

Supporting Information

Mesostructured Zeolite Y - High Hydrothermal Stability and Superior FCC Catalytic Performance

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Experimental Section

MAT Experiments: The MAT experiments were conducted at the National Centre for Upgrading Technology (NCUT) in Edmonton, Canada using a fluid fixed bed reactor system at 500°C. The feedstock was a VGO with API 22.2, CCR 0.42%, sulfur content 0.48 wt%, IBP 241C and FBP 603C. To obtain different feed conversions (at least three for each zeolite), the catalyst/oil ratio was varied, while keeping the catalyst contact time constant at 60 s, with different amounts of oil delivered into the reactor through a syringe pump. The collected liquid products were weighed, and analyzed by simulated distillation (ASTM D 2887) to determine the yields of gasoline (IBP/216 °C), LCO (216/343°C) and heavy cycle oil (HCO, +343°C). Gaseous products analyzed by a gas chromatograph included dry gas (H₂-C₂) and liquefied petroleum gas (LPG, C₃ and C₄). Coke deposited on the catalyst after cracking was determined by *in situ* combustion through the use of a CO₂ absorber. For each MAT test, the conversion was calculated based on the portion of the feed converted to 216°C products including gas and coke.

Table S1: Micropore volume, mesopore volume and unit cell size of the samples described in Figures 8 and 9.

	Micropore volume [Pores of 0–20 Å, cc/g]	Mesopore volume ^[a] [Pores of 20–135 Å, cc/g]	BET [m ² /g]	External Surface Area [m ² /g]	Unit cell size [Å]
Zeolite NH ₄ Y	0.38	0.03	970	22	24.70
Mesostructured zeolite Y ^[b]	0.37	0.16	916	243	24.67
Mesostructured zeolite USY ^[b]	0.27	0.16	812	152	24.55
Steamed meso- structured zeolite USY ^[b,c]	0.24	0.16	661	136	24.35
Conventional USY (CBV500)	0.32	0.04	857	75	24.55

[a] The 20-135 Å mesopore range was chosen to capture the characteristic mesoporosity introduced by this technique. [b] The zeolites contained ~ 5% rare earth oxides. [c] Steaming was conducted at 1450 °F under 100% steam for 4 h.

Table S2: XPS analysis results of a deep-bed calcined mesostructured NH₄-Y.

	C	O	Si	Al	N	Si/Al
Surface	5.67	63.28	21.93	7.25	1.87	3.02
250 nm deep	0.55	65.22	25.82	7.55	0.85	3.42

Table S3: Yields at 78% conversion for the catalyst comparison shown in Figure 10.

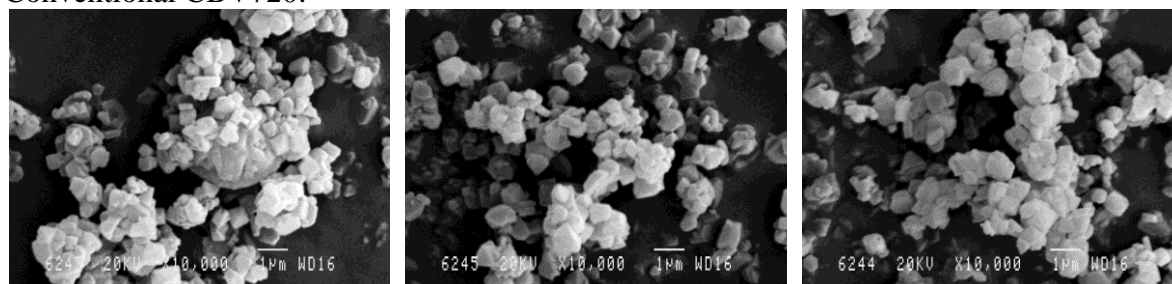
Products at 78% Conversion	Catalyst with mesostructured zeolite [wt%]	Catalyst with conventional zeolite [wt%]	Absolute difference [wt%]	Relative difference [%]
Gasoline	54.67	52.18	+2.50	+4.8
Diesel	16.45	15.40	+1.05	+6.8
Coke	2.77	2.97	-0.20	-6.7
Gases	20.56	22.86	-2.30	-10.1
Bottoms	5.55	6.60	-1.05	-15.9

Table S4: Properties of the mesoporous zeolites prepared by the newly developed surfactant-free process.

