0.40(2)
O1	0.3749(3)	0.0591(3)	-0.2395(6)	1.0	0.81(5)
O2	0.3169(3)	0.0536(4)	-0.0673(5)	1.0	0.81(5)
O3	0.2028(1)	0.0607(4)	0.0218(6)	1.0	0.81(5)
O4	0.0911(3)	0.0639(3)	-0.0762(5)	1.0	0.81(5)
O5	0.1188(2)	0.0555(3)	-0.2648(6)	1.0	0.81(5)
O6	0.2462(3)	0.0567(4)	-0.2303(6)	1.0	0.81(5)
O7	0.3764(3)	-0.1604(4)	-0.2239(6)	1.0	0.81(5)
O8	0.3055(3)	-0.1506(4)	-0.0622(4)	1.0	0.81(5)
O9	0.1943(1)	-0.1569(5)	0.0362(7)	1.0	0.81(5)
O10	0.0883(4)	-0.1647(3)	-0.0745(5)	1.0	0.81(5)
O11	0.1192(3)	-0.1583(4)	-0.2622(7)	1.0	0.81(5)
O12	0.2474(3)	-0.1559(4)	-0.2359(6)	1.0	0.81(5)
O13	0.3140(5)	-0.0497(1)	-0.1843(8)	1.0	0.81(5)
O14	0.0819(4)	-0.0508(1)	-0.1679(8)	1.0	0.81(5)
O15	0.4209(3)	0.1263(2)	-0.3896(6)	1.0	0.81(5)
O16	0.4017(4)	-0.0024(3)	-0.4056(6)	1.0	0.81(5)
O17	0.3957(4)	-0.1323(2)	-0.4114(6)	1.0	0.81(5)
O18	0.1955(3)	0.1315(2)	-0.3701(5)	1.0	0.81(5)
O19	0.1996(4)	0.0025(2)	-0.3930(6)	1.0	0.81(5)
O20	0.1965(4)	-0.1274(2)	-0.4095(5)	1.0	0.81(5)
O21	0.0027(2)	0.0438(3)	-0.2064(4)	1.0	0.81(5)
O22	0.0035(2)	-0.1448(4)	-0.2083(5)	1.0	0.81(5)
O23	0.4276(6)	-1/4	-0.3421(8)	1.0	0.81(5)
O24	0.1932(5)	-1/4	-0.3437(7)	1.0	0.81(5)
O25	0.2834(6)	-1/4	0.0580(9)	1.0	0.81(5)
O26	0.1070(6)	-1/4	0.0697(7)	1.0	0.81(5)

Table S2

ZSM-5c_20, room temperature

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.0565(3)	0.4223(3)	-0.3308(7)	1.0	0.42(3)
T2	0.0334(4)	0.3148(4)	-0.1755(7)	1.0	0.42(3)
T3	0.0616(4)	0.2787(3)	0.0405(8)	1.0	0.42(3)
T4	0.0633(3)	0.1226(3)	0.0311(6)	1.0	0.42(3)
T5	0.0283(3)	0.0727(4)	-0.1776(7)	1.0	0.42(3)
T6	0.0602(4)	0.1924(4)	-0.3140(8)	1.0	0.42(3)
T7	-0.1725(2)	0.4259(3)	-0.3193(7)	1.0	0.42(3)
T8	-0.1261(4)	0.3114(3)	-0.1798(7)	1.0	0.42(3)
T9	-0.1725(3)	0.2718(3)	0.0358(7)	1.0	0.42(3)
T10	-0.1752(3)	0.1175(4)	0.0371(9)	1.0	0.42(3)
T11	-0.1291(3)	0.0708(4)	-0.1739(8)	1.0	0.42(3)
T12	-0.1682(5)	0.1881(3)	-0.3154(7)	1.0	0.42(3)
T13	0.4436(3)	0.4250(4)	-0.3326(7)	1.0	0.42(3)
T14	0.4728(3)	0.3098(4)	-0.1852(7)	1.0	0.42(3)
T15	0.4404(3)	0.2803(3)	0.0353(8)	1.0	0.42(3)
T16	0.4337(3)	0.1234(3)	0.0327(6)	1.0	0.42(3)
T17	0.4735(3)	0.0721(4)	-0.1793(7)	1.0	0.42(3)
T18	0.4394(4)	0.1881(4)	-0.3187(9)	1.0	0.42(3)
T19	0.6709(3)	0.4233(3)	-0.3163(6)	1.0	0.42(3)
T20	0.6318(3)	0.3108(4)	-0.1737(7)	1.0	0.42(3)
T21	0.6713(3)	0.2731(4)	0.0425(7)	1.0	0.42(3)
T22	0.6733(3)	0.1189(4)	0.0346(8)	1.0	0.42(3)
T23	0.6319(3)	0.0735(5)	-0.1808(8)	1.0	0.42(3)
T24	0.6778(5)	0.1931(4)	-0.3095(7)	1.0	0.42(3)
O1	0.0627(6)	0.3760(5)	-0.2352(11)	1.0	0.82(4)
O2	0.0609(9)	0.3160(6)	-0.0640(7)	1.0	0.82(4)
O3	0.0542(6)	0.2009(3)	0.0223(15)	1.0	0.82(4)
O4	0.0675(5)	0.0912(8)	-0.0776(9)	1.0	0.82(4)
O5	0.0507(8)	0.1211(4)	-0.2652(11)	1.0	0.82(4)
O6	0.0565(8)	0.2474(5)	-0.2288(9)	1.0	0.82(4)
O7	-0.1569(8)	0.3765(6)	-0.2294(11)	1.0	0.82(4)
O8	-0.1546(8)	0.3029(6)	-0.0700(9)	1.0	0.82(4)
O9	-0.1563(7)	0.1943(3)	0.0350(14)	1.0	0.82(4)
O10	-0.1660(4)	0.0867(8)	-0.0715(8)	1.0	0.82(4)
O11	-0.1558(7)	0.1199(6)	-0.2582(11)	1.0	0.82(4)
O12	-0.1462(10)	0.2483(7)	-0.2453(14)	1.0	0.82(4)
O13	-0.0464(3)	0.3178(8)	-0.1750(16)	1.0	0.82(4)
O14	-0.0503(2)	0.0802(6)	-0.1599(14)	1.0	0.82(4)
O15	0.1246(2)	0.4199(4)	-0.3920(8)	1.0	0.82(4)
O16	-0.0035(4)	0.3972(8)	-0.3999(12)	1.0	0.82(4)
O17	-0.1334(4)	0.4022(7)	-0.4163(10)	1.0	0.82(4)
O18	0.1326(3)	0.1956(8)	-0.3652(7)	1.0	0.82(4)
O19	0.0039(4)	0.2050(7)	-0.3956(12)	1.0	0.82(4)
O20	-0.1250(5)	0.1891(8)	-0.4148(7)	1.0	0.82(4)
O21	0.0450(5)	0.0016(4)	-0.2085(6)	1.0	0.82(4)
O22	-0.1444(7)	0.0036(4)	-0.2063(9)	1.0	0.82(4)
O23	-0.2511(2)	0.4262(8)	-0.3418(9)	1.0	0.82(4)
O24	-0.2456(4)	0.1946(7)	-0.3434(11)	1.0	0.82(4)
O25	-0.2500(2)	0.2829(7)	0.0581(10)	1.0	0.82(4)
O26	-0.2511(2)	0.1093(7)	0.0712(9)	1.0	0.82(4)
O27	0.4464(9)	0.3741(4)	-0.2422(10)	1.0	0.82(4)
O28	0.4506(7)	0.3130(6)	-0.0716(8)	1.0	0.82(4)
O29	0.4312(7)	0.2021(2)	0.0229(14)	1.0	0.82(4)
O30	0.4407(8)	0.0913(8)	-0.0752(9)	1.0	0.82(4)
O31	0.4431(7)	0.1176(3)	-0.2652(12)	1.0	0.82(4)
O32	0.4423(7)	0.2452(4)	-0.2367(11)	1.0	0.82(4)
O33	0.6600(8)	0.3778(6)	-0.2207(9)	1.0	0.82(4)

O34	0.6482(6)	0.3091(6)	-0.0576(7)	1.0	0.82(4)
O35	0.6548(6)	0.1958(7)	0.0351(14)	1.0	0.82(4)
O36	0.6652(6)	0.0904(7)	-0.0756(7)	1.0	0.82(4)
O37	0.6608(7)	0.1222(6)	-0.2636(9)	1.0	0.82(4)
O38	0.6660(18)	0.2488(6)	-0.2271(11)	1.0	0.82(4)
O39	0.5527(3)	0.3074(11)	-0.1906(12)	1.0	0.82(4)
O40	0.5526(3)	0.0822(6)	-0.1735(16)	1.0	0.82(4)
O41	0.3723(3)	0.4244(5)	-0.3862(9)	1.0	0.82(4)
O42	0.5010(4)	0.4078(9)	-0.4109(11)	1.0	0.82(4)
O43	0.6306(4)	0.3932(5)	-0.4087(8)	1.0	0.82(4)
O44	0.3709(5)	0.1930(7)	-0.3796(12)	1.0	0.82(4)
O45	0.5009(5)	0.1957(8)	-0.3930(10)	1.0	0.82(4)
O46	0.6307(5)	0.2067(7)	-0.4033(8)	1.0	0.82(4)
O47	0.4577(5)	-0.0035(3)	-0.2041(7)	1.0	0.82(4)
O48	0.6487(7)	-0.0011(5)	-0.2103(9)	1.0	0.82(4)

Table S3

ZSM-5c_37, room temperature

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.0556(2)	0.4224(2)	-0.3298(4)	1.0	0.27(3)
T2	0.0349(2)	0.3160(3)	-0.1725(5)	1.0	0.27(3)
T3	0.0627(3)	0.2786(2)	0.0428(5)	1.0	0.27(3)
T4	0.0637(2)	0.1230(2)	0.0319(4)	1.0	0.27(3)
T5	0.0281(2)	0.0735(2)	-0.1758(5)	1.0	0.27(3)
T6	0.0614(2)	0.1940(2)	-0.3114(5)	1.0	0.27(3)
T7	-0.1727(1)	0.4268(2)	-0.3201(5)	1.0	0.27(3)
T8	-0.1241(2)	0.3115(2)	-0.1809(5)	1.0	0.27(3)
T9	-0.1726(2)	0.2708(2)	0.0334(5)	1.0	0.27(3)
T10	-0.1758(2)	0.1164(2)	0.0378(6)	1.0	0.27(3)
T11	-0.1289(2)	0.0700(3)	-0.1717(6)	1.0	0.27(3)
T12	-0.1657(3)	0.1875(2)	-0.3156(5)	1.0	0.27(3)
T13	0.4444(2)	0.4255(2)	-0.3322(5)	1.0	0.27(3)
T14	0.4745(2)	0.3094(3)	-0.1859(5)	1.0	0.27(3)
T15	0.4412(2)	0.2805(2)	0.0358(5)	1.0	0.27(3)
T16	0.4330(2)	0.1241(2)	0.0336(5)	1.0	0.27(3)
T17	0.4746(2)	0.0732(3)	-0.1793(6)	1.0	0.27(3)
T18	0.4394(2)	0.1881(2)	-0.3187(6)	1.0	0.27(3)
T19	0.6709(2)	0.4229(2)	-0.3147(4)	1.0	0.27(3)
T20	0.6329(2)	0.3103(2)	-0.1725(5)	1.0	0.27(3)
T21	0.6709(2)	0.2728(2)	0.0442(5)	1.0	0.27(3)
T22	0.6728(2)	0.1186(2)	0.0357(6)	1.0	0.27(3)
T23	0.6328(2)	0.0746(3)	-0.1816(6)	1.0	0.27(3)
T24	0.680(3)	0.1942(3)	-0.3076(5)	1.0	0.27(3)
O1	0.0641(3)	0.3779(4)	-0.2322(7)	1.0	0.49(4)
O2	0.0631(6)	0.3174(4)	-0.0609(5)	1.0	0.49(4)
O3	0.0531(4)	0.2013(2)	0.0223(9)	1.0	0.49(4)
O4	0.0691(3)	0.0912(5)	-0.0767(6)	1.0	0.49(4)
O5	0.0492(6)	0.1227(3)	-0.2632(7)	1.0	0.49(4)
O6	0.0577(5)	0.2491(3)	-0.2261(7)	1.0	0.49(4)
O7	-0.1559(5)	0.3763(5)	-0.2316(9)	1.0	0.49(4)
O8	-0.1555(5)	0.3018(4)	-0.0728(6)	1.0	0.49(4)
O9	-0.1568(5)	0.1932(2)	0.0325(11)	1.0	0.49(4)
O10	-0.1673(2)	0.0838(5)	-0.0698(6)	1.0	0.49(4)
O11	-0.1555(4)	0.1200(4)	-0.2553(8)	1.0	0.49(4)
O12	-0.1415(7)	0.2484(5)	-0.2483(10)	1.0	0.49(4)
O13	-0.0449(2)	0.3197(5)	-0.1713(12)	1.0	0.49(4)
O14	-0.0502(1)	0.0806(4)	-0.1553(10)	1.0	0.49(4)
O15	0.1234(2)	0.4207(3)	-0.3923(5)	1.0	0.49(4)
O16	-0.0042(3)	0.3943(5)	-0.3965(8)	1.0	0.49(4)
O17	-0.1341(2)	0.4040(4)	-0.4185(7)	1.0	0.49(4)
O18	0.1336(2)	0.1960(5)	-0.3619(5)	1.0	0.49(4)

O19	0.0051(2)	0.2082(4)	-0.3940(8)	1.0	0.49(4)
O20	-0.12274(3)	0.1852(5)	-0.4153(5)	1.0	0.49(4)
O21	0.0445(4)	-0.0003(2)	-0.2083(4)	1.0	0.49(4)
O22	-0.1424(4)	-0.0048(6)	-0.2068(6)	1.0	0.49(4)
O23	-0.2511(1)	0.42739(4)	-0.3407(7)	1.0	0.49(4)
O24	-0.2432(2)	0.1962(5)	-0.3435(8)	1.0	0.49(4)
O25	-0.2500(1)	0.2824(5)	0.0572(7)	1.0	0.49(4)
O26	-0.2516(1)	0.1088(5)	0.0731(7)	1.0	0.49(4)
O27	0.4484(6)	0.3746(3)	-0.2413(8)	1.0	0.49(4)
O28	0.4542(4)	0.3123(4)	-0.0712(6)	1.0	0.49(4)
O29	0.4277(4)	0.2028(1)	0.0236(9)	1.0	0.49(4)
O30	0.443(5)	0.0924(5)	-0.0741(6)	1.0	0.49(4)
O31	0.4412(4)	0.1176(2)	-0.2646(8)	1.0	0.49(4)
O32	0.4417(4)	0.2456(3)	-0.2369(8)	1.0	0.49(4)
O33	0.6612(6)	0.3777(4)	-0.2183(6)	1.0	0.49(4)
O34	0.6462(4)	0.3092(3)	-0.0551(5)	1.0	0.49(4)
O35	0.6542(4)	0.1955(2)	0.0368(10)	1.0	0.49(4)
O36	0.6653(4)	0.0906(5)	-0.0752(5)	1.0	0.49(4)
O37	0.6641(4)	0.1226(4)	-0.2635(6)	1.0	0.49(4)
O38	0.6699(6)	0.2489(5)	-0.2230(7)	1.0	0.49(4)
O39	0.5543(2)	0.3053(7)	-0.1943(7)	1.0	0.49(4)
O40	0.5536(2)	0.0859(4)	-0.1768(11)	1.0	0.49(4)
O41	0.3726(2)	0.4201(3)	-0.3846(6)	1.0	0.49(4)
O42	0.5013(2)	0.4084(6)	-0.4111(8)	1.0	0.49(4)
O43	0.6309(2)	0.3914(3)	-0.4067(5)	1.0	0.49(4)
O44	0.3720(3)	0.1940(5)	-0.3828(9)	1.0	0.49(4)
O45	0.5025(3)	0.1948(5)	-0.3904(7)	1.0	0.49(4)
O46	0.6321(3)	0.2093(4)	-0.3999(5)	1.0	0.49(4)
O47	0.4603(3)	-0.0039(2)	-0.2022(5)	1.0	0.49(4)
O48	0.6479(4)	-0.00054(3)	-0.2107(6)	1.0	0.49(4)

