Structure-direction in the crystallization of ITW zeolite using 2–ethyl–1,3,4–trimethylimidazolium

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Supporting Information

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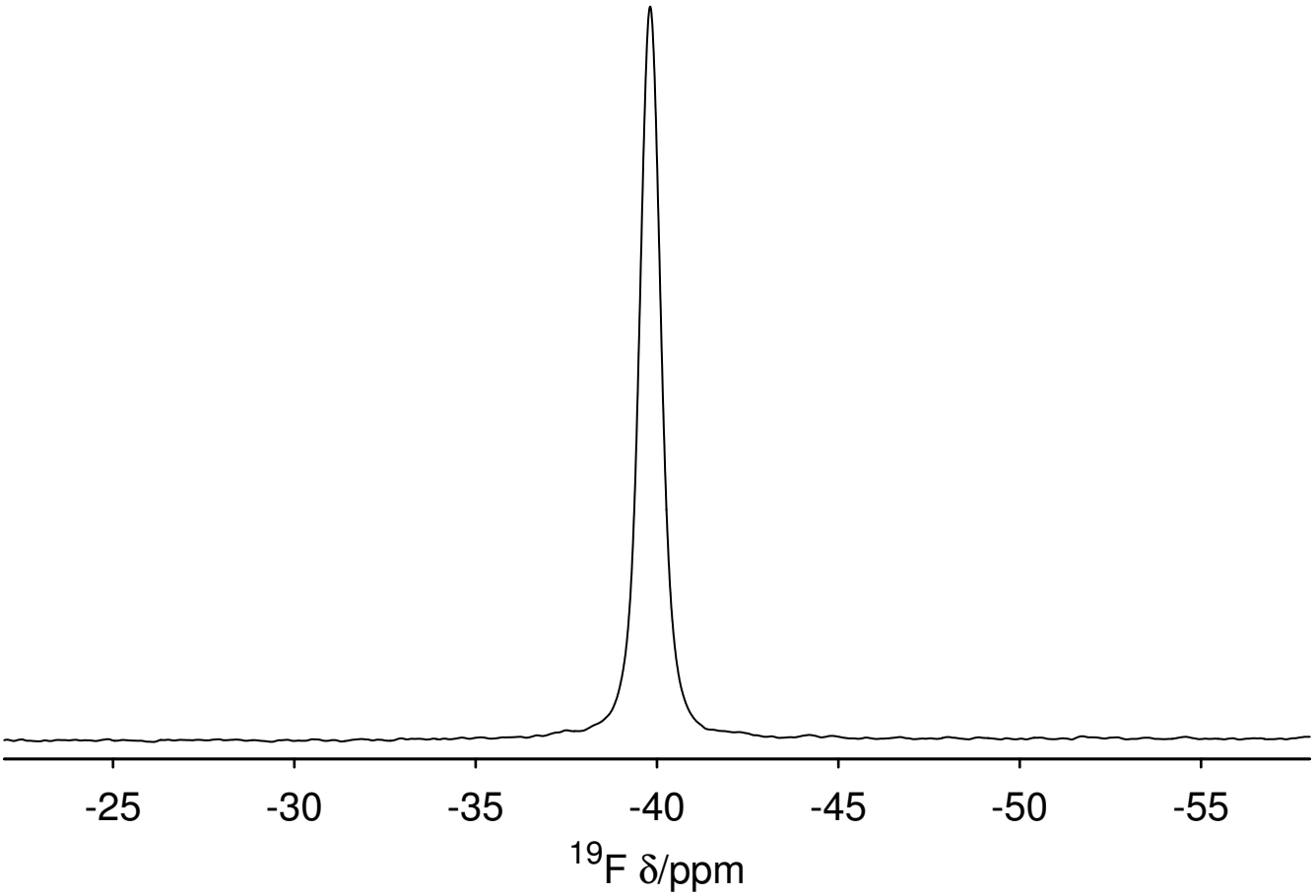

Figure S1: ^{19}F MAS NMR spectrum of as-made 2E134TMI-ITW.

