Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting information

Insight into the effect of tetrapropylammonium hydroxide on HZSM-5 zeolite and its application in the reaction between 2,5-dimethylfuran and ethanol to *p*-xylene

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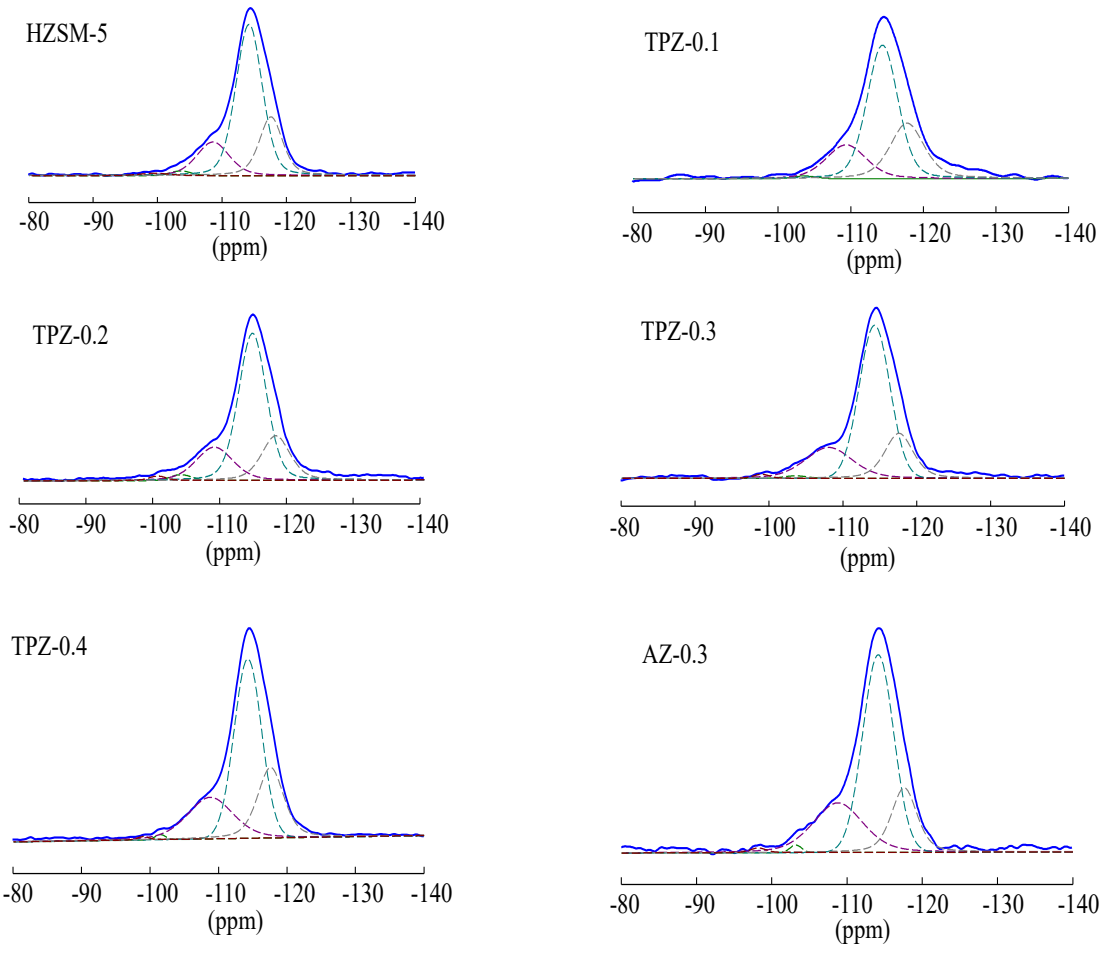

Figure S1 Deconvoluted ^{29}Si MAS NMR spectra of H-ZSM-5 zeolites before and after alkali modification.

Table S1 The Si distribution and content of different sample derived from ^{29}Si MAS NMR spectra deconvolution

sample	Framework Si/Al ratio[1)]	$Si(0Al)_A$ site		$Si(0Al)_B$ site		$Si(1Al)_{site}$		Si(1OH) site		Si(2Al) site	
		ppm	area(%)	ppm	area(%)	ppm	area(%)	ppm	area(%)	ppm	area(%)
HZSM-5	21	-117.6	21.89	-114.2	58.99	-108.6	16.88	-103.6	1.27	-99.51	0.96
TPZ-0.1	21	-117.8	24.87	-114.4	55.30	-108.9	18.05	-103.6	1.48	-99.61	0.30
TPZ-0.3	19	-117.8	19.80	-114.3	58.91	-108.6	18.53	-103.6	1.63	-100.1	1.14
TPZ-0.4	17	-117.6	18.9	-114.3	58.68	-108.1	18.90	-103.6	0.74	-99.00	0.94
TPZ-0.5	16	-117.6	23.47	-114.2	52.42	-108.8	23.08	-102.6	0.57	-99.00	0.46
AZ-0.3	15	-117.6	17.67	-114.2	55.29	-108.8	25.52	-103.6	0.76	-98.60	0.76