Table S4

ZSM-5c_69, room temperature

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.0555(2)	0.4220(2)	-0.3298(4)	1.0	0.19(6)
T2	0.0332(2)	0.3153(2)	-0.1714(4)	1.0	0.19(6)
T3	0.0626(2)	0.2790(2)	0.0431(5)	1.0	0.19(6)
T4	0.0636(2)	0.1233(2)	0.0313(4)	1.0	0.19(6)
T5	0.0281(2)	0.0735(2)	-0.1761(4)	1.0	0.19(6)
T6	0.0595(2)	0.1937(2)	-0.3117(4)	1.0	0.19(6)
T7	-0.1721(2)	0.4261(2)	-0.3201(4)	1.0	0.19(6)
T8	-0.1259(2)	0.3118(2)	-0.1781(4)	1.0	0.19(6)
T9	-0.1732(2)	0.2704(2)	0.0352(5)	1.0	0.19(6)
T10	-0.1758(2)	0.1165(2)	0.0360(5)	1.0	0.19(6)
T11	-0.1286(2)	0.0697(2)	-0.1728(5)	1.0	0.19(6)
T12	-0.1663(6)	0.1881(2)	-0.3137(4)	1.0	0.19(6)
T13	0.4439(2)	0.4255(2)	-0.3341(4)	1.0	0.19(6)
T14	0.4735(2)	0.3103(2)	-0.1855(4)	1.0	0.19(6)
T15	0.4403(2)	0.2800(2)	0.0345(5)	1.0	0.19(6)
T16	0.4330(2)	0.1236(2)	0.0323(4)	1.0	0.19(6)
T17	0.4737(2)	0.0722(2)	-0.1799(5)	1.0	0.19(6)
T18	0.4394(2)	0.188(2)	-0.3184(5)	1.0	0.19(6)

T19	0.6707(2)	0.4228(2)	-0.3149(4)	1.0	0.19(6)
T20	0.6324(2)	0.3110(2)	-0.1704(4)	1.0	0.19(6)
T21	0.6703(2)	0.2722(2)	0.0452(4)	1.0	0.19(6)
T22	0.6723(2)	0.1184(2)	0.0352(5)	1.0	0.19(6)
T23	0.6317(2)	0.0734(2)	-0.1812(5)	1.0	0.19(6)
T24	0.6791(2)	0.1939(2)	-0.3055(4)	1.0	0.19(6)
O1	0.0626(3)	0.3761(3)	-0.2334(6)	1.0	0.65(4)
O2	0.0636(4)	0.3171(3)	-0.0612(4)	1.0	0.65(4)
O3	0.0528(3)	0.2015(1)	0.0230(9)	1.0	0.65(4)
O4	0.0695(3)	0.0924(5)	-0.0778(5)	1.0	0.65(4)
O5	0.0486(4)	0.1217(2)	-0.2651(6)	1.0	0.65(4)
O6	0.0535(5)	0.2477(3)	-0.2253(6)	1.0	0.65(4)
O7	-0.1570(4)	0.3755(4)	-0.2314(7)	1.0	0.65(4)
O8	-0.1578(4)	0.3032(3)	-0.0704(5)	1.0	0.65(4)
O9	-0.1560(4)	0.1932(2)	0.0315(9)	1.0	0.65(4)
O10	-0.1680(2)	0.0843(4)	-0.0720(5)	1.0	0.65(4)
O11	-0.1544(4)	0.1192(3)	-0.2577(6)	1.0	0.65(4)
O12	-0.1416(6)	0.2475(4)	-0.2439(7)	1.0	0.65(4)
O13	-0.046(2)	0.3208(4)	-0.1671(9)	1.0	0.65(4)
O14	-0.0507(1)	0.0806(4)	-0.1549(8)	1.0	0.65(4)
O15	0.1231(2)	0.4204(3)	-0.3910(5)	1.0	0.65(4)
O16	-0.0045(2)	0.3957(4)	-0.3984(7)	1.0	0.65(4)
O17	-0.1345(2)	0.4025(4)	-0.4182(6)	1.0	0.65(4)
O18	0.1322(2)	0.1979(4)	-0.3606(4)	1.0	0.65(4)
O19	0.0039(2)	0.2071(4)	-0.3955(7)	1.0	0.65(4)
O20	-0.1247(3)	0.1887(4)	-0.4149(5)	1.0	0.65(4)
O21	0.0445(3)	0.0010(2)	-0.2072(4)	1.0	0.65(4)
O22	-0.1420(4)	0.0048(2)	-0.2072(6)	1.0	0.65(4)
O23	-0.2514(1)	0.4280(4)	-0.3414(5)	1.0	0.65(4)
O24	-0.2441(2)	0.1967(4)	-0.3390(7)	1.0	0.65(4)
O25	-0.2506(8)	0.2805(4)	0.0607(6)	1.0	0.65(4)
O26	-0.2517(7)	0.1097(4)	0.0717(6)	1.0	0.65(4)
O27	0.4472(4)	0.3743(2)	-0.2436(6)	1.0	0.65(4)
O28	0.4511(4)	0.3138(3)	-0.0717(4)	1.0	0.65(4)
O29	0.4296(4)	0.2021(1)	0.0203(8)	1.0	0.65(4)
O30	0.4416(4)	0.0902(5)	-0.0748(5)	1.0	0.65(4)
O31	0.4408(4)	0.1172(2)	-0.2648(7)	1.0	0.65(4)
O32	0.4431(4)	0.2452(2)	-0.2364(6)	1.0	0.65(4)
O33	0.6618(4)	0.377(7)	-0.2186(5)	1.0	0.65(4)
O34	0.6472(4)	0.3105(3)	-0.0534(4)	1.0	0.65(4)
O35	0.6528(4)	0.1952(2)	0.0344(9)	1.0	0.65(4)

O36	0.6644(4)	0.0891(5)	-0.0747(4)	1.0	0.65(4)
O37	0.6628(4)	0.1219(3)	-0.2627(6)	1.0	0.65(4)
O38	0.6670(5)	0.2480(4)	-0.2206(6)	1.0	0.65(4)
O39	0.5535(1)	0.3078(5)	-0.1902(7)	1.0	0.65(4)
O40	0.5526(2)	0.0847(3)	-0.1758(9)	1.0	0.65(4)
O41	0.3722(3)	0.4209(3)	-0.3871(6)	1.0	0.65(4)
O42	0.5011(2)	0.4085(5)	-0.4128(6)	1.0	0.65(4)
O43	0.6307()	0.3912(3)	-0.4068(5)	1.0	0.65(4)
O44	0.3715(3)	0.1947(4)	-0.3810(7)	1.0	0.65(4)
O45	0.5019(3)	0.1941(4)	-0.3913(6)	1.0	0.65(4)
O46	0.6316(2)	0.2090(4)	-0.3989(5)	1.0	0.65(4)
O47	0.4596(3)	-0.0038(2)	-0.2048(5)	1.0	0.65(4)
O48	0.6470(4)	-0.0016(2)	-0.2108(6)	1.0	0.65(4)

Table S5

ZSM-5c_15, 200 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42322(9)	0.05659(6)	-0.3372(1)	1.0	1.6(1)
T2	0.31197(9)	0.02987(6)	-0.1846(1)	1.0	1.6(1)
T3	0.28075(9)	0.05903(6)	0.0334(1)	1.0	1.6(1)
T4	0.12365(9)	0.06557(6)	0.0266(1)	1.0	1.6(1)
T5	0.07138(9)	0.02760(6)	-0.1823(1)	1.0	1.6(1)
T6	0.18962(9)	0.06149(6)	-0.3174(1)	1.0	1.6(1)
T7	0.42337(9)	-0.17244(6)	-0.3214(1)	1.0	1.6(1)
T8	0.30987(9)	-0.12936(6)	-0.1803(1)	1.0	1.6(1)
T9	0.27108(9)	-0.17117(6)	0.0364(1)	1.0	1.6(1)
T10	0.11608(9)	-0.17428(6)	0.0304(1)	1.0	1.6(1)
T11	0.07051(9)	-0.12930(6)	-0.1822(1)	1.0	1.6(1)
T12	0.18817(9)	-0.17267(6)	-0.3165(1)	1.0	1.6(1)
O1	0.3720(2)	0.0608(2)	-0.2465(4)	1.0	3.1(2)
O2	0.3168(2)	0.0531(2)	-0.0714(2)	1.0	3.1(2)
O3	0.2023(1)	0.0609(2)	0.0178(4)	1.0	3.1(2)
O4	0.0911(2)	0.0645(2)	-0.0811(2)	1.0	3.1(2)
O5	0.1168(1)	0.0554(2)	-0.2709(4)	1.0	3.1(2)
O6	0.2435(2)	0.0553(3)	-0.2317(4)	1.0	3.1(2)
O7	0.3737(2)	-0.1628(2)	-0.2298(4)	1.0	3.1(2)
O8	0.3051(2)	-0.1496(3)	-0.0658(2)	1.0	3.1(2)
O9	0.1934(1)	-0.1566(4)	0.0324(5)	1.0	3.1(2)
O10	0.0884(2)	-0.1657(2)	-0.0799(2)	1.0	3.1(2)
O11	0.1169(1)	-0.1581(3)	-0.2688(4)	1.0	3.1(2)
O12	0.2447(2)	-0.1544(3)	-0.2378(4)	1.0	3.1(2)
O13	0.3150(3)	-0.0498(1)	-0.1900(5)	1.0	3.1(2)
O14	0.0820(2)	-0.0508(1)	-0.1716(5)	1.0	3.1(2)
O15	0.4230(2)	0.1258(1)	-0.3959(4)	1.0	3.1(2)
O16	0.4027(2)	-0.0029(2)	-0.4098(4)	1.0	3.1(2)
O17	0.3962(2)	-0.1328(1)	-0.4162(3)	1.0	3.1(2)
O18	0.1962(2)	0.1315(1)	-0.3732(3)	1.0	3.1(2)
O19	0.1997(3)	0.0023(2)	-0.3967(4)	1.0	3.1(2)
O20	0.19692(2)	-0.1277(1)	-0.4140(3)	1.0	3.1(2)
O21	-0.0044(1)	0.0429(2)	-0.2073(3)	1.0	3.1(2)
O22	-0.0053(1)	-0.1436(2)	-0.2092(3)	1.0	3.1(2)
O23	0.4297(4)	-1/4	-0.3472(5)	1.0	3.1(2)
O24	0.1933(4)	-1/4	-0.3459(5)	1.0	3.1(2)
O25	0.2827(4)	-1/4	0.0525(6)	1.0	3.1(2)
O26	0.1061(4)	-1/4	0.0657(4)	1.0	3.1(2)

Table S6

ZSM-5c_15, 400 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42313(9)	0.05656(6)	-0.3368(2)	1.0	2.3(1)
T2	0.31189(9)	0.02984(6)	-0.1843(2)	1.0	2.3(1)
T3	0.28067(9)	0.05900(6)	0.0337(2)	1.0	2.3(1)
T4	0.12357(9)	0.06554(6)	0.0269(2)	1.0	2.3(1)
T5	0.07130(9)	0.02757(6)	-0.1819(2)	1.0	2.3(1)
T6	0.18954(9)	0.06146(6)	-0.3170(2)	1.0	2.3(1)
T7	0.42329(9)	-0.17247(6)	-0.3210(2)	1.0	2.3(1)
T8	0.30979(9)	-0.12939(6)	-0.1800(2)	1.0	2.3(1)
T9	0.27099(9)	-0.17120(6)	0.0367(2)	1.0	2.3(1)
T10	0.11600(9)	-0.17431(6)	0.0307(2)	1.0	2.3(1)
T11	0.07043(9)	-0.12933(6)	-0.1818(2)	1.0	2.3(1)
T12	0.18809(9)	-0.17270(6)	-0.3161(2)	1.0	2.3(1)
O1	0.3716(2)	0.0612(2)	-0.2466(4)	1.0	4.3(2)
O2	0.3174(2)	0.0523(2)	-0.0707(2)	1.0	4.3(2)
O3	0.2023(1)	0.0606(3)	0.0169(4)	1.0	4.3(2)
O4	0.0904(2)	0.0646(2)	-0.0806(3)	1.0	4.3(2)
O5	0.1167(1)	0.0555(2)	-0.2704(4)	1.0	4.3(2)
O6	0.2431(2)	0.0555(3)	-0.2303(4)	1.0	4.3(2)
O7	0.37354(2)	-0.1631(2)	-0.2294(4)	1.0	4.3(2)
O8	0.3052(2)	-0.1487(3)	-0.0652(2)	1.0	4.3(2)
O9	0.1932(1)	-0.1562(4)	0.0324(5)	1.0	4.3(2)
O10	0.0881(3)	-0.1662(2)	-0.0798(3)	1.0	4.3(2)
O11	0.1167(2)	-0.1583(3)	-0.2686(4)	1.0	4.3(2)
O12	0.2445(2)	-0.1548(3)	-0.2369(4)	1.0	4.3(2)
O13	0.3150(4)	-0.0498(1)	-0.1912(5)	1.0	4.3(2)
O14	0.0826(2)	-0.0509(1)	-0.1707(5)	1.0	4.3(2)
O15	0.4235(2)	0.1256(1)	-0.3962(4)	1.0	4.3(2)
O16	0.4025(2)	-0.0029(2)	-0.4095(4)	1.0	4.3(2)
O17	0.3957(2)	-0.1329(2)	-0.4159(4)	1.0	4.3(2)
O18	0.1965(2)	0.1317(1)	-0.3724(3)	1.0	4.3(2)
O19	0.2002(3)	0.0023(2)	-0.3959(4)	1.0	4.3(2)
O20	0.1971(2)	-0.1275(1)	-0.4134(3)	1.0	4.3(2)
O21	-0.0046(1)	0.0422(2)	-0.2076(3)	1.0	4.3(2)
O22	-0.0055(1)	-0.1429(3)	-0.2090(4)	1.0	4.3(2)
O23	0.4302(4)	-1/4	-0.3470(5)	1.0	4.3(2)
O24	0.1933(4)	-1/4	-0.3458(5)	1.0	4.3(2)
O25	0.2823(5)	-1/4	0.0516(6)	1.0	4.3(2)
O26	0.1062(5)	-1/4	0.0664(5)	1.0	4.3(2)

