Supporting Information for:

IMPACT OF COMPOSITION AND STRUCTURAL PARAMETERS ON THE CATALYTIC ACTIVITY OF MFI TYPE TITANOSILIKALITES

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Table S1. Coordinates of atoms, displacement parameters $U_{eq} \times 10^2$ (Å^2), and site occupancies p (s.o.f.) in the structures of TS samples according to the XRPD data

Parameter	Sample		Parameter	Sample	
	TS-1P	TS-1P(75)		TS-1P	TS-1P(75)
Si1			O19		
x	0.42279(18)	0.42269(18)	x	0.1906(4)	0.1906(4)
y	0.05810(16)	0.05800(16)	y	0.0008(4)	0.0013(4)
z	-0.3358(3)	-0.3356(3)	z	-0.4040(6)	-0.4043(6)
p	0.081(9)	0.090(10)	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si2			O20		
x	0.30510(17)	0.30500(17)	x	0.1983(4)	0.1991(4)
y	0.02800(17)	0.02810(17)	y	-0.1316(4)	-0.1313(4)
z	-0.1880(3)	-0.1883(3)	z	-0.4218(6)	-0.4217(6)
p	1.0	1.0	p	1.0	1.0

U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si3			O21		
x	0.27631(18)	0.27661(19)	x	-0.0047(4)	-0.0047(4)
y	0.05611(18)	0.05621(18)	y	0.0457(4)	0.0456(4)
z	0.0310(3)	0.0312(3)	z	-0.2085(6)	-0.2087(6)
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si4			O22		
x	0.11781(18)	0.11791(18)	x	-0.0001(3)	-0.0001(3)
y	0.06250(16)	0.06190(17)	y	-0.1577(4)	-0.1579(4)
z	0.0288(3)	0.0291(3)	z	-0.2057(6)	-0.2058(6)
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si5			O23		
x	0.07120(18)	0.07130(18)	x	0.4227(6)	0.4230(6)
y	0.02759(17)	0.02759(17)	y	-0.2500	-0.2500
z	-0.1855(2)	-0.1852(2)	z	-0.3556(7)	-0.3550(8)
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si6			O24		
x	0.18790(18)	0.18770(18)	x	0.1984(5)	0.1980(5)
y	0.06009(16)	0.06059(16)	y	-0.2500	-0.2500
z	-0.3257(3)	-0.3255(3)	z	-0.3516(8)	-0.3516(8)
p	0.074(10)	0.077(10)	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si7			O25		
x	0.42510(18)	0.42490(18)	x	0.2950(5)	0.2947(6)
y	-0.17120(18)	-0.17130(18)	y	-0.2500	-0.2500
z	-0.3287(2)	-0.3288(2)	z	0.0655(8)	0.0656(8)
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si8			O26		
x	0.30670(18)	0.30680(18)	x	0.1167(5)	0.1172(5)
y	-0.13161(17)	-0.13161(17)	y	-0.2500	-0.2500
z	-0.1866(3)	-0.1863(3)	z	0.0687(8)	0.0690(8)
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.0202(7)	0.0211(8)
Si9			N1		
x	0.27710(18)	0.27700(18)	x	0.4762	0.4762
y	-0.1750(2)	-0.1750(2)	y	0.2500	0.2500
z	0.0307(2)	0.0309(2)	z	-0.1090	-0.1090
p	1.0	1.0	p	1.0	1.0
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.101	0.101
Si10			C1		
x	0.12440(17)	0.12440(17)	x	0.4950	0.4950
y	-0.1740(2)	-0.1739(2)	y	0.2330	0.2330
z	0.0321(2)	0.0322(2)	z	-0.2210	-0.2210
p	1.0	1.0	p	0.30	0.30
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.101	0.101