1) The framework Si/Al ratio was calculated by the following formula:

$$Si/Al_{NMR} = \sum_{n=0}^{4} I_{Si(nAl)} \Big/ \sum_{n=0}^{4} 0.25n[I_{Si(nAl)}]$$

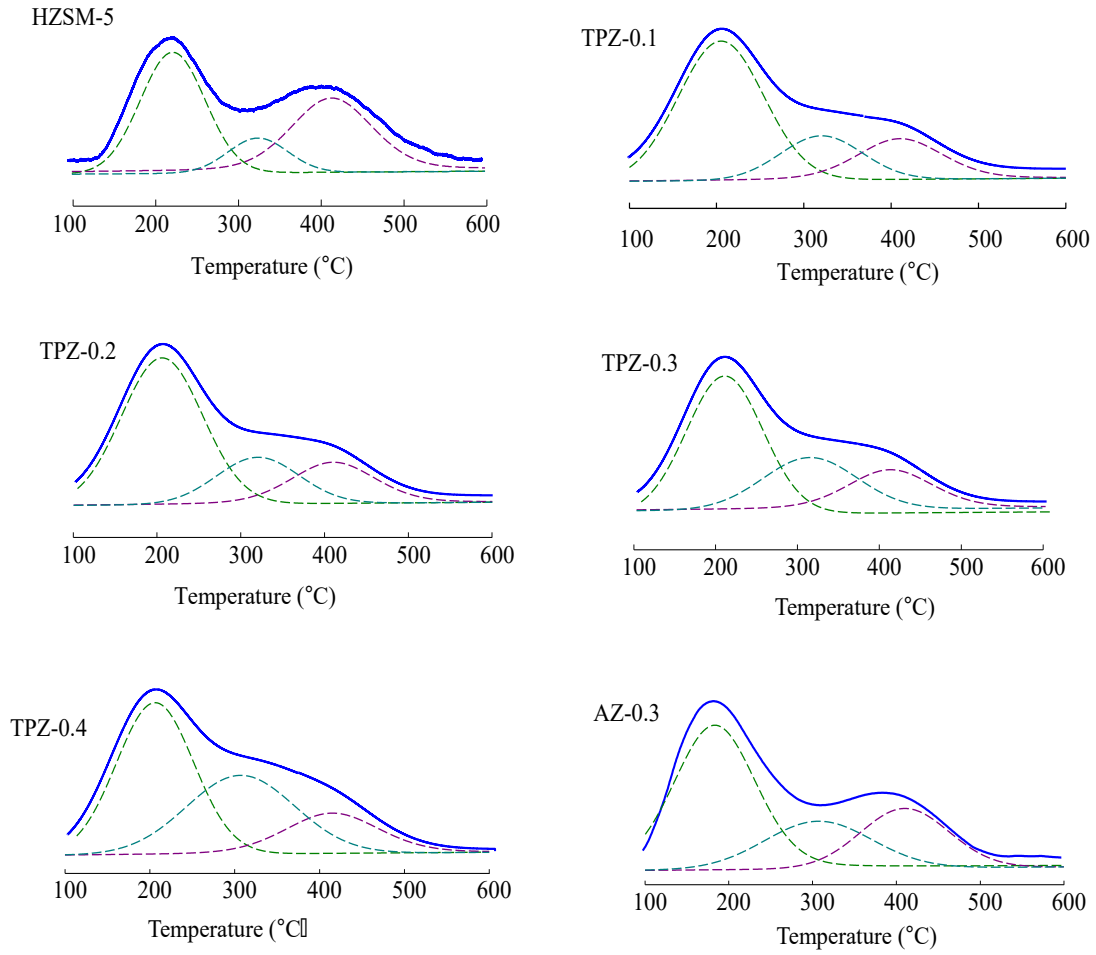

Figure S2 Deconvoluted NH_3-TPD spectra of H-ZSM-5 zeolites before and after TPAOH and NaOH

modification with different concentration.