Table S7

ZSM-5c_15, 600 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42304(9)	0.05658(6)	-0.3368(2)	1.0	2.7(1)
T2	0.31180(9)	0.02986(6)	-0.1842(2)	1.0	2.7(1)
T3	0.28057(9)	0.05901(6)	0.0338(2)	1.0	2.7(1)
T4	0.12347(9)	0.06556(6)	0.0270(2)	1.0	2.7(1)
T5	0.07121(9)	0.02758(6)	-0.1819(2)	1.0	2.7(1)
T6	0.18944(9)	0.06148(6)	-0.3170(2)	1.0	2.7(1)
T7	0.42319(9)	-0.17245(6)	-0.3210(2)	1.0	2.7(1)
T8	0.30970(9)	-0.12937(6)	-0.1799(2)	1.0	2.7(1)
T9	0.27090(9)	-0.17119(6)	0.0367(2)	1.0	2.7(1)
T10	0.11590(9)	-0.17429(6)	0.0307(2)	1.0	2.7(1)
T11	0.07033(9)	-0.12931(6)	-0.1818(2)	1.0	2.7(1)
T12	0.18799(9)	-0.17268(6)	-0.3161(2)	1.0	2.7(1)
O1	0.3712(2)	0.0616(2)	-0.2471(4)	1.0	5.0(2)
O2	0.3178(2)	0.0519(2)	-0.0705(2)	1.0	5.0(2)
O3	0.2022(1)	0.0605(3)	0.0158(4)	1.0	5.0(2)
O4	0.0899(2)	0.0648(2)	-0.0805(3)	1.0	5.0(2)
O5	0.1165(1)	0.0554(2)	-0.2705(4)	1.0	5.0(2)
O6	0.2428(2)	0.0556(3)	-0.2294(3)	1.0	5.0(2)
O7	0.3732(2)	-0.1636(2)	-0.2293(4)	1.0	5.0(2)
O8	0.3053(2)	-0.1482(3)	-0.0649(2)	1.0	5.0(2)
O9	0.1930(1)	-0.1554(3)	0.0323(4)	1.0	5.0(2)
O10	0.0880(3)	-0.1666(2)	-0.0799(3)	1.0	5.0(2)
O11	0.1164(2)	-0.1582(3)	-0.2688(4)	1.0	5.0(2)
O12	0.2441(2)	-0.15480(3)	-0.2362(4)	1.0	5.0(2)
O13	0.3151(3)	-0.0498(1)	-0.1919(5)	1.0	5.0(2)
O14	0.0829(2)	-0.0509(1)	-0.1700(5)	1.0	5.0(2)
O15	0.4241(2)	0.1255(1)	-0.3965(4)	1.0	5.0(2)
O16	0.4022(2)	-0.0028(2)	-0.4097(4)	1.0	5.0(2)
O17	0.3953(2)	-0.1330(2)	-0.4157(3)	1.0	5.0(2)
O18	0.1967(2)	0.1319(1)	-0.3719(3)	1.0	5.0(2)
O19	0.2007(3)	0.0025(2)	-0.3956(4)	1.0	5.0(2)
O20	0.1974(2)	-0.1275(1)	-0.4132(3)	1.0	5.0(2)
O21	-0.0048(1)	0.0416(2)	-0.2078(3)	1.0	5.0(2)
O22	-0.0058(1)	-0.1424(2)	-0.2089(3)	1.0	5.0(2)
O23	0.4306(4)	-1/4	-0.3471(5)	1.0	5.0(2)
O24	0.1933(4)	-1/4	-0.3455(5)	1.0	5.0(2)
O25	0.2815(4)	-1/4	0.0510(6)	1.0	5.0(2)
O26	0.1067(4)	-1/4	0.0666(4)	1.0	5.0(2)

Table S8**ZSM-5c_15, 800 °C**

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.4229(1)	0.05661(6)	-0.3369(2)	1.0	2.9(1)
T2	0.3117(1)	0.02990(6)	-0.1844(2)	1.0	2.9(1)
T3	0.2805(1)	0.05905(6)	0.0336(2)	1.0	2.9(1)
T4	0.1234(1)	0.06559(6)	0.0268(2)	1.0	2.9(1)
T5	0.0711(1)	0.02762(6)	-0.1821(2)	1.0	2.9(1)
T6	0.1893(1)	0.06152(6)	-0.3172(2)	1.0	2.9(1)
T7	0.4231(1)	-0.17242(6)	-0.3212(2)	1.0	2.9(1)
T8	0.3096(1)	-0.12934(6)	-0.1801(2)	1.0	2.9(1)
T9	0.2708(1)	-0.17115(6)	0.0366(2)	1.0	2.9(1)
T10	0.1158(1)	-0.17426(6)	0.0306(2)	1.0	2.9(1)
T11	0.0702(1)	-0.12927(6)	-0.1820(2)	1.0	2.9(1)
T12	0.1879(1)	-0.17264(6)	-0.3162(2)	1.0	2.9(1)
O1	0.3709(2)	0.0618(2)	-0.2475(4)	1.0	5.9(3)
O2	0.3179(2)	0.0520(3)	-0.0706(3)	1.0	5.9(3)
O3	0.2022(1)	0.0604(3)	0.0152(4)	1.0	5.9(3)
O4	0.0898(2)	0.0649(2)	-0.0807(3)	1.0	5.9(3)
O5	0.1163(1)	0.0554(2)	-0.2708(4)	1.0	5.9(3)
O6	0.2425(2)	0.0555(3)	-0.2293(4)	1.0	5.9(3)
O7	0.3731(2)	-0.1636(2)	-0.2295(4)	1.0	5.9(3)
O8	0.3052(2)	-0.1481(3)	-0.0650(2)	1.0	5.9(3)
O9	0.1930(1)	-0.1554(3)	0.0323(5)	1.0	5.9(3)
O10	0.0881(3)	-0.1666(2)	-0.0803(3)	1.0	5.9(3)
O11	0.1162(2)	-0.1580(3)	-0.2693(4)	1.0	5.9(3)
O12	0.2439(2)	-0.1546(3)	-0.2362(4)	1.0	5.9(3)
O13	0.3151(3)	-0.0498(1)	-0.1920(5)	1.0	5.9(3)
O14	0.0829(3)	-0.0508(1)	-0.1700(5)	1.0	5.9(3)
O15	0.4243(2)	0.1255(1)	-0.3969(4)	1.0	5.9(3)
O16	0.4023(3)	-0.0028(2)	-0.4099(4)	1.0	5.9(3)
O17	0.3951(3)	-0.1330(2)	-0.4158(3)	1.0	5.9(3)
O18	0.1967(2)	0.1319(1)	-0.3720(3)	1.0	5.9(3)
O19	0.2008(3)	0.0025(2)	-0.3958(4)	1.0	5.9(3)
O20	0.1976(3)	-0.1275(1)	-0.4134(3)	1.0	5.9(3)
O21	-0.0050(1)	0.0416(2)	-0.2081(3)	1.0	5.9(3)
O22	-0.0059(1)	-0.1424(3)	-0.2088(3)	1.0	5.9(3)
O23	0.4306(4)	-1/4	-0.3472(5)	1.0	5.9(3)
O24	0.1932(4)	-1/4	-0.3455(5)	1.0	5.9(3)
O25	0.2815(4)	-1/4	0.0510(6)	1.0	5.9(3)
O26	0.1066(4)	-1/4	0.0666(4)	1.0	5.9(3)

Table S9

ZSM-5c_20, 200 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42323(8)	0.05658(5)	-0.3368(1)	1.0	0.9(6)
T2	0.31199(8)	0.02987(5)	-0.1843(1)	1.0	0.9(6)
T3	0.28076(8)	0.05902(5)	0.0337(1)	1.0	0.9(6)
T4	0.12366(8)	0.06556(5)	0.0270(1)	1.0	0.9(6)
T5	0.07140(8)	0.02759(5)	-0.1819(1)	1.0	0.9(6)
T6	0.18963(8)	0.06149(5)	-0.3170(1)	1.0	0.9(6)
T7	0.42338(8)	-0.17245(5)	-0.3210(1)	1.0	0.9(6)
T8	0.30989(8)	-0.12937(5)	-0.1800(1)	1.0	0.9(6)
T9	0.27109(8)	-0.17118(5)	0.0367(1)	1.0	0.9(6)
T10	0.11609(8)	-0.17428(5)	0.0307(1)	1.0	0.9(6)
T11	0.07052(8)	-0.12930(5)	-0.1818(1)	1.0	0.9(6)
T12	0.18818(8)	-0.17267(5)	-0.3161(1)	1.0	0.9(6)
O1	0.3719(2)	0.0608(2)	-0.2463(3)	1.0	1.9(1)
O2	0.3171(1)	0.0531(2)	-0.0710(2)	1.0	1.9(1)
O3	0.2023(1)	0.0606(2)	0.0176(3)	1.0	1.9(1)
O4	0.0909(2)	0.0648(2)	-0.0808(2)	1.0	1.9(1)
O5	0.1168(1)	0.0553(2)	-0.2705(3)	1.0	1.9(1)
O6	0.2435(1)	0.0555(2)	-0.2311(3)	1.0	1.9(1)
O7	0.3737(2)	-0.1629(2)	-0.2293(3)	1.0	1.9(1)
O8	0.3052(2)	-0.1494(2)	-0.0653(2)	1.0	1.9(1)
O9	0.1934(1)	-0.1559(3)	0.0326(4)	1.0	1.9(1)
O10	0.0883(2)	-0.1659(2)	-0.0796(2)	1.0	1.9(1)
O11	0.1170(1)	-0.1580(3)	-0.2683(3)	1.0	1.9(1)
O12	0.2447(2)	-0.1548(2)	-0.2372(3)	1.0	1.9(1)
O13	0.3149(3)	-0.0498(1)	-0.1900(4)	1.0	1.9(1)
O14	0.0823(2)	-0.0508(1)	-0.1704(4)	1.0	1.9(1)
O15	0.4232(1)	0.1258(1)	-0.3956(3)	1.0	1.9(1)
O16	0.4027(2)	-0.0027(1)	-0.4099(3)	1.0	1.9(1)
O17	0.3960(2)	-0.1328(1)	-0.4157(3)	1.0	1.9(1)
O18	0.1962(2)	0.1317(1)	-0.3726(2)	1.0	1.9(1)
O19	0.1999(2)	0.0025(1)	-0.3966(3)	1.0	1.9(1)
O20	0.1970(2)	-0.1275(1)	-0.4134(2)	1.0	1.9(1)
O21	-0.0044(1)	0.0426(2)	-0.2074(2)	1.0	1.9(1)
O22	-0.0053(1)	-0.1434(2)	-0.2091(3)	1.0	1.9(1)
O23	0.4299(3)	-1/4	-0.3471(4)	1.0	1.9(1)
O24	0.1932(3)	-1/4	-0.3457(4)	1.0	1.9(1)
O25	0.2821(3)	-1/4	0.0528(5)	1.0	1.9(1)
O26	0.1066(3)	-1/4	0.0665(3)	1.0	1.9(1)

Table S10

ZSM-5c_20, 400 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42320(8)	0.05658(5)	-0.3364(1)	1.0	1.4(1)
T2	0.31196(8)	0.02986(5)	-0.1838(1)	1.0	1.4(1)
T3	0.28073(8)	0.05901(5)	0.0342(1)	1.0	1.4(1)
T4	0.12363(8)	0.06556(5)	0.0274(1)	1.0	1.4(1)
T5	0.07137(8)	0.02758(5)	-0.1815(1)	1.0	1.4(1)
T6	0.18960(8)	0.06148(5)	-0.3166(1)	1.0	1.4(1)
T7	0.42335(8)	-0.17245(5)	-0.3206(1)	1.0	1.4(1)
T8	0.30986(8)	-0.12937(5)	-0.1795(1)	1.0	1.4(1)
T9	0.27106(8)	-0.17119(5)	0.0371(1)	1.0	1.4(1)
T10	0.11607(8)	-0.17429(5)	0.0311(1)	1.0	1.4(1)
T11	0.07050(8)	-0.12931(5)	-0.1814(1)	1.0	1.4(1)
T12	0.18815(8)	-0.17268(5)	-0.3157(1)	1.0	1.4(1)
O1	0.3717(2)	0.0614(2)	-0.2462(3)	1.0	2.9(1)
O2	0.3176(1)	0.0522(2)	-0.0702(2)	1.0	2.9(1)
O3	0.2023(1)	0.0604(2)	0.0167(3)	1.0	2.9(1)
O4	0.0901(2)	0.0649(2)	-0.0800(2)	1.0	2.9(1)
O5	0.1168(1)	0.0553(2)	-0.2698(3)	1.0	2.9(1)
O6	0.2433(1)	0.0555(2)	-0.2298(3)	1.0	2.9(1)
O7	0.3736(2)	-0.1636(2)	-0.2287(3)	1.0	2.9(1)
O8	0.3055(2)	-0.1484(2)	-0.0645(2)	1.0	2.9(1)
O9	0.1932(1)	-0.1552(3)	0.0322(4)	1.0	2.9(1)
O10	0.0878(2)	-0.1665(2)	-0.0793(2)	1.0	2.9(1)
O11	0.1168(1)	-0.1581(3)	-0.2679(3)	1.0	2.9(1)
O12	0.24451(2)	-0.1548(3)	-0.2360(3)	1.0	2.9(1)
O13	0.3152(3)	-0.0499(1)	-0.1912(4)	1.0	2.9(1)
O14	0.0829(2)	-0.0509(1)	-0.1693(4)	1.0	2.9(1)
O15	0.4237(2)	0.1257(1)	-0.3958(3)	1.0	2.9(1)
O16	0.4023(2)	-0.0027(1)	-0.4094(3)	1.0	2.9(1)
O17	0.3953(2)	-0.1329(1)	-0.4151(3)	1.0	2.9(1)
O18	0.1966(2)	0.1320(1)	-0.3715(3)	1.0	2.9(1)
O19	0.2005(2)	0.0027(1)	-0.3957(3)	1.0	2.9(1)
O20	0.1973(2)	-0.1274(1)	-0.4127(3)	1.0	2.9(1)
O21	-0.0045(1)	0.0418(2)	-0.2076(2)	1.0	2.9(1)
O22	-0.0056(1)	-0.1425(2)	-0.2090(3)	1.0	2.9(1)
O23	0.4307(3)	-1/4	-0.3468(4)	1.0	2.9(1)
O24	0.1934(3)	-1/4	-0.3449(4)	1.0	2.9(1)
O25	0.2815(4)	-1/4	0.0516(5)	1.0	2.9(1)
O26	0.1072(4)	-1/4	0.0670(4)	1.0	2.9(1)