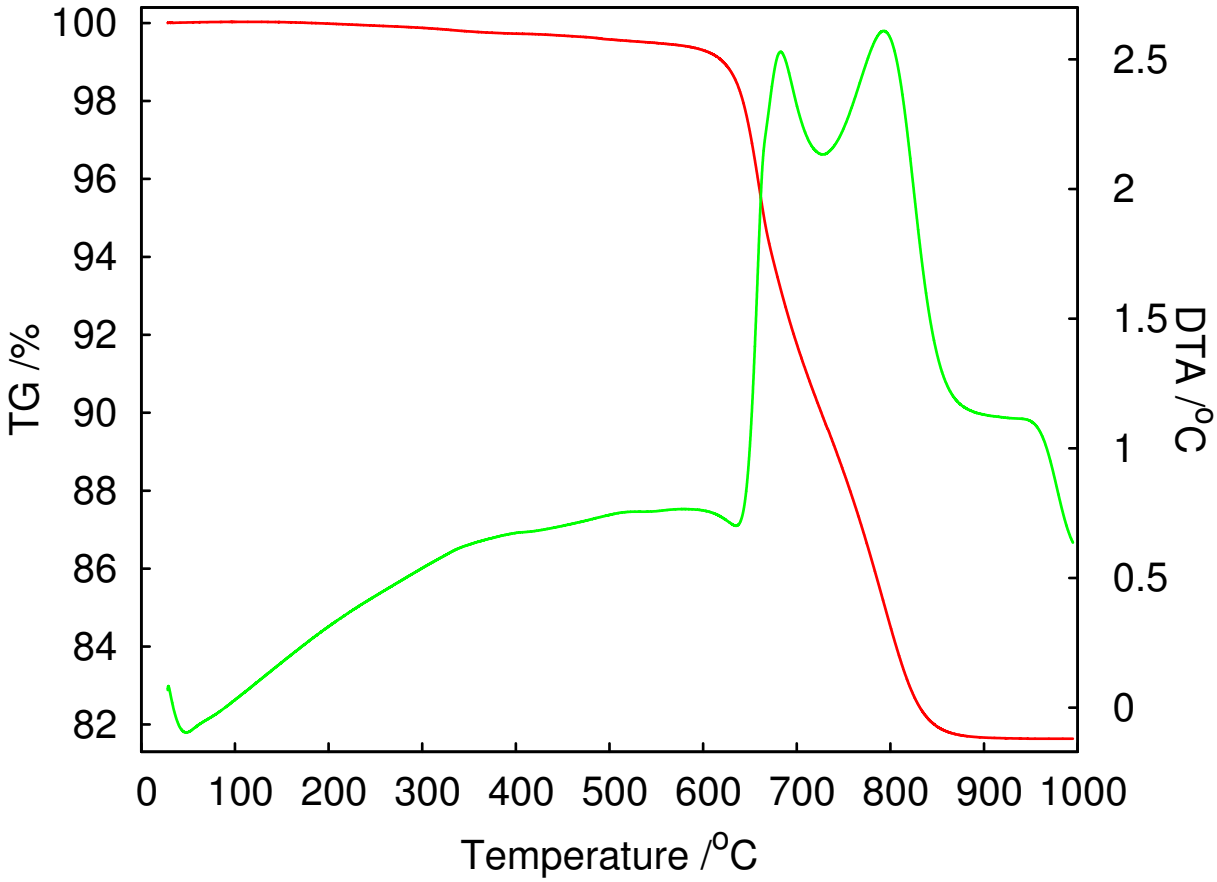

Figure S2: Thermogravimetric (red) and thermodifferential analysis (green) in air of 2E134TMI-ITW.

Table S1: Crystallographic and Experimental Parameters for the Rietveld Refinement of as-made 2E134TMI-ITW.

wavelength (Å)	0.82548
temperature (K)	293
2θ range	2.00-62.00
no. of data points	6001
no. of reflections	1419
Space Group	Cm
unit cell parameters (Å)	
a	10.53225(6)
b	14.96434(9)
c	8.82685(6)
β	106.0718(5)
Cell volume (Å^3)	1336.810(15)
Residuals	
R_{wp}	5.86
R_p	4.42
R_{F^2}	6.507
reduced χ^2	5.416

Table S2: Fractional Atomic Positions, Occupancy Factors and Isotropic Displacement Parameters of as-made 2E134TMI-ITW.

Site	x/a	y/b	z/c	Occupancy*	U_{iso}x100
Si1	0.88103(85)	0.1012(5)	0.5681(4)	1.0	0.769(24)
Si2	0.61976(96)	0.2445(5)	0.9839(12)	1.0	0.769(24)
Si3	0.77714(35)	0.1001(5)	1.2031(10)	1.0	0.769(24)
Si4	0.82377(96)	0.2573(5)	0.7743(13)	1.0	0.769(24)
Si5	0.56705(88)	0.3965(5)	1.188785	1.0	0.769(24)
Si6	0.660153	0.3974(5)	0.5413(10)	1.0	0.769(24)
O14	0.7275(17)	0.000000	1.1480(17)	1.0	0.58(5)
O1	0.7979(14)	0.13046(85)	0.3966(18)	1.0	0.58(5)
O2	0.9604(14)	0.27883(32)	0.8809(23)	1.0	0.58(5)
O3	0.7045(17)	0.500000	0.5779(18)	1.0	0.58(5)
O4	0.6155(12)	0.33163(78)	1.0684(17)	1.0	0.58(5)
O5	0.8994(12)	0.12666(80)	1.1553(17)	1.0	0.58(5)
O6	0.7234(22)	0.25171(141	) 0.8824(25)	1.0	0.58(5)
F1	0.4774(23)	0.500000	0.3939(24)	1.0	2.50(27)
O7	0.8085(12)	0.15852(74)	0.6811(18)	1.0	0.58(5)
O8	1.0234(12)	0.13213(79)	0.5966(17)	1.0	0.58(5)
O9	0.6647(14)	0.16648(85)	1.1153(16)	1.0	0.58(5)
O10	0.7874(14)	0.34212(82)	0.6570(17)	1.0	0.58(5)
O11	0.8651(18)	0.000000	0.6287(22)	1.0	0.58(5)
O12	0.5904(18)	0.500000	1.1448(20)	1.0	0.58(5)
O13	0.6580(13)	0.62364(86)	0.3715(17)	1.0	0.58(5)
C2	0.9892(13)	0.5008(5)	0.4293(12)	0.5	0.40(15)
N1	0.9795(13)	0.4150(5)	0.3894(13)	0.5	0.40(15)
C5	0.9302(12)	0.4078(5)	0.2258(13)	0.5	0.40(15)
C4	0.9106(10)	0.4907(6)	0.1670(12)	0.5	0.40(15)
N3	0.9492(11)	0.5484(5)	0.2967(12)	0.5	0.40(15)
C6	1.0137(17)	0.3365(6)	0.4943(15)	0.5	0.40(15)
C7	0.9457(14)	0.6467(5)	0.2816(13)	0.5	0.40(15)
C8	0.8576(12)	0.5231(7)	0.0013(12)	0.5	0.40(15)
C9	1.0373(17)	0.5376(6)	0.5929(12)	0.5	0.40(15)
C10	1.0632(21)	0.4630(8)	0.7227(13)	0.5	0.40(15)