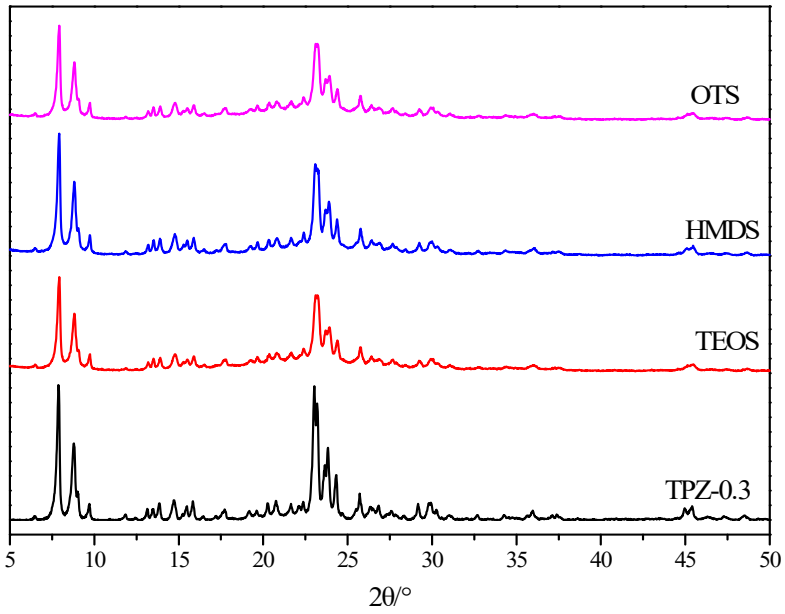

Figure S3 XRD patterns of HZSM-5 modified by 0.3M TPAOH (TPZ-0.3), and its surface modified samples with different silylation agents (TEOS, HMDS and OTS).

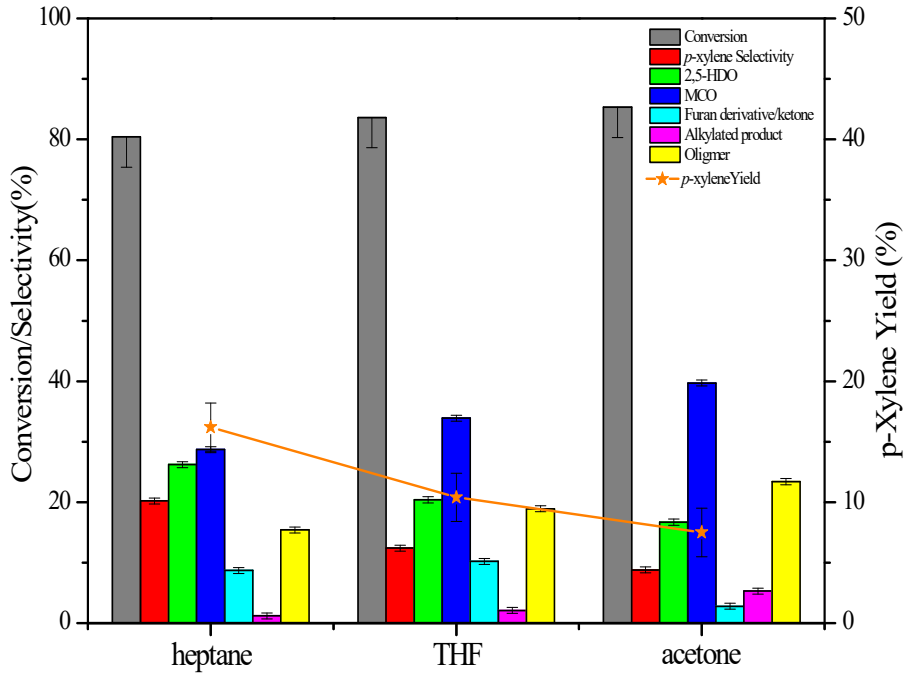

Figure S4 Reaction performances for DMF reaction with ethanol under various solvent. Reaction conditions: 3.75 M reactant (DMF+ethanol) in solvent, molar ratios DMF/ethanol 1:2, temperature 300 °C , reaction time 10 h, 0.4 g HZSM-5 zeolite.

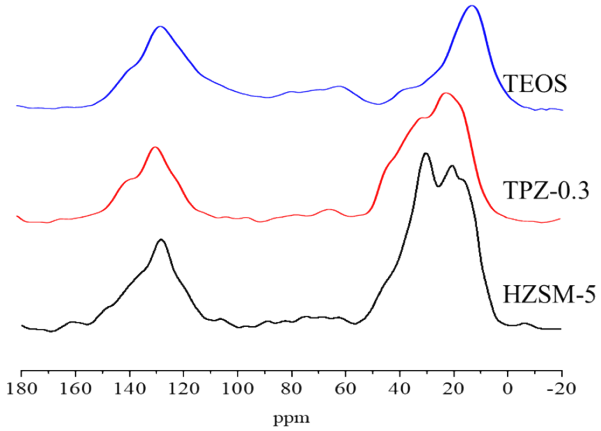

Figure S5 ^{13}C CP/MAS NMR spectra of coked HZSM-5 samples modified by different methods