Table S11

ZSM-5c_20, 600 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42318(8)	0.05660(5)	-0.3362(1)	1.0	1.6(1)
T2	0.31194(8)	0.02988(5)	-0.1837(1)	1.0	1.6(1)
T3	0.28071(8)	0.05903(5)	0.0343(1)	1.0	1.6(1)
T4	0.12361(8)	0.06558(5)	0.02760(1)	1.0	1.6(1)
T5	0.07135(8)	0.02760(5)	-0.1813(1)	1.0	1.6(1)
T6	0.18959(8)	0.06150(5)	-0.3164(1)	1.0	1.6(1)
T7	0.42333(8)	-0.17243(5)	-0.3204(1)	1.0	1.6(1)
T8	0.30984(8)	-0.12935(5)	-0.1794(1)	1.0	1.6(1)
T9	0.27104(8)	-0.17117(5)	0.0373(1)	1.0	1.6(1)
T10	0.11604(8)	-0.17427(5)	0.03135(1)	1.0	1.6(1)
T11	0.07047(8)	-0.12929(5)	-0.1812(1)	1.0	1.6(1)
T12	0.18813(8)	-0.17266(5)	-0.3155(1)	1.0	1.6(1)
O1	0.3715(2)	0.0618(2)	-0.2462(3)	1.0	3.6(2)
O2	0.3182(1)	0.0521(2)	-0.06993(2)	1.0	3.6(2)
O3	0.2023(1)	0.0603(2)	0.0158(3)	1.0	3.6(2)
O4	0.0897(2)	0.0651(2)	-0.0799(2)	1.0	3.6(2)
O5	0.1166(1)	0.0554(2)	-0.2699(3)	1.0	3.6(2)
O6	0.2430(1)	0.0556(2)	-0.2289(3)	1.0	3.6(2)
O7	0.3735(2)	-0.1638(2)	-0.2284(3)	1.0	3.6(2)
O8	0.3056(2)	-0.1481(2)	-0.0641(2)	1.0	3.6(2)
O9	0.1931(1)	-0.15519(3)	0.0326(4)	1.0	3.6(2)
O10	0.0878(2)	-0.1667(2)	-0.0793(2)	1.0	3.6(2)
O11	0.1165(1)	-0.1581(3)	-0.2682(3)	1.0	3.6(2)
O12	0.2443(2)	-0.1548(3)	-0.2356(3)	1.0	3.6(2)
O13	0.3154(3)	-0.0498(1)	-0.1913(4)	1.0	3.6(2)
O14	0.0832(2)	-0.0509(1)	-0.1690(4)	1.0	3.6(2)
O15	0.4241(1)	0.1257(1)	-0.3958(3)	1.0	3.6(2)
O16	0.4021(2)	-0.0027(1)	-0.4092(3)	1.0	3.6(2)
O17	0.3949(2)	-0.1331(1)	-0.4150(3)	1.0	3.6(2)
O18	0.1966(2)	0.1321(1)	-0.3710(3)	1.0	3.6(2)
O19	0.2007(2)	0.0026(1)	-0.3953(3)	1.0	3.6(2)
O20	0.1974(2)	-0.1274(1)	-0.4127(3)	1.0	3.6(2)
O21	-0.0042(1)	0.0414(2)	-0.2081(2)	1.0	3.6(2)
O22	-0.0057(1)	-0.1421(2)	-0.2090(3)	1.0	3.6(2)
O23	0.4309(3)	-1/4	-0.3467(4)	1.0	3.6(2)
O24	0.1934(3)	-1/4	-0.3451(4)	1.0	3.6(2)
O25	0.2816(4)	-1/4	0.0517(5)	1.0	3.6(2)
O26	0.1070(4)	-1/4	0.0676(4)	1.0	3.6(2)

Table S12

ZSM-5c_20, 800 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42317(9)	0.05661(6)	-0.3363(1)	1.0	2.6(1)
T2	0.31192(9)	0.02990(6)	-0.1838(1)	1.0	2.6(1)
T3	0.28070(9)	0.05905(6)	0.0342(1)	1.0	2.6(1)
T4	0.12360(9)	0.06560(6)	0.0275(1)	1.0	2.6(1)
T5	0.07133(9)	0.02762(6)	-0.1814(1)	1.0	2.6(1)
T6	0.18957(9)	0.06152(6)	-0.3165(1)	1.0	2.6(1)
T7	0.42332(9)	-0.17241(6)	-0.3205(1)	1.0	2.6(1)
T8	0.30982(9)	-0.12934(6)	-0.1795(1)	1.0	2.6(1)
T9	0.27103(9)	-0.17115(6)	0.0372(1)	1.0	2.6(1)
T10	0.11603(9)	-0.17425(6)	0.0312(1)	1.0	2.6(1)
T11	0.07046(9)	-0.12927(6)	-0.1813(1)	1.0	2.6(1)
T12	0.18812(9)	-0.17264(6)	-0.3156(1)	1.0	2.6(1)
O1	0.3713(2)	0.0622(2)	-0.2465(3)	1.0	5.5(2)
O2	0.3183(2)	0.0518(2)	-0.0699(2)	1.0	5.5(2)
O3	0.2024(1)	0.0603(2)	0.0154(4)	1.0	5.5(2)
O4	0.0895(2)	0.0652(2)	-0.0799(2)	1.0	5.5(2)
O5	0.1165(1)	0.05540(2)	-0.2701(3)	1.0	5.5(2)
O6	0.2428(2)	0.0556(3)	-0.2286(3)	1.0	5.5(2)
O7	0.3734(2)	-0.1642(2)	-0.2285(3)	1.0	5.5(2)
O8	0.3056(2)	-0.1475(3)	-0.0640(5)	1.0	5.5(2)
O9	0.1931(1)	-0.1548(3)	0.0325(4)	1.0	5.5(2)
O10	0.0878(2)	-0.1670(2)	-0.0796(2)	1.0	5.5(2)
O11	0.1164(1)	-0.1581(3)	-0.2685(3)	1.0	5.5(2)
O12	0.2441(2)	-0.1547(3)	-0.2353(3)	1.0	5.5(2)
O13	0.3156(3)	-0.0498(1)	-0.1923(4)	1.0	5.5(2)
O14	0.0835(2)	-0.0509(1)	-0.1687(5)	1.0	5.5(2)
O15	0.4244(2)	0.1256(1)	-0.3962(3)	1.0	5.5(2)
O16	0.4019(2)	-0.0027(2)	-0.4092(4)	1.0	5.5(2)
O17	0.3947(2)	-0.1331(1)	-0.4150(3)	1.0	5.5(2)
O18	0.1967(2)	0.1323(1)	-0.3707(3)	1.0	5.5(2)
O19	0.2009(3)	0.0027(2)	-0.3953(4)	1.0	5.5(2)
O20	0.1975(2)	-0.1274(1)	-0.4127(3)	1.0	5.5(2)
O21	-0.0048(1)	0.0410(2)	-0.2082(3)	1.0	5.5(2)
O22	-0.0058(1)	-0.1417(2)	-0.2090(3)	1.0	5.5(2)
O23	0.4314(3)	-1/4	-0.3468(5)	1.0	5.5(2)
O24	0.1936(4)	-1/4	-0.3449(5)	1.0	5.5(2)
O25	0.2814(4)	-1/4	0.0508(5)	1.0	5.5(2)
O26	0.1073(4)	-1/4	0.0676(4)	1.0	5.5(2)

Table S13

ZSM-5c_37, 200 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42312(5)	0.0565(3)	-0.3365(1)	1.0	0.89(8)
T2	0.31188(5)	0.0298(3)	-0.1839(1)	1.0	0.89(8)
T3	0.28066(5)	0.0589(3)	0.0341(1)	1.0	0.89(8)
T4	0.12356(5)	0.0655(3)	0.0273(1)	1.0	0.89(8)
T5	0.07129(5)	0.0275(3)	-0.1816(1)	1.0	0.89(8)
T6	0.18953(5)	0.0614(3)	-0.3167(1)	1.0	0.89(8)
T7	0.42328(5)	-0.1724(30)	-0.3207(1)	1.0	0.89(8)
T8	0.30978(5)	-0.1294(3)	-0.1796(1)	1.0	0.89(8)
T9	0.27099(5)	-0.1712(3)	0.0370(1)	1.0	0.89(8)
T10	0.11599(5)	-0.1743(3)	0.0310(1)	1.0	0.89(8)
T11	0.07042(5)	-0.1293(3)	-0.1815(1)	1.0	0.89(8)
T12	0.18808(5)	-0.1727(3)	-0.3158(1)	1.0	0.89(8)
O1	0.3717(1)	0.0609(1)	-0.2463(2)	1.0	2.0(1)
O2	0.3174(1)	0.0526(1)	-0.0704(1)	1.0	2.0(1)
O3	0.2022(6)	0.0605(1)	0.0168(2)	1.0	2.0(1)
O4	0.0904(1)	0.0649(1)	-0.0804(1)	1.0	2.0(1)
O5	0.1168(9)	0.0551(1)	-0.2700(2)	1.0	2.0(1)
O6	0.2432(1)	0.0556(1)	-0.2300(2)	1.0	2.0(1)
O7	0.3736(1)	-0.1631(1)	-0.2290(2)	1.0	2.0(1)
O8	0.3052(1)	-0.1491(1)	-0.0649(5)	1.0	2.0(1)
O9	0.1932(6)	-0.1554(1)	0.0323(2)	1.0	2.0(1)
O10	0.0879(1)	-0.1664(1)	-0.0793(1)	1.0	2.0(1)
O11	0.1169(1)	-0.1579(1)	-0.2680(2)	1.0	2.0(1)
O12	0.2446(1)	-0.1550(1)	-0.2366(2)	1.0	2.0(1)
O13	0.3146(1)	-0.04994(6)	-0.1903(2)	1.0	2.0(1)
O14	0.0825(1)	-0.05094(6)	-0.1694(2)	1.0	2.0(1)
O15	0.4234(1)	0.12576(9)	-0.3956(2)	1.0	2.0(1)
O16	0.4025(1)	-0.0026(1)	-0.4099(2)	1.0	2.0(1)
O17	0.3955(1)	-0.1329(1)	-0.4154(1)	1.0	2.0(1)
O18	0.1966(1)	0.13178(9)	-0.3719(1)	1.0	2.0(1)
O19	0.2004(1)	0.0025(1)	-0.3958(2)	1.0	2.0(1)
O20	0.1973(1)	-0.12751(9)	-0.4129(1)	1.0	2.0(1)
O21	-0.00457(7)	0.0421(1)	-0.2073(1)	1.0	2.0(1)
O22	-0.00550(8)	-0.1431(1)	-0.2088(1)	1.0	2.0(1)
O23	0.4300(2)	-1/4	-0.3468(2)	1.0	2.0(1)
O24	0.1930(2)	-1/4	-0.3453(2)	1.0	2.0(1)
O25	0.2814(2)	-1/4	0.0528(3)	1.0	2.0(1)
O26	0.1070(2)	-1/4	0.0670(2)	1.0	2.0(1)

Table S14

ZSM-5c_37, 400 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42314(5)	0.0565(3)	-0.3362(1)	1.0	1.44(8)
T2	0.31190(5)	0.02985(3)	-0.1836(1)	1.0	1.44(8)
T3	0.28068(5)	0.05900(3)	0.0344(1)	1.0	1.44(8)
T4	0.12358(5)	0.06555(3)	0.0276(1)	1.0	1.44(8)
T5	0.07131(5)	0.02757(3)	-0.1813(1)	1.0	1.44(8)
T6	0.18955(5)	0.06147(3)	-0.3164(1)	1.0	1.44(8)
T7	0.42330(5)	-0.17241(3)	-0.3204(1)	1.0	1.44(8)
T8	0.30980(5)	-0.12938(3)	-0.1793(1)	1.0	1.44(8)
T9	0.27101(5)	-0.17119(3)	0.0373(1)	1.0	1.44(8)
T10	0.11601(5)	-0.17430(3)	0.0313(1)	1.0	1.44(8)
T11	0.07044(5)	-0.12931(3)	-0.1812(1)	1.0	1.44(8)
T12	0.18810(5)	-0.17268(3)	-0.3155(1)	1.0	1.44(8)
O1	0.3716(1)	0.0613(1)	-0.2461(2)	1.0	3.5(1)
O2	0.3178(1)	0.0523(1)	-0.0700(1)	1.0	3.5(1)
O3	0.20234(6)	0.0605(1)	0.0162(2)	1.0	3.5(1)
O4	0.0900(1)	0.0651(1)	-0.0800(1)	1.0	3.5(1)
O5	0.11685(9)	0.0552(1)	-0.2697(2)	1.0	3.5(1)
O6	0.2432(1)	0.0556(1)	-0.2293(2)	1.0	3.5(1)
O7	0.3736(1)	-0.1634(1)	-0.2285(2)	1.0	3.5(1)
O8	0.3053(1)	-0.1487(1)	-0.0644(1)	1.0	3.5(1)
O9	0.19318(6)	-0.1552(1)	0.0325(2)	1.0	3.5(1)
O10	0.0878(1)	-0.1666(1)	-0.0792(1)	1.0	3.5(1)
O11	0.1168(1)	-0.1579(1)	-0.2678(2)	1.0	3.5(1)
O12	0.2445(1)	-0.1550(1)	-0.2360(2)	1.0	3.5(1)
O13	0.3149(1)	-0.04991(6)	-0.1905(2)	1.0	3.5(1)
O14	0.0828(1)	-0.05094(6)	-0.1688(2)	1.0	3.5(1)
O15	0.4237(1)	0.12573(9)	-0.3956(2)	1.0	3.5(1)
O16	0.4022(1)	-0.0026(1)	-0.4095(2)	1.0	3.5(1)
O17	0.3951(1)	-0.1330(1)	-0.4150(1)	1.0	3.5(1)
O18	0.1967(1)	0.13194(9)	-0.3713(1)	1.0	3.5(1)
O19	0.2007(1)	0.0025(1)	-0.3953(2)	1.0	3.5(1)
O20	0.1975(1)	-0.12749(9)	-0.4126(1)	1.0	3.5(1)
O21	-0.00463(7)	0.0418(1)	-0.2075(1)	1.0	3.5(1)
O22	-0.00559(8)	-0.1426(1)	-0.2088(1)	1.0	3.5(1)
O23	0.4304(2)	-1/4	-0.3465(2)	1.0	3.5(1)
O24	0.1931(2)	-1/4	-0.3449(2)	1.0	3.5(1)
O25	0.28132(2)	-1/4	0.0526(3)	1.0	3.5(1)
O26	0.1071(2)	-1/4	0.0675(2)	1.0	3.5(1)

