

Electronic Supplementary Information

A study on factors influencing cross and self products selectivity in aldol condensation over propylsulfonic acid functionalized silica

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Calculation of *n*-heptanal conversion:

The conversion of *n*-heptanal was calculated on the basis of its weight percent; the initial theoretical weight percent of *n*-heptanal (100 X wt. of *n*-heptanal/ wt. of *n*-heptanal + wt. of benzaldehyde) was divided by initial GC peak area to get the response factor. Final unreacted weight percent of *n*-heptanal remained in the reaction mixture was calculated by multiplying the response factor with the GC peak area for *n*-heptanal after the reaction.

Conversion (%) of *n*-heptanal = 100 X [Initial wt.% of *n*-heptanal – Final wt.% of *n*-heptanal]/ Initial wt.% of *n*-heptanal.

Capping of surface silanols of SFS-3 catalyst

The capping of surface silanols of SFS-3 catalyst was carried out by reaction of *iso*-butyl trimethoxy silane with silanols. SFS-3 catalyst was dried at 100 °C for 1 h as pre-treatment prior to functionalization. The pre-treated 1 g SFS-3 catalyst was suspended in 15 mL toluene and 0.045g (0.25mmol) *iso*-butyl trimethoxy silane (Aldrich, 97%) was added in the solution under stirring. The reaction mass was kept at 100°C for 24h under nitrogen atmosphere with continuous stirring. The solid was filtered, washed with toluene and dried at 120°C for 14 h.

The modified SFS-3 catalyst was named as CSFS-3. The surface Brønsted acidity of CSFS-3 was determined by titration of the sample protons and was found to be 0.41 mmol/ g.

Table 1S. CHS and TGA weight loss data of SFS samples.

Sample	C, H, S content (wt.%)	S content (mmol/ g) ^a	Weight losses in different temperature range in TGA analysis and amount of S species				
			40-120°C (H ₂ O loss; wt.%)	330-430°C (PrSH loss)		430-580°C (PrSA loss)	
				wt.%	mmol PrSH/g ^b	wt.%	mmol PrSA/g ^c
SG	-	-	10.7	-*	-	-*	-
SFS-1	0.786, 0.632, 0.398	0.124	20.3	-*	-	2.30	0.18
SFS-2	1.458, 1.258, 0.804	0.25	18.8	0.86	0.11	2.07	0.17
SFS-3	1.828, 2.582, 1.131	0.35	18.7	0.69	0.09	3.45	0.28
SFS-4	2.125, 1.476, 1.321	0.41	14.0	1.17	0.15	3.4	0.27
SFS-5	2.261, 1.957, 1.435	0.45	17.1	1.18	0.16	3.81	0.31

^aCalculated from sulphur wt. % obtained by CHS analysis as follows, (wt % of sulphur X 1000)/ (100 X 32) = mmol S/ g of SFS sample.

^bAmount of PrSH in the 1 g of SFS sample was calculated from weight loss (wt. %) observed in 330-430°C temperature range in TGA as follows, (Weight loss in wt % X 1000)/ (100 X 75) = mmol PrSA/ g of SFS sample.

^cAmount of PrSA in the 1 g of SFS sample was calculated from weight loss (wt. %) observed in 430-580°C temperature range in TGA as follows, (Weight loss in wt % X 1000)/ (100 X 123) = mmol PrSA/ g of SFS sample.

* There was no significant weight loss in these temperature ranges.