Si11			C2		
x	0.07290(19)	0.07280(19)	*x*	0.5680	0.5680
y	-0.13020(17)	-0.13020(17)	*y*	0.2500	0.2500
z	-0.1789(2)	-0.1792(2)	*z*	-0.2410	-0.2410
p	1.0	1.0	*p*	0.60	0.60
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.101	0.101
Si12			C3		
x	0.18540(17)	0.18550(17)	*x*	0.5780	0.5780
y	-0.17350(17)	-0.17340(18)	*y*	0.2500	0.2500
z	-0.3217(2)	-0.3221(2)	*z*	-0.3620	-0.3620
p	1.0	1.0	*p*	0.60	0.60
U_{eq}	0.0191(5)	0.0189(5)	U_{eq}	0.101	0.101
O1			C4		
x	0.3750(4)	0.3751(4)	*x*	0.3990	0.3990
y	0.0459(3)	0.0455(3)	*y*	0.2740	0.2740
z	-0.2407(6)	-0.2406(6)	*z*	-0.1000	-0.1000
p	1.0	1.0	*p*	0.30	0.30
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O2			C5		
x	0.3059(4)	0.3062(4)	*x*	0.3550	0.3550
y	0.0618(3)	0.0619(3)	*y*	0.2280	0.2280
z	-0.0800(6)	-0.0801(6)	*z*	-0.1500	-0.1500
p	1.0	1.0	*p*	0.30	0.30
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O3			C6		
x	0.1974(4)	0.1975(4)	*x*	0.2780	0.2780
y	0.0603(4)	0.0600(4)	*y*	0.2500	0.2500
z	0.0249(6)	0.0243(6)	*z*	-0.1470	-0.1470
p	1.0	1.0	*p*	0.60	0.60
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O4			C7		
x	0.0954(4)	0.0952(4)	*x*	0.4960	0.4960
y	0.0639(3)	0.0641(3)	*y*	0.4120	0.4120
z	-0.0848(6)	-0.0846(6)	*z*	0.0450	0.0450
p	1.0	1.0	*p*	0.30	0.30
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O5			C8		
x	0.1151(4)	0.1151(4)	*x*	0.4730	0.4730
y	0.0599(3)	0.0597(3)	*y*	0.3340	0.3340
z	-0.2742(6)	-0.2739(6)	*z*	-0.0190	-0.0190
p	1.0	1.0	*p*	0.30	0.30
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O6			C9		
x	0.2474(4)	0.2475(4)	*x*	0.4960	0.4960
y	0.0671(4)	0.0674(4)	*y*	0.4120	0.4120
z	-0.2482(6)	-0.2483(6)	*z*	0.0450	0.0450
p	1.0	1.0	*p*	0.50	0.50
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O7			C10		
x	0.3744(4)	0.3744(4)	*x*	0.5080	0.5080
y	-0.1563(4)	-0.1561(4)	*y*	0.1990	0.1990
z	-0.2390(6)	-0.2389(6)	*z*	-0.0320	-0.0320
p	1.0	1.0	*p*	0.50	0.50
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101

O8			C11		
x	0.3106(4)	0.3108(4)	*x*	0.4900	0.4900
y	-0.1523(4)	-0.1519(4)	*y*	0.1240	0.1240
z	-0.0716(6)	-0.0713(6)	*z*	-0.0450	-0.0450
p	1.0	1.0	*p*	0.50	0.50
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O9			C12		
x	0.2009(4)	0.2009(4)	*x*	0.5290	0.5290
y	-0.1513(4)	-0.1510(4)	*y*	0.0880	0.0880
z	0.0260(5)	0.0254(5)	*z*	0.0330	0.0330
p	1.0	1.0	*p*	0.50	0.50
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O10			C21		
x	0.0923(4)	0.0926(4)	*x*	0.4130	0.4130
y	-0.1650(4)	-0.1657(4)	*y*	0.2290	0.2290
z	-0.0754(5)	-0.0763(5)	*z*	-0.1660	-0.1660
p	1.0	1.0	*p*	0.20	0.20
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O11			C22		
x	0.1158(4)	0.1157(4)	*x*	0.3550	0.3550
y	-0.1531(3)	-0.1524(3)	*y*	0.2720	0.2720
z	-0.2733(6)	-0.2741(6)	*z*	-0.1500	-0.1500
p	1.0	1.0	*p*	0.20	0.20
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O12			C23		
x	0.2434(3)	0.2433(3)	*x*	0.2850	0.2850
y	-0.1595(4)	-0.1597(4)	*y*	0.2500	0.2500
z	-0.2440(5)	-0.2436(5)	*z*	-0.1950	-0.1950
p	1.0	1.0	*p*	0.40	0.40
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O13			C24		
x	0.3059(4)	0.3057(4)	*x*	0.5340	0.5340
y	-0.0517(3)	-0.0516(4)	*y*	0.2790	0.2790
z	-0.1927(6)	-0.1929(6)	*z*	-0.1850	-0.1850
p	1.0	1.0	*p*	0.20	0.20
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O14			C25		
x	0.0790(4)	0.0787(4)	*x*	0.5460	0.5460
y	-0.0509(3)	-0.0509(3)	*y*	0.2250	0.2250
z	-0.1674(5)	-0.1666(5)	*z*	-0.2630	-0.2630
p	1.0	1.0	*p*	0.20	0.20
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O15			C26		
x	0.4155(4)	0.4150(4)	*x*	0.6010	0.6010
y	0.1300(4)	0.1299(4)	*y*	0.2500	0.2500
z	-0.3879(5)	-0.3877(5)	*z*	-0.3320	-0.3320
p	1.0	1.0	*p*	0.40	0.40
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O16			C27		
x	0.4047(4)	0.4052(4)	*x*	0.4680	0.4680
y	-0.0008(4)	-0.0011(4)	*y*	0.3150	0.3150
z	-0.4117(5)	-0.4116(5)	*z*	-0.0600	-0.0600
p	1.0	1.0	*p*	0.20	0.20