Table S15

ZSM-5c_37, 600 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42308(5)	0.05656(2)	-0.3362(1)	1.0	2.3(1)
T2	0.31183(5)	0.02985(2)	-0.1837(1)	1.0	2.3(1)
T3	0.28061(5)	0.0590(2)	0.0343(1)	1.0	2.3(1)
T4	0.12351(5)	0.06554(2)	0.0275(1)	1.0	2.3(1)
T5	0.07124(5)	0.02757(2)	-0.1819(1)	1.0	2.3(1)
T6	0.18948(5)	0.06147(2)	-0.3164(1)	1.0	2.3(1)
T7	0.42323(5)	-0.17246(2)	-0.3204(1)	1.0	2.3(1)
T8	0.30973(5)	-0.12938(2)	-0.1794(1)	1.0	2.3(1)
T9	0.27094(5)	-0.17119(2)	0.0373(1)	1.0	2.3(1)
T10	0.11594(5)	-0.17430(2)	0.0313(1)	1.0	2.3(1)
T11	0.07037(5)	-0.12932(2)	-0.1812(1)	1.0	2.3(1)
T12	0.18803(5)	-0.17269(2)	-0.3158(1)	1.0	2.3(1)
O1	0.3713(1)	0.0616(12)	-0.2465(2)	1.0	5.4(1)
O2	0.3181(1)	0.0520(1)	-0.0699(1)	1.0	5.4(1)
O3	0.20232(6)	0.0604(1)	0.0155(2)	1.0	5.4(1)
O4	0.0897(1)	0.0652(1)	-0.0800(1)	1.0	5.4(1)
O5	0.11669(9)	0.0552(1)	-0.2699(2)	1.0	5.4(1)
O6	0.2429(1)	0.0556(1)	-0.2287(1)	1.0	5.4(1)
O7	0.3734(1)	-0.1638(1)	-0.2286(2)	1.0	5.4(1)
O8	0.3054(1)	-0.1484(1)	-0.0642(1)	1.0	5.4(1)
O9	0.19306(6)	-0.1548(1)	0.0323(2)	1.0	5.4(1)
O10	0.0876(1)	-0.1669(1)	-0.0794(1)	1.0	5.4(1)
O11	0.1165(1)	-0.1580(1)	-0.2681(2)	1.0	5.4(1)
O12	0.2443(1)	-0.1549(1)	-0.2356(2)	1.0	5.4(1)
O13	0.3151(1)	-0.04993(5)	-0.1911(2)	1.0	5.4(1)
O14	0.0830(1)	-0.05096(5)	-0.1685(2)	1.0	5.4(1)
O15	0.4241(1)	0.1256(8)	-0.3960(2)	1.0	5.4(1)
O16	0.4021(1)	-0.0027(1)	-0.4096(2)	1.0	5.4(1)
O17	0.3948(1)	-0.1331(9)	-0.4150(1)	1.0	5.4(1)
O18	0.1969(1)	0.1320(8)	-0.3710(1)	1.0	5.4(1)
O19	0.2010(1)	0.00264(1)	-0.3952(2)	1.0	5.4(1)
O20	0.1976(1)	-0.12744(9)	-0.4126(1)	1.0	5.4(1)
O21	-0.0048(7)	0.0413(1)	-0.2078(1)	1.0	5.4(1)
O22	-0.0058(7)	-0.1422(1)	-0.2088(1)	1.0	5.4(1)
O23	0.4308(1)	-1/4	-0.3467(2)	1.0	5.4(1)
O24	0.1932(2)	-1/4	-0.3449(2)	1.0	5.4(1)
O25	0.2809(2)	-1/4	0.0521(2)	1.0	5.4(1)
O26	0.10745(2)	-1/4	0.0676(2)	1.0	5.4(1)

Table S16

ZSM-5c_37, 800 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42308(5)	0.05658(2)	-0.3363(1)	1.0	2.8(1)
T2	0.31183(5)	0.02987(2)	-0.1838(1)	1.0	2.8(1)
T3	0.28061(5)	0.05902(2)	0.0342(1)	1.0	2.8(1)
T4	0.12351(5)	0.06557(2)	0.0275(1)	1.0	2.8(1)
T5	0.07124(5)	0.02759(2)	-0.1814(1)	1.0	2.8(1)
T6	0.18948(5)	0.06149(2)	-0.3165(1)	1.0	2.8(1)
T7	0.42323(5)	-0.17240(2)	-0.3205(1)	1.0	2.8(1)
T8	0.30973(5)	-0.12936(2)	-0.1795(1)	1.0	2.8(1)
T9	0.27094(5)	-0.17117(2)	0.0372(1)	1.0	2.8(1)
T10	0.11594(5)	-0.17427(2)	0.0312(1)	1.0	2.8(1)
T11	0.07037(5)	-0.12929(2)	-0.1813(1)	1.0	2.8(1)
T12	0.18803(5)	-0.17266(2)	-0.3156(1)	1.0	2.8(1)
O1	0.3712(1)	0.0619(1)	-0.2467(2)	1.0	5.2(2)
O2	0.3183(1)	0.0520(1)	-0.0699(1)	1.0	5.2(2)
O3	0.2023(6)	0.0604(1)	0.0150(2)	1.0	5.2(2)
O4	0.0896(1)	0.0654(1)	-0.0801(1)	1.0	5.2(2)
O5	0.1165(9)	0.0552(1)	-0.2701(2)	1.0	5.2(2)
O6	0.2427(1)	0.0556(1)	-0.2285(2)	1.0	5.2(2)
O7	0.3733(1)	-0.1640(1)	-0.2286(2)	1.0	5.2(2)
O8	0.3054(1)	-0.1482(1)	-0.0642(1)	1.0	5.2(2)
O9	0.1930(6)	-0.1548(1)	0.0324(2)	1.0	5.2(2)
O10	0.0877(1)	-0.1671(1)	-0.0796(1)	1.0	5.2(2)
O11	0.1164(1)	-0.1579(1)	-0.2685(2)	1.0	5.2(2)
O12	0.2442(1)	-0.1549(1)	-0.2356(2)	1.0	5.2(2)
O13	0.3153(1)	-0.04989(5)	-0.1914(2)	1.0	5.2(2)
O14	0.0832(1)	-0.05095(6)	-0.1684(2)	1.0	5.2(2)
O15	0.4243(1)	0.12566(8)	-0.3962(2)	1.0	5.2(2)
O16	0.4020(1)	-0.0027(1)	-0.4097(2)	1.0	5.2(2)
O17	0.3947(1)	-0.1331(1)	-0.4151(1)	1.0	5.2(2)
O18	0.1968(1)	0.1321(9)	-0.3709(1)	1.0	5.2(2)
O19	0.2011(1)	0.0026(1)	-0.3953(2)	1.0	5.2(2)
O20	0.1976(1)	-0.1278(9)	-0.4128(1)	1.0	5.2(2)
O21	0.0048(7)	0.0412(1)	-0.2079(1)	1.0	5.2(2)
O22	0.0058(8)	-0.1420(1)	-0.2088(1)	1.0	5.2(2)
O23	0.4310(1)	-1/z	-0.3469(2)	1.0	5.2(2)
O24	0.1932(2)	-1/4	-0.3450(2)	1.0	5.2(2)
O25	0.2809(2)	-1/4	0.0519(3)	1.0	5.2(2)
O26	0.1073(2)	-1/4	0.0678(2)	1.0	5.2(2)

Table S17

ZSM-5c_69, 200 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42307(6)	0.05661(4)	-0.3376(1)	1.0	0.90(7)
T2	0.31183(6)	0.02990(4)	-0.1850(1)	1.0	0.90(7)
T3	0.28060(6)	0.05905(4)	0.0330(1)	1.0	0.90(7)
T4	0.12350(6)	0.06559(4)	0.0262(1)	1.0	0.90(7)
T5	0.07124(6)	0.02762(4)	-0.1827(1)	1.0	0.90(7)
T6	0.18947(6)	0.06151(4)	-0.3178(1)	1.0	0.90(7)
T7	0.42322(6)	-0.17242(4)	-0.3218(1)	1.0	0.90(7)
T8	0.30972(6)	-0.12934(4)	-0.1807(1)	1.0	0.90(7)
T9	0.27093(6)	-0.17115(4)	0.0359(1)	1.0	0.90(7)
T10	0.11593(6)	-0.17426(4)	0.0299(1)	1.0	0.90(7)
T11	0.07036(6)	-0.12928(4)	-0.1826(1)	1.0	0.90(7)
T12	0.18802(6)	-0.17265(4)	-0.3169(1)	1.0	0.90(7)
O1	0.3713(1)	0.0610(1)	-0.2479(2)	1.0	1.8(1)
O2	0.3170(1)	0.0532(1)	-0.0719(1)	1.0	1.8(1)
O3	0.2022(7)	0.0605(2)	0.0168(2)	1.0	1.8(1)
O4	0.0911(1)	0.0651(1)	-0.0819(2)	1.0	1.8(1)
O5	0.1165(1)	0.0550(1)	-0.2717(2)	1.0	1.8(1)
O6	0.2430(1)	0.0552(2)	-0.2315(2)	1.0	1.8(1)
O7	0.3732(1)	-0.1632(1)	-0.2304(2)	1.0	1.8(1)
O8	0.3051(1)	-0.1494(2)	-0.0660(1)	1.0	1.8(1)
O9	0.19325(8)	-0.1551(2)	0.0318(3)	1.0	1.8(1)
O10	0.0884(1)	-0.1663(1)	-0.0806(2)	1.0	1.8(1)
O11	0.1166(1)	-0.1578(2)	-0.2695(2)	1.0	1.8(1)
O12	0.2442(1)	-0.1545(2)	-0.2374(2)	1.0	1.8(1)
O13	0.3148(2)	-0.04988(7)	-0.1907(3)	1.0	1.8(1)
O14	0.0824(1)	-0.05087(7)	-0.1705(3)	1.0	1.8(1)
O15	0.4236(1)	0.1258(1)	-0.3967(2)	1.0	1.8(1)
O16	0.4030(1)	-0.0026(1)	-0.4112(2)	1.0	1.8(1)
O17	0.3959(1)	-0.1329(1)	-0.4166(2)	1.0	1.8(1)
O18	0.1963(1)	0.1318(1)	-0.3731(2)	1.0	1.8(1)
O19	0.1999(2)	0.0026(1)	-0.3976(2)	1.0	1.8(1)
O20	0.1973(1)	-0.1276(1)	-0.4141(2)	1.0	1.8(1)
O21	-0.00476(9)	0.0423(1)	-0.2073(2)	1.0	1.8(1)
O22	-0.0056(1)	-0.1430(2)	-0.2089(2)	1.0	1.8(1)
O23	0.4302(2)	-1/4	-0.3478(3)	1.0	1.8(1)
O24	0.1930(2)	-1/4	-0.3458(3)	1.0	1.8(1)
O25	0.2810(3)	-1/4	0.0520(3)	1.0	1.8(1)
O26	0.10743(3)	-1/4	0.0659(3)	1.0	1.8(1)

Table S18

ZSM-5c_69, 400 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42322(6)	0.05658(4)	-0.3362(1)	1.0	1.83(8)
T2	0.31198(6)	0.02987(4)	-0.1836(1)	1.0	1.83(8)
T3	0.28075(6)	0.05902(4)	0.0344(1)	1.0	1.83(8)
T4	0.12365(6)	0.06556(4)	0.0276(1)	1.0	1.83(8)
T5	0.07139(6)	0.02759(4)	-0.1813(1)	1.0	1.83(8)
T6	0.18962(6)	0.06149(4)	-0.3164(1)	1.0	1.83(8)
T7	0.42337(6)	-0.17245(4)	-0.3204(1)	1.0	1.83(8)
T8	0.30988(6)	-0.12937(4)	-0.1793(1)	1.0	1.83(8)
T9	0.27108(6)	-0.17118(4)	0.03739(1)	1.0	1.83(8)
T10	0.11608(6)	-0.17429(4)	0.0314(1)	1.0	1.83(8)
T11	0.07051(6)	-0.12931(4)	-0.1812(1)	1.0	1.83(8)
T12	0.18817(6)	-0.17267(4)	-0.3155(1)	1.0	1.83(8)
O1	0.3717(1)	0.0614(1)	-0.2461(2)	1.0	3.9(1)
O2	0.3178(1)	0.0523(1)	-0.0700(1)	1.0	3.9(1)
O3	0.20238(7)	0.0605(1)	0.0164(2)	1.0	3.9(1)
O4	0.0901(1)	0.0651(1)	-0.0800(2)	1.0	3.9(1)
O5	0.1168(1)	0.0552(1)	-0.2698(2)	1.0	3.9(1)
O6	0.2432(1)	0.0556(2)	-0.2293(2)	1.0	3.9(1)
O7	0.3737(1)	-0.1635(1)	-0.2284(2)	1.0	3.9(1)
O8	0.3054(1)	-0.1485(2)	-0.0643(1)	1.0	3.9(1)
O9	0.19327(8)	-0.1553(2)	0.0326(3)	1.0	3.9(1)
O10	0.0879(1)	-0.1667(1)	-0.0792(2)	1.0	3.9(1)
O11	0.1168(1)	-0.1579(2)	-0.2679(2)	1.0	3.9(1)
O12	0.2445(1)	-0.1548(2)	-0.2359(2)	1.0	3.9(1)
O13	0.3152(2)	-0.0498(7)	-0.1907(3)	1.0	3.9(1)
O14	0.0830(1)	-0.0509(7)	-0.1687(3)	1.0	3.9(1)
O15	0.4237(1)	0.1256(1)	-0.3957(2)	1.0	3.9(1)
O16	0.4022(1)	-0.0027(1)	-0.4094(2)	1.0	3.9(1)
O17	0.3950(1)	-0.1331(1)	-0.4150(2)	1.0	3.9(1)
O18	0.1966(1)	0.1320(1)	-0.3712(2)	1.0	3.9(1)
O19	0.2006(2)	0.0026(1)	-0.3955(2)	1.0	3.9(1)
O20	0.1974(1)	-0.1275(1)	-0.4126(2)	1.0	3.9(1)
O21	-0.00457(9)	0.0416(1)	-0.2076(2)	1.0	3.9(1)
O22	-0.00556(9)	-0.1424(1)	-0.2087(2)	1.0	3.9(1)
O23	0.4306(2)	-1/4	-0.3465(3)	1.0	3.9(1)
O24	0.1933(2)	-1/4	-0.3448(3)	1.0	3.9(1)
O25	0.2816(2)	-1/4	0.0523(3)	1.0	3.9(1)
O26	0.1071(2)	-1/4	0.0677(2)	1.0	3.9(1)