* not refined

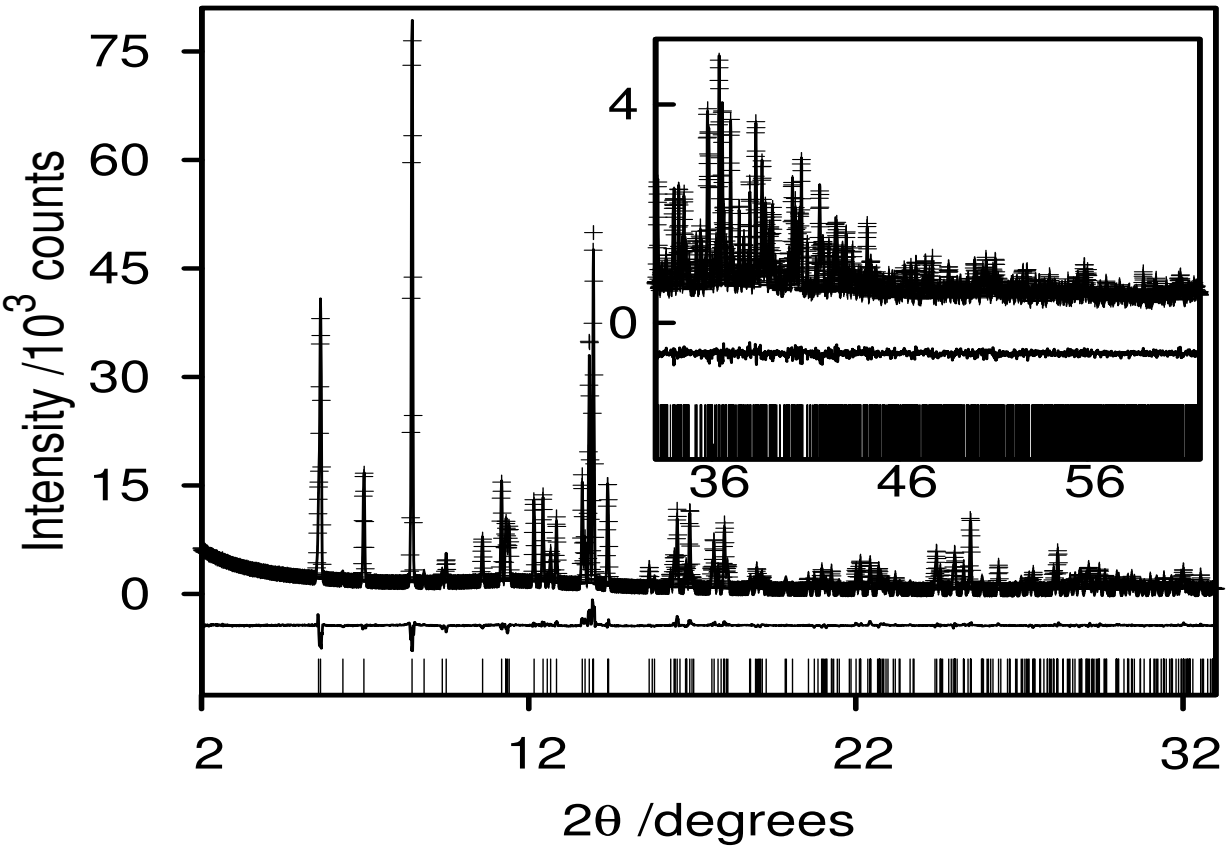

Figure S3: Observed (+) and calculated (solid line) powder X-ray diffractograms for as-made 2E134TMI-ITW refined in space group Cm. Vertical tic marks indicate the positions of allowed reflections. The lower trace is the difference plot. λ=0.82548 Å.