U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O17			C28		
x	0.4043(4)	0.4042(4)	*x*	0.5160	0.5160
y	-0.1352(4)	-0.1356(4)	*y*	0.3350	0.3350
z	-0.4315(6)	-0.4316(6)	*z*	0.0200	0.0200
p	1.0	1.0	*p*	0.20	0.20
U_{eq}	0.0202(7)	0.0211(8)	U_{eq}	0.101	0.101
O18					
x	0.1855(4)	0.1849(4)			
y	0.1303(4)	0.1308(4)			
z	-0.3860(6)	-0.3850(6)			
p	1.0	1.0			
U_{eq}	0.0202(7)	0.0211(8)			

Table S2. Main interatomic distances *d* (Å) in the structures of TS samples according to the XRPD data

Parameter	Sample		Parameter	Sample	
	TS-1P	TS-1P(75)		TS-1P	TS-1P(75)
Si1 – O21	1.590(8)	1.592(9)	Si7 – O22	1.592(8)	1.596(8)
– O16	1.595(8)	1.596(8)	– O7	1.602(8)	1.603(8)
– O15	1.601(8)	1.601(8)	– O17	1.609(8)	1.606(8)
– O1	1.613(8)	1.611(9)	– O23	1.612(4)	1.608(4)
$[Si1–O]_{av}$	1.600	1.600	$[Si7–O]_{av}$	1.604	1.603
Si2 – O13	1.590(8)	1.590(8)	Si8 – O12	1.585(8)	1.589(8)
– O2	1.597(9)	1.600(9)	– O13	1.595(8)	1.598(8)
– O1	1.610(8)	1.609(9)	– O8	1.598(8)	1.596(8)
– O6	1.612(9)	1.609(9)	– O7	1.606(8)	1.604(8)
$[Si2–O]_{av}$	1.602	1.602	$[Si8–O]_{av}$	1.596	1.597
Si3 – O19	1.577(8)	1.580(8)	Si9 – O8	1.593(8)	1.596(8)
– O3	1.587(9)	1.591(9)	– O9	1.600(9)	1.601(9)
– O2	1.606(9)	1.610(9)	– O25	1.607(5)	1.605(5)
– O20	1.709(8)	1.695(8)	– O18	1.613(8)	1.622(8)
$[Si3–O]_{av}$	1.620	1.619	$[Si9–O]_{av}$	1.603	1.606
Si4 – O16	1.534(8)	1.522(8)	Si10 – O10	1.589(8)	1.596(8)
– O4	1.588(9)	1.592(9)	– O26	1.600(5)	1.602(5)
– O3	1.597(9)	1.598(9)	– O15	1.600(8)	1.596(8)
– O17	1.606(8)	1.622(8)	– O9	1.602(9)	1.603(9)
$[Si4–O]_{av}$	1.581	1.584	$[Si10–O]_{av}$	1.598	1.599
Si5 – O14	1.591(8)	1.591(8)	Si11 – O14	1.593(8)	1.594(8)
– O21	1.594(8)	1.597(9)	– O11	1.597(8)	1.598(8)
– O4	1.607(9)	1.606(9)	– O10	1.599(8)	1.600(8)
– O5	1.614(8)	1.611(9)	– O22	1.604(8)	1.603(8)
$[Si5–O]_{av}$	1.602	1.601	$[Si11–O]_{av}$	1.598	1.599
Si6 – O19	1.581(8)	1.586(8)	Si12 – O12	1.586(8)	1.589(8)
– O6	1.588(9)	1.590(9)	– O11	1.592(8)	1.596(8)
– O5	1.615(9)	1.612(9)	– O24	1.598(5)	1.597(5)
– O18	1.617(8)	1.612(8)	– O20	1.602(8)	1.601(8)
$[Si6–O]_{av}$	1.600	1.600	$[Si12–O]_{av}$	1.595	1.596