Table S19

ZSM-5c_69, 600 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ui*100
T1	0.42325(6)	0.05660(4)	-0.3361(1)	1.0	1.99(8)
T2	0.31201(6)	0.02988(4)	-0.1835(1)	1.0	1.99(8)
T3	0.28078(6)	0.05903(4)	0.0345(1)	1.0	1.99(8)
T4	0.12368(6)	0.06558(4)	0.0277(1)	1.0	1.99(8)
T5	0.07142(6)	0.02760(4)	-0.1812(1)	1.0	1.99(8)
T6	0.18965(6)	0.06150(4)	-0.3163(1)	1.0	1.99(8)
T7	0.42340(6)	-0.17243(4)	-0.3203(1)	1.0	1.99(8)
T8	0.30991(6)	-0.12935(4)	-0.1792(1)	1.0	1.99(8)
T9	0.27111(6)	-0.17117(4)	0.0374(1)	1.0	1.99(8)
T10	0.11611(6)	-0.17427(4)	0.0314(1)	1.0	1.99(8)
T11	0.07054(6)	-0.12929(4)	-0.1811(1)	1.0	1.99(8)
T12	0.18820(6)	-0.17266(4)	-0.3154(1)	1.0	1.99(8)
O1	0.3716(1)	0.0618(1)	-0.2461(2)	1.0	4.3(1)
O2	0.3181(1)	0.0522(1)	-0.0698(1)	1.0	4.3(1)
O3	0.2024(7)	0.0605(1)	0.0160(2)	1.0	4.3(1)
O4	0.0899(1)	0.0652(1)	-0.0798(2)	1.0	4.3(1)
O5	0.1168(1)	0.0553(1)	-0.2698(2)	1.0	4.3(1)
O6	0.2431(1)	0.0555(2)	-0.2289(2)	1.0	4.3(1)
O7	0.3736(1)	-0.1639(1)	-0.2283(2)	1.0	4.3(1)
O8	0.3056(1)	-0.1483(2)	-0.0640(1)	1.0	4.3(1)
O9	0.1932(8)	-0.1550(2)	0.0325(3)	1.0	4.3(1)
O10	0.0878(1)	-0.1669(1)	-0.0792(2)	1.0	4.3(1)
O11	0.1167(1)	-0.1581(2)	-0.2680(2)	1.0	4.3(1)
O12	0.2444(1)	-0.1547(2)	-0.2356(2)	1.0	4.3(1)
O13	0.3155(2)	-0.04986(7)	-0.1909(3)	1.0	4.3(1)
O14	0.0834(1)	-0.05093(7)	-0.1685(3)	1.0	4.3(1)
O15	0.4240(1)	0.1256(1)	-0.3958(2)	1.0	4.3(1)
O16	0.4020(1)	-0.0027(1)	-0.4092(2)	1.0	4.3(1)
O17	0.3949(1)	-0.1331(1)	-0.4149(2)	1.0	4.3(1)
O18	0.1967(1)	0.1322(1)	-0.3708(2)	1.0	4.3(1)
O19	0.2008(2)	0.0027(1)	-0.3954(2)	1.0	4.3(1)
O20	0.1974(1)	-0.1274(1)	-0.4125(2)	1.0	4.3(1)
O21	-0.00463(9)	0.0413(1)	-0.2078(2)	1.0	4.3(1)
O22	-0.0056(1)	-0.1420(1)	-0.2088(2)	1.0	4.3(1)
O23	0.4310(2)	-1/4	-0.3466(3)	1.0	4.3(1)
O24	0.1936(2)	-1/4	-0.3448(3)	1.0	4.3(1)
O25	0.2814(3)	-1/4	0.0520(3)	1.0	4.3(1)
O26	0.1074(3)	-1/4	0.0679(2)	1.0	4.3(1)

Table S20

ZSM-5c_69, 800 °C

Site	x/a	y/b	z/c	Fraction	Ui/Ue*100
T1	0.42324(6)	0.05660(4)	-0.3358(1)	1.0	2.72(8)
T2	0.31200(6)	0.02988(4)	-0.1833(1)	1.0	2.72(8)
T3	0.28077(6)	0.05904(4)	0.0347(1)	1.0	2.72(8)
T4	0.12367(6)	0.06558(4)	0.0280(1)	1.0	2.72(8)
T5	0.07141(6)	0.02761(4)	-0.1809(1)	1.0	2.72(8)
T6	0.18965(6)	0.06151(4)	-0.3160(1)	1.0	2.72(8)
T7	0.42339(6)	-0.17243(4)	-0.3200(1)	1.0	2.72(8)
T8	0.30990(6)	-0.12935(4)	-0.1790(1)	1.0	2.72(8)
T9	0.27110(6)	-0.17116(4)	0.0377(1)	1.0	2.72(8)
T10	0.11610(6)	-0.17427(4)	0.0317(1)	1.0	2.72(8)
T11	0.07053(6)	-0.12929(4)	-0.1808(1)	1.0	2.72(8)
T12	0.18819(6)	-0.17266(4)	-0.3151(1)	1.0	2.72(8)
O1	0.3715(1)	0.0620(1)	-0.2460(2)	1.0	6.2(1)
O2	0.3185(1)	0.0519(1)	-0.0694(1)	1.0	6.2(1)
O3	0.20244(7)	0.0604(1)	0.0153(2)	1.0	6.2(1)
O4	0.0895(1)	0.0654(1)	-0.0794(2)	1.0	6.2(1)
O5	0.1168(1)	0.0551(1)	-0.2695(2)	1.0	6.2(1)
O6	0.2430(1)	0.0556(1)	-0.2282(2)	1.0	6.2(1)
O7	0.3736(1)	-0.1641(1)	-0.2278(2)	1.0	6.2(1)
O8	0.30573(1)	-0.1479(2)	-0.0636(1)	1.0	6.2(1)
O9	0.19319(8)	-0.1548(2)	0.0327(3)	1.0	6.2(1)
O10	0.0878(1)	-0.1672(1)	-0.0791(1)	1.0	6.2(1)
O11	0.1166(1)	-0.1579(2)	-0.2679(2)	1.0	6.2(1)
O12	0.2443(1)	-0.1547(2)	-0.2350(2)	1.0	6.2(1)
O13	0.3157(2)	-0.04985(7)	-0.1912(3)	1.0	6.2(1)
O14	0.0835(1)	-0.05095(7)	-0.1677(3)	1.0	6.2(1)
O15	0.4242(1)	0.1256(1)	-0.3959(2)	1.0	6.2(1)
O16	0.4018(1)	-0.0027(1)	-0.4090(2)	1.0	6.2(1)
O17	0.3944(1)	-0.1332(1)	-0.4145(2)	1.0	6.2(1)
O18	0.1968(1)	0.13229(1)	-0.3702(2)	1.0	6.2(1)
O19	0.2011(1)	0.0027(1)	-0.3949(2)	1.0	6.2(1)
O20	0.1977(1)	-0.1274(1)	-0.4123(2)	1.0	6.2(1)
O21	-0.00470(8)	0.0409(1)	-0.2078(1)	1.0	6.2(1)
O22	-0.00572(9)	-0.1417(1)	-0.2086(2)	1.0	6.2(1)
O23	0.4312(2)	-1/4	-0.3464(3)	1.0	6.2(1)
O24	0.1936(2)	-1/4	-0.3442(3)	1.0	6.2(1)
O25	0.2812(2)	-1/4	0.0518(3)	1.0	6.2(1)
O26	0.1076(2)	-1/4	0.0684(2)	1.0	6.2(1)

Table S21**ZSM-5c_15, room temperature**

Bond distances (Å)	H*-ZSM-5_15
T1-O1	1.600(3)
T1-O15	1.588(3)
T1-O16	1.593(3)
T1-O21	1.586(3)
T2-O1	1.592(3)
T2-O2	1.593(3)
T2-O6	1.593(3)
T2-O13	1.590(2)
T3-O2	1.583(3)
T3-O3	1.601(3)
T3-O19	1.587(3)
T3-O20	1.600(3)
T4-O3	1.587(3)
T4-O4	1.587(3)
T4-O16	1.611(3)
T4-O17	1.595(3)
T5-O4	1.595(3)
T5-O5	1.596(3)
T5-O14	1.583(3)
T5-O21	1.591(3)
T6-O5	1.587(3)
T6-O6	1.584(4)
T6-O18	1.596(3)
T6-O19	1.602(3)
T7-O7	1.598(3)
T7-O17	1.602(3)
T7-O22	1.593(3)
T7-O23	1.585(2)
T8-O7	1.597(3)
T8-O8	1.591(3)
T8-O12	1.597(3)
T8-O13	1.593(2)
T9-O8	1.592(3)
T9-O9	1.590(4)
T9-O18	1.580(3)
T9-O25	1.607(2)
T10-O9	1.598(4)

T10-O10	1.586(3)
T10-O15	1.591(3)
T10-O26	1.595(2)
T11-O10	1.596(3)
T11-O11	1.595(3)
T11-O14	1.586(3)
T11-O22	1.594(3)
T12-O11	1.585(3)
T12-O12	1.596(3)
T12-O20	1.594(3)
T12-O24	1.602(2)
<T-O >	1.592
T-O-T angles (°)	
T1_O1_T2	149.9(5)
T2_O2_T3	147.7(4)
T3_O3_T4	167.7(6)
T4_O4_T5	152.5(5)
T5_O5_T6	149.3(5)
T2_O6_T6	155.9(6)
T7_O7_T8	150.8(5)
T8_O8_T9	158.5(5)
T9_O9_T10	157.1(8)
T10_O10_T11	159.3(5)
T11_O11_T12	154.6(5)
T8_O12_T12	168.8(6)
T2_O13_T8	173.3(7)
T5_O14_T11	162.2(5)
T1_O15_T10	148.5(5)
T1_O16_T4	174.1(6)
T4_O17_T7	153.2(5)
T6_O18_T9	146.0(4)
T3_O19_T6	171.2(7)
T3_O20_T12	150.7(5)
T1_O21_T5	146.7(4)
T7_O22_T11	151.4(5)
T7_O23_T7	155.1(7)
T12_O24_T12	148.9(7)
T9_O25_T9	156.3(8)
T10_O26_T10	142.6(6)
<T-O-T>	155.8

Table S22**ZSM-5c_20, ZSM-5c_37 and ZSM-5c_69, room temperature**

Bond distances (Å)	ZSM-5c_20	ZSM-5c_37	ZSM-5c_69
T1-O1	1.591(2)	1.592(2)	1.592(3)
T1-O15	1.594(2)	1.594(2)	1.594(4)
T1-O16	1.592(2)	1.592(2)	1.591(3)
T1-O47	1.592(2)	1.592(2)	1.591(3)
T2-O1	1.593(3)	1.593(2)	1.594(3)
T2-O2	1.591(2)	1.592(2)	1.595(4)
T2-O6	1.593(2)	1.593(2)	1.595(3)
T2-O13	1.594(2)	1.593(2)	1.596(4)
T3-O2	1.592(2)	1.593(2)	1.593(3)
T3-O3	1.593(2)	1.593(2)	1.593(3)
T3-O45	1.593(2)	1.594(2)	1.594(3)
T3-O46	1.593(2)	1.592(2)	1.591(4)
T4-O3	1.593(2)	1.593(2)	1.593(3)
T4-O4	1.592(2)	1.593(2)	1.593(4)
T4-O42	1.594(2)	1.594(2)	1.594(3)
T4-O43	1.594(2)	1.593(2)	1.592(4)
T5-O4	1.592(2)	1.593(2)	1.593(4)
T5-O5	1.592(2)	1.593(2)	1.593(3)
T5-O14	1.594(2)	1.593(2)	1.594(4)
T5-O21	1.592(2)	1.593(2)	1.598(3)
T6-O5	1.593(3)	1.593(2)	1.591(3)
T6-O6	1.594(2)	1.594(2)	1.597(3)
T6-O18	1.594(2)	1.594(2)	1.594(4)
T6-O19	1.592(2)	1.592(2)	1.592(4)
T7-O7	1.593(2)	1.593(2)	1.593(3)
T7-O17	1.594(2)	1.594(2)	1.594(4)
T7-O23	1.594(2)	1.593(2)	1.593(4)
T7-O48	1.594(2)	1.594(2)	1.594(3)
T8-O7	1.592(2)	1.593(2)	1.593(3)
T8-O8	1.594(2)	1.592(2)	1.592(4)
T8-O12	1.594(2)	1.594(2)	1.594(3)
T8-O13	1.594(2)	1.594(2)	1.595(4)
T9-O8	1.594(2)	1.593(2)	1.595(3)
T9-O9	1.594(2)	1.593(2)	1.593(3)
T9-O25	1.593(2)	1.593(2)	1.594(4)
T9-O44	1.591(2)	1.591(2)	1.589(3)
T10-O9	1.593(2)	1.593(2)	1.593(3)
T10-O10	1.594(2)	1.594(2)	1.594(4)

T10-O26	1.593(2)	1.594(2)	1.596(4)
T10-O41	1.592(2)	1.592(2)	1.591(3)
T11-O10	1.595(2)	1.594(2)	1.594(4)
T11-O11	1.592(2)	1.593(2)	1.594(3)
T11-O14	1.593(2)	1.593(2)	1.594(4)
T11-O22	1.592(2)	1.593(2)	1.592(3)
T12-O11	1.593(2)	1.593(2)	1.593(3)
T12-O12	1.593(2)	1.593(2)	1.593(3)
T12-O20	1.593(2)	1.593(2)	1.593(4)
T12-O24	1.594(2)	1.593(2)	1.593(4)
T13-O21	1.592(2)	1.593(2)	1.593(3)
T13-O27	1.591(2)	1.592(2)	1.592(3)
T13-O41	1.592(2)	1.592(2)	1.591(4)
T13-O42	1.594(2)	1.594(2)	1.593(4)
T14-O27	1.591(2)	1.592(2)	1.591(3)
T14-O28	1.593(2)	1.593(2)	1.593(4)
T14-O32	1.593(2)	1.593(2)	1.592(3)
T14-O39	1.594(2)	1.594(2)	1.594(4)
T15-O19	1.592(2)	1.592(2)	1.590(4)
T15-O20	1.594(2)	1.594(2)	1.595(3)
T15-O28	1.593(2)	1.593(2)	1.593(3)
T15-O29	1.593(2)	1.593(2)	1.593(3)
T16-O16	1.593(2)	1.593(2)	1.593(4)
T16-O17	1.594(2)	1.594(2)	1.594(3)
T16O29	1.593(2)	1.593(2)	1.593(3)
T16-O30	1.593(2)	1.593(2)	1.593(3)
T17-O30	1.593(2)	1.593(2)	1.592(4)
T17-O31	1.590(2)	1.592(2)	1.591(3)
T17-O40	1.593(2)	1.593(2)	1.593(4)
T17-O47	1.592(2)	1.592(2)	1.591(3)
T18-O31	1.592(2)	1.593(2)	1.592(3)
T18-O32	1.593(2)	1.593(2)	1.594(3)
T18-O44	1.591(2)	1.591(2)	1.590(4)
T18-O45	1.593(2)	1.593(2)	1.593(4)
T19-O22	1.593(3)	1.593(2)	1.593(3)
T19-O23	1.595(2)	1.594(2)	1.595(4)
T19-O33	1.593(2)	1.593(2)	1.593(3)
T19-O43	1.593(2)	1.593(2)	1.596(3)
T20-O33	1.593(2)	1.593(2)	1.597(3)
T20-O34	1.591(2)	1.592(2)	1.592(1)
T20-O38	1.595(3)	1.593(2)	1.594(3)

T20-O39	1.594(2)	1.593(2)	1.593(4)
T21-O18	1.593(2)	1.594(2)	1.595(3)
T21-O25	1.593(2)	1.593(2)	1.593(4)
T21-O34	1.592(2)	1.593(2)	1.593(3)
T21-O35	1.594(2)	1.594(2)	1.595(3)
T22-O15	1.593(2)	1.594(2)	1.593(3)
T22-O26	1.593(2)	1.593(2)	1.593(4)
T22-O35	1.593(2)	1.593(2)	1.594(3)
T22-O36	1.593(2)	1.593(2)	1.593(4)
T23-O36	1.593(2)	1.593(2)	1.593(4)
T23-O37	1.593(2)	1.593(2)	1.593(3)
T23-O40	1.593(2)	1.593(2)	1.592(4)
T23-O48	1.592(2)	1.593(2)	1.592(3)
T24-O24	1.595(2)	1.594(2)	1.595(4)
T24-O37	1.593(2)	1.593(2)	1.593(3)
T24-O38	1.594(2)	1.594(2)	1.594(3)
T24-O46	1.591(2)	1.592(2)	1.590(4)
<T-O>	1.592	1.593	1.593
T-O-T angles (°)			
T1_O1_T2	147.4(8)	145.1(6)	146.7(1)
T2_O2_T3	144.8(7)	143.1(5)	142.7(1)
T3_O3_T4	162.5(7)	159.1(3)	159.9(1)
T4_O4_T5	149.0(7)	145.3(5)	143.9(1)
T5_O5_T6	151.0(6)	153.9(5)	152.0(1)
T2_O6_T6	157.5(7)	157.7(6)	158.8(1)
T7_O7_T8	157.0(8)	158.0(7)	157.0(1)
T8_O8_T9	158.5(9)	160.0(7)	158.6(1)
T9_O9_T10	155.5(7)	155.3(6)	152.9(1)
T10_O10_T11	156.9(6)	154.2(3)	153.6(1)
T11_O11_T12	154.9(8)	158.1(7)	157.7(1)
T8_O12_T12	171.1(1)	172.6(8)	172.6(1)
T2_O13_T8	169.4(8)	168.9(7)	167.0(1)
T5_O14_T11	160.5(6)	158.3(5)	156.9(1)
T1_O15_T22	150.1(6)	149.5(5)	148.6(1)
T1_O16_T16	178.6(7)	173.5(5)	174.4(1)
T7_O17_T16	148.0(7)	146.2(6)	148.2(1)
T6_O18_T21	145.0(7)	141.4(5)	141.5(1)
T6_O19_T15	172.9(6)	172.4(5)	171.0(1)
T12_O20_T15	143.5(7)	139.8(6)	142.6(1)
T5_O21_T13	145.4(4)	144.4(3)	144.3(1)
T11_O22_T19	149.2(6)	149.6(5)	150.1(1)

T7_O23_T19	154.4(5)	156.7(5)	156.2(1)
T12_O24_T24	150.8(6)	148.4(3)	150.1(1)
T9_O25_T21	155.2(7)	155.9(6)	156.0(1)
T10_O26_T22	143.3(5)	142.2(2)	142.8(1)
T13_O27_T14	152.1(8)	152.8(7)	155.3(1)
T14_O28_T15	152.6(8)	154.5(6)	151.0(1)
T15_O29_T16	168.1(9)	163.7(6)	163.7(1)
T16_O30_T17	161.0(9)	163.5(7)	159.7(1)
T17_O31_T18	146.6(6)	145.6(5)	147.0(1)
T14_O32_T18	155.6(7)	153.3(5)	154.7(1)
T19_O33_T20	149.6(6)	147.7(2)	148.6(1)
T20_O34_T21	151.3(6)	150.8(5)	150.1(1)
T21_O35_T22	155.2(7)	154.8(6)	152.7(1)
T22_O36_T23	160.6(7)	160.4(5)	159.8(1)
T23_O37_T24	151.2(7)	151.3(6)	152.2(1)
T20_O38_T24	159.0(7)	154.9(5)	155.8(1)
T14_O39_T20	168.8(8)	164.3(6)	167.1(1)
T17_O40_T23	163.6(5)	162.0(1)	162.7(1)
T10_O41_T13	149.4(6)	149.8(5)	148.0(1)
T4_O42_T13	168.3(9)	166.2(8)	163.(1)
T4_O43_T19	152.1(5)	151.8(3)	152.5(1)
T9_O44_T18	152.0(8)	152.6(7)	151.3(1)
T3_O45_T18	166.0(8)	165.3(7)	164.3(1)
T3_O46_T24	154.7(5)	156.8(3)	156.6(1)
T1_O47_T17	150.4(6)	153.4(4)	150.9(1)
T7_O48_T23	148.6(6)	149.4(5)	149.6(1)
<T-O-T>	155.6	154.88	154.6

Table S23

ZSM-5c_15

Bond distances (Å)	200 °C	400 °C	600 °C	800 °C
T1-O1	1.595(2)	1.594(2)	1.5926(8)	1.5921(9)
T1-O15	1.589(2)	1.590(2)	1.5914(9)	1.5916(11)
T1-O16	1.589(2)	1.590(2)	1.5906(7)	1.5908(9)
T1-O21	1.596(2)	1.594(2)	1.5936(9)	1.5941(11)
T2-O1	1.590(2)	1.591(2)	1.5918(7)	1.5918(9)
T2-O2	1.591(2)	1.590(2)	1.5915(1)	1.5919(12)
T2-O6	1.597(2)	1.596(2)	1.5959(8)	1.5964(10)
T2-O13	1.592(2)	1.593(2)	1.5933(1)	1.5927(13)
T3-O2	1.587(2)	1.589(2)	1.5913(8)	1.5929(10)
T3-O3	1.591(2)	1.590(2)	1.5901(1)	1.5896(13)

T3-O19	1.589(2)	1.591(2)	1.5927(7)	1.5931(9)
T3-O20	1.605(2)	1.602(2)	1.5999(8)	1.5992(10)
T4-O3	1.590(2)	1.590(2)	1.5921(1)	1.5926(13)
T4-O4	1.586(2)	1.588(2)	1.5904(9)	1.5916(11)
T4-O16	1.603(2)	1.598(2)	1.5959(7)	1.5959(9)
T4-O17	1.596(2)	1.595(2)	1.5935(8)	1.5924(10)
T5-O4	1.594(2)	1.594(2)	1.5937(8)	1.5933(10)
T5-O5	1.598(2)	1.596(2)	1.5952(7)	1.5953(8)
T5-O14	1.586(2)	1.588(2)	1.5904(1)	1.5903(13)
T5-O21	1.591(2)	1.590(2)	1.5916(1)	1.5919(12)
T6-O5	1.596(2)	1.595(2)	1.5945(9)	1.5953(12)
T6-O6	1.585(2)	1.589(2)	1.5930(8)	1.5933(9)
T6-O18	1.590(2)	1.591(2)	1.5917(9)	1.5905(11)
T6-O19	1.602(2)	1.597(2)	1.5946(7)	1.5952(9)
T7-O7	1.595(2)	1.594(2)	1.5944(8)	1.5948(9)
T7-O17	1.593(2)	1.593(2)	1.5935(7)	1.5932(9)
T7-O22	1.597(2)	1.597(2)	1.5963(9)	1.5953(11)
T7-O23	1.590(1)	1.590(1)	1.5917(1)	1.5922(13)
T8-O7	1.591(2)	1.591(2)	1.5915(8)	1.5907(9)
T8-O8	1.590(2)	1.588(2)	1.5894(1)	1.5898(12)
T8-O12	1.600(2)	1.599(2)	1.5987(8)	1.5988(10)
T8-O13	1.595(2)	1.596(2)	1.5968(1)	1.5969(13)
T9-O8	1.592(2)	1.594(2)	1.5945(8)	1.5936(10)
T9-O9	1.589(2)	1.591(2)	1.5940(1)	1.5934(13)
T9-O18	1.588(2)	1.589(2)	1.5906(7)	1.5913(9)
T9-O25	1.604(1)	1.599(1)	1.5968(1)	1.5975(13)
T10-O9	1.596(2)	1.594(2)	1.5943(1)	1.5936(13)
T10-O10	1.590(2)	1.592(2)	1.5936(9)	1.5938(11)
T10-O15	1.590(2)	1.591(2)	1.5920(6)	1.5920(8)
T10-O26	1.595(1)	1.595(3)	1.5943(1)	1.5953(12)
T11-O10	1.593(2)	1.593(2)	1.5933(8)	1.5937(10)
T11-O11	1.597(2)	1.596(2)	1.5960(7)	1.5969(8)
T11-O14	1.588(2)	1.589(2)	1.5904(1)	1.5906(13)
T11-O22	1.594(2)	1.593(2)	1.5930(1)	1.5922(12)
T12-O11	1.595(2)	1.595(2)	1.5956(9)	1.5959(11)
T12-O12	1.593(2)	1.594(2)	1.5946(7)	1.5940(9)
T12-O20	1.595(2)	1.594(2)	1.5938(8)	1.5938(10)
T12-O24	1.595(1)	1.594(1)	1.594(10)	1.5941(13)
<T-O>	1.593	1.592	1.593	1.593
T-O-T angles (°)				
T1_O1_T2	150.1(3)	149.8(3)	149.64(2)	149.61(2)

T2_O2_T3	146.9(2)	146.6(2)	146.06(3)	145.80(4)
T3_O3_T4	168.0(2)	166.8(3)	165.62(1)	165.23(2)
T4_O4_T5	152.2(3)	151.6(3)	151.20(2)	151.05(4)
T5_O5_T6	147.2(3)	147.2(3)	147.17(1)	147.00(1)
T2_O6_T6	154.2(2)	153.2(3)	152.39(1)	152.17(1)
T7_O7_T8	151.2(3)	150.9(3)	150.61(1)	150.55(1)
T8_O8_T9	157.8(3)	157.4(3)	157.0(2)	157.03(2)
T9_O9_T10	156.6(5)	156.0(5)	154.96(2)	154.97(4)
T10_O10_T11	158.3(3)	157.5(3)	156.96(2)	156.89(2)
T11_O11_T12	151.8(3)	151.6(3)	151.30(2)	151.02(4)
T8_O12_T12	167.1(2)	166.3(4)	165.69(2)	165.53(1)
T2_O13_T8	170.6(3)	169.4(2)	168.62(1)	168.60(1)
T5_O14_T11	160.7(3)	159.7(2)	158.87(2)	158.75(2)
T1_O15_T10	146.8(3)	146.4(3)	145.84(2)	145.58(2)
T1_O16_T4	173.5(3)	173.7(3)	173.68(3)	173.60(3)
T4_O17_T7	152.3(3)	152.1(2)	151.90(3)	151.80(5)
T6_O18_T9	146.2(3)	146.0(3)	145.76(1)	145.73(1)
T3_O19_T6	171.7(5)	172.6(5)	173.17(3)	173.24(5)
T3_O20_T12	150.4(3)	150.9(3)	151.26(4)	151.23(1)
T1_O21_T5	145.8(2)	145.5(4)	145.30(3)	145.06(7)
T7_O22_T11	149.8(3)	149.6(3)	149.39(2)	149.47(2)
T7_O23_T7	153.2(2)	152.7(5)	152.33(2)	152.33(2)
T12_O24_T12	150.4(5)	150.2(5)	150.37(4)	150.46(3)
T9_O25_T9	157.1(5)	158.2(6)	159.29(2)	159.19(2)
T10_O26_T10	142.4(3)	142.2(3)	142.32(3)	142.21(2)
<T-O-T>	155.0	154.7	154.4	154.3

Table S24

ZSM-5c_20

Bond distances (Å)	200 °C	400 °C	600 °C	800 °C
T1-O1	1.593(1)	1.592(2)	1.592(1)	1.591(2)
T1-O15	1.589(1)	1.590(2)	1.590(2)	1.590(2)
T1-O16	1.590(1)	1.590(2)	1.590(2)	1.590(2)
T1-O21	1.595(1)	1.593(2)	1.592(2)	1.591(2)
T2-O1	1.590(1)	1.592(2)	1.592(2)	1.593(2)
T2-O2	1.589(1)	1.590(2)	1.591(2)	1.589(2)
T2-O6	1.596(1)	1.594(2)	1.593(2)	1.593(2)
T2-O13	1.592(1)	1.593(1)	1.592(1)	1.592(2)
T3-O2	1.588(1)	1.589(1)	1.591(1)	1.592(2)
T3-O3	1.591(1)	1.591(2)	1.590(1)	1.589(2)
T3-O19	1.589(1)	1.591(2)	1.591(1)	1.592(2)

T3-O20	1.602(1)	1.598(2)	1.596(2)	1.594(3)
T4-O3	1.590(1)	1.59(2)	1.591(1)	1.591(2)
T4-O4	1.587(2)	1.589(2)	1.591(1)	1.591(2)
T4-O16	1.601(2)	1.597(2)	1.595(2)	1.594(2)
T4-O17	1.594(2)	1.594(2)	1.592(2)	1.592(2)
T5-O4	1.594(2)	1.594(2)	1.593(2)	1.593(2)
T5-O5	1.596(2)	1.594(2)	1.593(2)	1.592(2)
T5-O14	1.586(2)	1.589(2)	1.590(2)	1.591(2)
T5-O21	1.591(2)	1.590(2)	1.591(2)	1.591(2)
T6-O5	1.595(2)	1.593(2)	1.593(2)	1.593(2)
T6-O6	1.585(2)	1.590(2)	1.592(2)	1.593(2)
T6-O18	1.591(2)	1.592(2)	1.591(2)	1.591(2)
T6-O19	1.600(1)	1.595(1)	1.593(2)	1.591(2)
T7-O7	1.594(1)	1.594(2)	1.594(2)	1.594(2)
T7-O17	1.593(2)	1.593(2)	1.593(2)	1.592(2)
T7-O22	1.597(2)	1.596(2)	1.595(2)	1.595(2)
T7-O23	1.590(1)	1.591(1)	1.591(1)	1.592(1)
T8-O7	1.592(1)	1.593(2)	1.593(2)	1.593(2)
T8-O8	1.590(1)	1.589(2)	1.589(3)	1.588(2)
T8-O12	1.599(1)	1.597(1)	1.597(2)	1.596(2)
T8-O13	1.593(1)	1.595(1)	1.595(1)	1.596(1)
T9-O8	1.591(1)	1.594(2)	1.597(3)	1.593(2)
T9-O9	1.591(2)	1.595(2)	1.595(2)	1.596(2)
T9-O18	1.589(2)	1.588(2)	1.589(2)	1.590(2)
T9-O25	1.601(1)	1.596(1)	1.595(1)	1.593(1)
T10-O9	1.597(2)	1.596(2)	1.593(3)	1.593(2)
T10-O10	1.589(3)	1.593(2)	1.593(3)	1.594(2)
T10-O15	1.590(2)	1.591(2)	1.592(2)	1.592(2)
T10-O26	1.594(1)	1.593(1)	1.594(1)	1.594(1)
T11-O10	1.594(2)	1.593(2)	1.593(2)	1.593(2)
T11-O11	1.593(2)	1.593(2)	1.594(2)	1.593(2)
T11-O14	1.589(1)	1.590(2)	1.590(2)	1.591(2)
T11-O22	1.593(1)	1.594(1)	1.593(2)	1.593(2)
T12-O11	1.594(1)	1.595(2)	1.594(2)	1.595(2)
T12-O12	1.593(1)	1.595(2)	1.594(2)	1.594(2)
T12-O20	1.593(2)	1.592(2)	1.592(2)	1.592(2)
T12-O24	1.594(1)	1.593(1)	1.599(1)	1.592(1)
<T-O>	1.592	1.592	1.592	1.592
T-O-T angles (°)				
T1-O1-T2	150.2(3)	149.7(3)	149.2(3)	148.9(3)
T2-O2-T3	146.7(2)	146.3(2)	145.7(2)	145.6(2)

T3-O3-T4	167.4(2)	166.1(3)	165.1(3)	164.7(2)
T4-O4-T5	151.6(2)	151.1(3)	150.7(3)	150.5(3)
T5-O5-T6	147.4(2)	147.5(2)	147.1(2)	147.1(3)
T2-O6-T6	154.0(3)	153.2(2)	152.5(3)	152.2(3)
T7-O7-T8	151.0(3)	150.4(3)	150.0(3)	149.7(3)
T8-O8-T9	157.5(3)	156.9(3)	156.7(3)	156.4(3)
T9-O9-T10	155.8(2)	154.7(5)	154.6(3)	154.1(5)
T10-O10-T11	157.9(3)	156.9(3)	156.6(3)	156.2(3)
T11-O11-T12	152.0(3)	151.8(3)	151.2(3)	151.0(3)
T8-O12-T12	166.8(2)	165.9(2)	165.7(2)	165.3(3)
T2-O13-T8	170.5(2)	168.9(2)	168.5(2)	167.6(2)
T5-O14-T11	160.0(3)	158.9(3)	158.4(3)	157.8(3)
T1-O15-T10	146.5(2)	146.2(2)	145.6(2)	145.4(3)
T1-O16-T4	173.0(2)	173.5(3)	173.6(2)	173.9(2)
T4-O17-T7	152.3(3)	152.0(3)	151.8(3)	151.6(3)
T6-O18-T9	145.8(2)	145.6(2)	145.3(2)	145.0(3)
T3-O19-T6	171.7(2)	172.5(2)	172.9(2)	173.2(5)
T3-O20-T12	150.8(3)	151.3(3)	151.2(3)	151.3(3)
T1-O21-T5	145.7(2)	145.5(2)	145.0(2)	144.9(2)
T7-O22-T11	149.8(3)	149.3(3)	149.1(3)	148.9(3)
T7-O23-T7	152.9(3)	152.3(2)	152.1(2)	151.8(4)
T12-O24-T12	150.3(3)	150.5(1)	150.2(3)	150.4(5)
T9-O25-T9	157.6(5)	159.4(5)	159.3(5)	160.1(5)
T10-O26-T10	142.3(3)	142.5(1)	142.1(3)	142.2(4)
<T-O-T>	154.9	154.5	154.2	154.0

Table S25

ZSM-5c_37

Bond distances (Å)	200 °C	400 °C	600 °C	800 °C
T1-O1	1.592(1)	1.592(1)	1.591(1)	1.591(1)
T1-O15	1.591(1)	1.591(1)	1.592(1)	1.592(1)
T1-O16	1.591(1)	1.592(1)	1.592(1)	1.592(1)
T1-O21	1.594(1)	1.592(1)	1.592(1)	1.592(1)
T2-O1	1.591(1)	1.591(1)	1.592(1)	1.592(1)
T2-O2	1.591(1)	1.592(1)	1.592(1)	1.592(1)
T2-O6	1.596(1)	1.594(1)	1.594(1)	1.593(1)
T2-O13	1.593(1)	1.593(1)	1.593(1)	1.593(1)
T3-O2	1.589(1)	1.590(1)	1.592(1)	1.592(1)
T3-O3	1.593(1)	1.593(1)	1.592(1)	1.591(1)
T3-O19	1.590(1)	1.590(1)	1.591(1)	1.590(1)
T3-O20	1.601(1)	1.599(1)	1.597(1)	1.596(1)

T4-O3	1.592(1)	1.592(1)	1.593(1)	1.593(1)
T4-O4	1.589(1)	1.591(1)	1.592(1)	1.593(1)
T4-O16	1.597(1)	1.595(1)	1.593(1)	1.592(1)
T4-O17	1.594(2)	1.593(1)	1.593(1)	1.592(1)
T5-O4	1.595(1)	1.595(1)	1.594(1)	1.594(1)
T5-O5	1.596(1)	1.595(1)	1.594(1)	1.593(1)
T5-O14	1.589(1)	1.590(1)	1.591(1)	1.592(1)
T5-O21	1.591(1)	1.591(1)	1.591(1)	1.591(1)
T6-O5	1.594(1)	1.593(1)	1.593(1)	1.593(1)
T6-O6	1.591(1)	1.593(1)	1.594(1)	1.595(1)
T6-O18	1.592(1)	1.591(1)	1.591(1)	1.591(1)
T6-O19	1.597(1)	1.595(1)	1.593(1)	1.593(1)
T7-O7	1.594(1)	1.594(1)	1.594(1)	1.594(1)
T7-O17	1.594(1)	1.594(1)	1.594(1)	1.593(1)
T7-O22	1.597(1)	1.596(1)	1.596(1)	1.595(1)
T7-O23	1.590(8)	1.590(8)	1.591(8)	1.591(8)
T8-O7	1.593(1)	1.593(1)	1.593(1)	1.593(1)
T8-O8	1.590(1)	1.590(1)	1.590(1)	1.590(1)
T8-O12	1.600(1)	1.598(1)	1.597(1)	1.597(1)
T8-O13	1.593(1)	1.594(1)	1.594(1)	1.594(1)
T9-O8	1.592(1)	1.592(1)	1.592(1)	1.591(1)
T9-O9	1.596(1)	1.596(1)	1.598(1)	1.598(1)
T9-O18	1.589(1)	1.589(1)	1.590(1)	1.591(1)
T9-O25	1.598(8)	1.597(8)	1.594(8)	1.594(8)
T10-O9	1.598(1)	1.596(1)	1.595(1)	1.594(1)
T10-O10	1.591(1)	1.593(1)	1.594(1)	1.594(1)
T10-O15	1.590(1)	1.590(1)	1.591(1)	1.591(1)
T10-O26	1.593(1)	1.594(1)	1.593(1)	1.594(1)
T11-O10	1.595(1)	1.594(1)	1.595(1)	1.595(1)
T11-O11	1.595(1)	1.590(1)	1.594(1)	1.594(1)
T11-O14	1.589(1)	1.593(1)	1.590(1)	1.590(1)
T11-O22	1.594(1)	1.593(1)	1.593(1)	1.593(1)
T12-O11	1.595(1)	1.594(1)	1.595(1)	1.595(1)
T12-O12	1.595(1)	1.595(1)	1.595(1)	1.594(1)
T12-O20	1.593(1)	1.593(1)	1.592(1)	1.592(1)
T12-O24	1.593(9)	1.593(9)	1.592(9)	1.592(9)
<T-O>	1.593	1.593	1.593	1.592
T-O-T angles (°)				
T1-O1-T2	150.2(1)	149.9(1)	149.6(1)	149.4(1)
T2-O2-T3	146.4(4)	146.0(1)	145.6(1)	145.4(1)
T3-O3-T4	166.3(2)	165.5(2)	164.8(2)	164.4(1)

T4-O4-T5	151.2(1)	150.9(1)	150.5(1)	150.3(1)
T5-O5-T6	147.6(1)	147.5(1)	147.4(1)	147.2(1)
T2-O6-T6	153.2(2)	152.8(1)	152.3(1)	152.0(1)
T7-O7-T8	150.9(1)	150.5(1)	150.2(1)	150.0(1)
T8-O8-T9	157.4(1)	157.1(1)	156.8(1)	156.7(1)
T9-O9-T10	155.0(2)	154.7(2)	154.1(2)	154.1(2)
T10-O10-T11	157.2(1)	156.8(1)	156.3(1)	156.1(1)
T11-O11-T12	152.1(1)	151.9(1)	151.5(1)	151.3(1)
T8-O12-T12	166.3(3)	166.0(2)	165.6(2)	165.5(2)
T2-O13-T8	170.1(2)	169.4(2)	168.8(2)	168.5(2)
T5-O14-T11	159.3(1)	158.8(1)	158.2(1)	157.9(1)
T1-O15-T10	146.4(1)	146.1(1)	145.7(1)	145.5(1)
T1-O16-T4	173.0(2)	173.2(2)	173.3(2)	173.4(2)
T4-O17-T7	152.1(1)	151.9(1)	151.7(1)	151.6(1)
T6-O18-T9	145.9(1)	145.7(1)	145.5(1)	145.3(1)
T3-O19-T6	172.5(2)	172.9(2)	173.2(2)	173.4(2)
T3-O20-T12	151.2(1)	151.2(1)	151.4(1)	151.3(1)
T1-O21-T5	145.8(1)	145.6(1)	145.3(1)	145.2(1)
T7-O22-T11	149.8(1)	149.6(1)	149.3(1)	149.2(1)
T7-O23-T7	152.7(2)	152.4(2)	152.0(2)	151.9(2)
T12-O24-T12	150.3(2)	150.4(2)	150.4(2)	150.4(2)
T9-O25-T9	158.5(2)	159.0(2)	159.6(2)	159.6(2)
T10-O26-T10	142.3(2)	142.2(2)	142.2(2)	142.0(2)
<T-O-T>	154.7	154.5	154.2	154.1

Table S26

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Bond distances (Å)	200 °C	400 °C	600 °C	800 °C
T1-O1	1.591(1)	1.591(1)	1.591(1)	1.591(1)
T1-O15	1.591(1)	1.590(1)	1.590(1)	1.591(1)
T1-O16	1.591(1)	1.592(1)	1.592(1)	1.593(1)
T1-O21	1.596(1)	1.592(1)	1.591(1)	1.589(1)
T2-O1	1.589(1)	1.592(1)	1.592(1)	1.593(1)
T2-O2	1.588(1)	1.590(1)	1.590(1)	1.591(1)
T2-O6	1.598(1)	1.594(1)	1.593(1)	1.592(1)
T2-O13	1.592(1)	1.592(1)	1.592(1)	1.592(1)
T3-O2	1.589(1)	1.590(1)	1.590(1)	1.592(1)
T3-O3	1.591(1)	1.592(1)	1.591(1)	1.592(1)
T3-O19	1.590(1)	1.590(1)	1.590(1)	1.590(1)
T3-O20	1.601(1)	1.598(1)	1.596(1)	1.594(1)
T4-O3	1.591(1)	1.591(1)	1.591(1)	1.592(1)

T4-O4	1.588(1)	1.590(1)	1.591(1)	1.599(1)
T4-O16	1.599(1)	1.595(1)	1.594(1)	1.520(1)
T4-O17	1.593(1)	1.594(1)	1.593(1)	1.592(1)
T5-O4	1.594(1)	1.594(1)	1.593(1)	1.594(1)
T5-O5	1.597(1)	1.594(1)	1.593(1)	1.591(1)
T5-O14	1.588(1)	1.590(1)	1.591(1)	1.592(1)
T5-O21	1.590(1)	1.590(1)	1.590(1)	1.590(1)
T6-O5	1.597(1)	1.593(1)	1.593(1)	1.593(1)
T6-O6	1.585(1)	1.591(1)	1.591(1)	1.594(1)
T6-O18	1.591(1)	1.591(1)	1.591(1)	1.591(1)
T6-O19	1.600(1)	1.595(1)	1.593(1)	1.591(1)
T7-O7	1.594(1)	1.594(1)	1.594(1)	1.594(1)
T7-O17	1.591(1)	1.594(1)	1.593(1)	1.594(1)
T7-O22	1.599(1)	1.596(1)	1.595(1)	1.594(1)
T7-O23	1.591(1)	1.590(1)	1.591(1)	1.591(1)
T8-O7	1.590(1)	1.593(1)	1.593(1)	1.594(1)
T8-O8	1.591(1)	1.589(1)	1.589(1)	1.589(1)
T8-O12	1.600(1)	1.597(1)	1.596(1)	1.595(1)
T8-O13	1.592(1)	1.594(1)	1.594(1)	1.595(1)
T9-O8	1.590(1)	1.591(1)	1.591(1)	1.591(1)
T9-O9	1.595(1)	1.595(1)	1.596(1)	1.597(1)
T9-O18	1.590(1)	1.589(1)	1.588(1)	1.589(1)
T9-O25	1.599(1)	1.596(1)	1.595(1)	1.593(1)
T10-O9	1.601(1)	1.595(1)	1.594(1)	1.594(1)
T10-O10	1.589(1)	1.592(1)	1.593(1)	1.594(1)
T10-O15	1.589(1)	1.590(1)	1.591(1)	1.590(1)
T10-O26	1.593(1)	1.594(1)	1.594(1)	1.594(1)
T11-O10	1.595(1)	1.594(1)	1.594(1)	1.594(1)
T11-O11	1.595(1)	1.594(1)	1.594(1)	1.593(1)
T11-O14	1.589(1)	1.590(1)	1.590(1)	1.591(1)
T11-O22	1.593(1)	1.593(1)	1.593(1)	1.593(1)
T12-O11	1.594(1)	1.594(1)	1.594(1)	1.594(1)
T12-O12	1.594(1)	1.594(1)	1.594(1)	1.594(1)
T12-O20	1.592(1)	1.592(1)	1.591(1)	1.591(1)
T12-O24	1.592(1)	1.592(1)	1.592(1)	1.591(1)
<T-O>	1.592	1.592	1.592	1.591
T-O-T angles (°)				
T1-O1-T2	150.5(2)	149.7(2)	149.3(2)	149.1(2)
T2-O2-T3	146.6(1)	146.1(1)	145.8(1)	145.4(1)
T3-O3-T4	167.3(2)	165.6(2)	165.1(2)	164.2(2)
T4-O4-T5	151.4(2)	150.8(2)	150.6(2)	150.1(2)

T5-O5-T6	147.1(3)	147.4(2)	147.3(2)	147.4(2)
T2-O6-T6	153.7(2)	152.9(2)	152.6(2)	152.3(2)
T7-O7-T8	151.1(2)	150.3(2)	150.0(2)	149.7(2)
T8-O8-T9	157.4(2)	157.1(2)	156.7(2)	156.5(2)
T9-O9-T10	154.6(3)	154.8(3)	154.3(3)	154.0(3)
T10-O10-T11	157.4(2)	156.7(2)	156.3(2)	155.8(2)
T11-O11-T12	151.6(2)	151.7(2)	151.4(2)	151.3(2)
T8-O12-T12	166.1(2)	166.0(2)	165.8(2)	165.5(2)
T2-O13-T8	170.4(4)	169.1(2)	168.6(2)	168.0(2)
T5-O14-T11	159.2(2)	158.5(2)	158.1(2)	157.6(2)
T1-O15-T10	146.0(2)	146.1(2)	145.8(1)	145.9(3)
T1-O16-T4	172.4(2)	173.4(2)	173.6(2)	173.8(2)
T4-O17-T7	152.1(2)	151.8(2)	151.7(2)	151.5(2)
T6-O18-T9	145.6(3)	145.5(3)	145.2(2)	145.1(3)
T3-O19-T6	171.6(3)	172.7(3)	172.8(3)	173.3(3)
T3-O20-T12	151.0(2)	151.2(2)	151.2(2)	151.3(2)
T1-O21-T5	145.9(1)	145.6(1)	145.3(1)	145.2(1)
T7-O22-T11	149.8(2)	149.6(2)	149.2(2)	149.2(2)
T7-O23-T7	152.6(3)	152.3(2)	152.0(3)	151.8(2)
T12-O24-T12	150.8(3)	150.4(3)	150.3(3)	150.6(3)
T9-O25-T9	158.6(2)	159.0(1)	159.5(2)	160.0(2)
T10-O26-T10	142.6(2)	142.1(2)	142.1(2)	142.0(2)
<T-O-T>	154.7	154.4	154.2	154.1