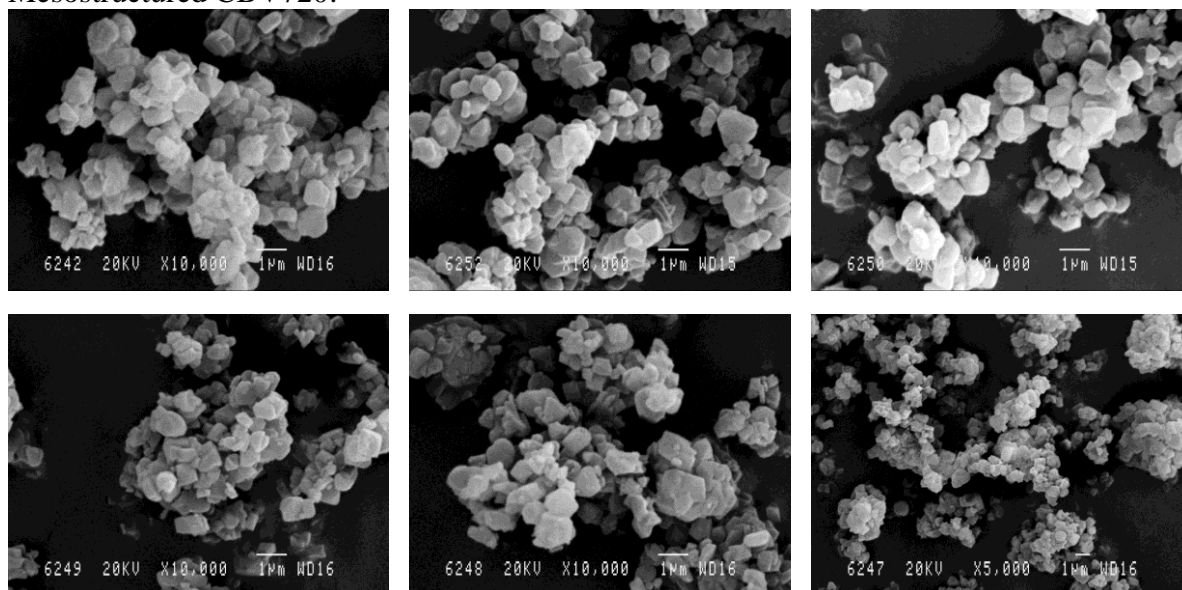
	Micropore volume [Pores of 0–20 Å, cc/g]	Mesopore volume ^[a] [Pores of 20–135 Å, cc/g]	Crystallinity [%]	Unit cell size [Å]
Zeolite NaY	0.40	0.03	95	24.66
Mesostructured zeolite USY	0.34	0.15	72	24.50
Steamed mesostructured zeolite USY ^[b]	0.18	0.14	57	24.25
Conventional USY (CBV500)	0.33	0.06	86	24.54

[a] The 20–135 Å mesopore range was chosen to capture the characteristic mesoporosity introduced by this technique. [b] Steaming was conducted at 1450 °F under 100% steam for 8 h.

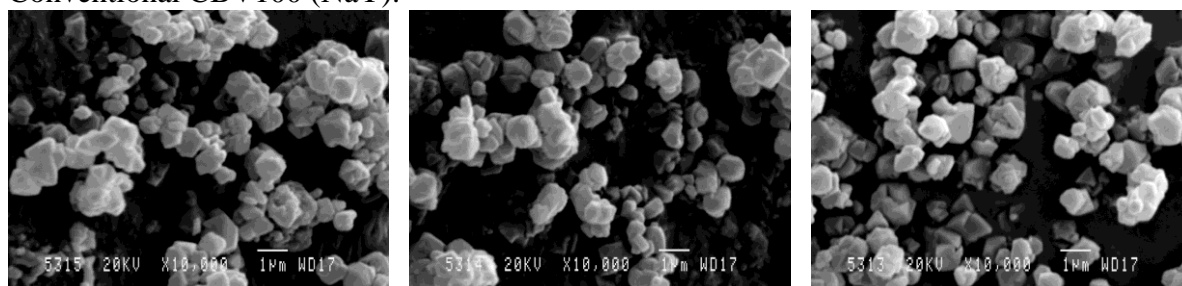
Conventional CBV720:



Mesostructured CBV720:



Conventional CBV100 (NaY):



Mesostructured CBV100:

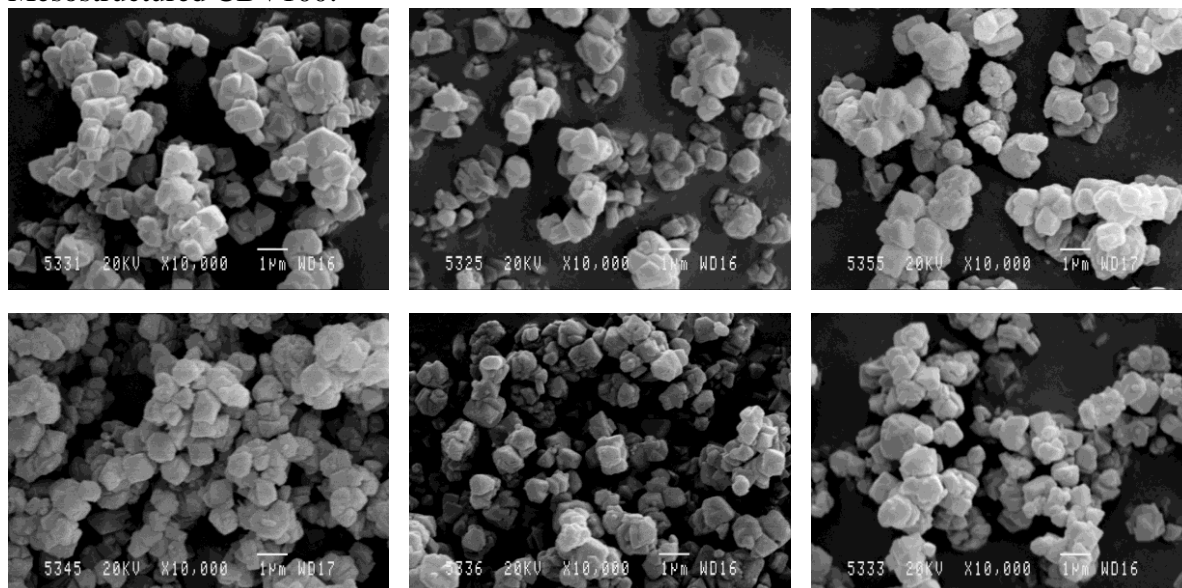


Figure S1. Additional SEM images of conventional and mesostructured Y zeolites.

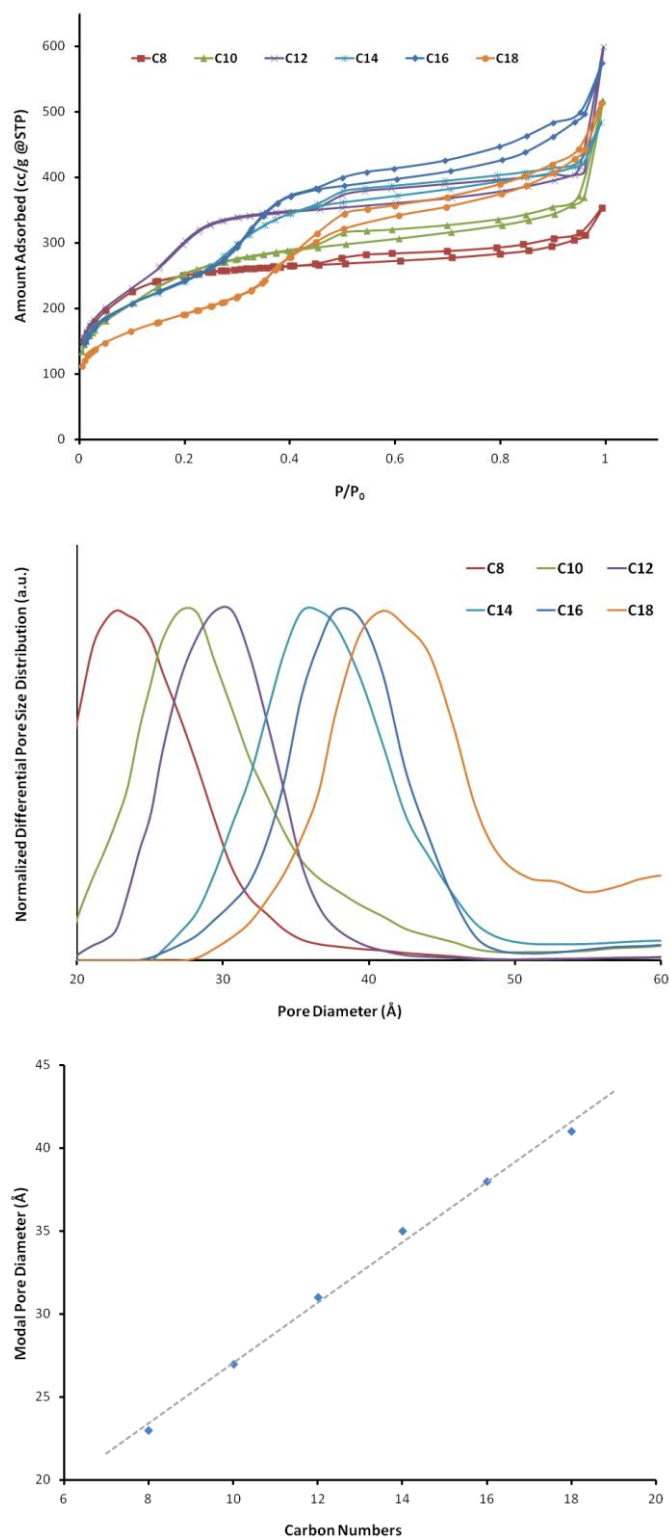


Figure S2. Nitrogen adsorption isotherms (top), NLDFT pore size distributions (middle, normalized peak heights to better demonstrate the size correspondence with surfactant size), and a linear correlation of the modal mesopore diameters with the carbon numbers of the long alkyl chains in the surfactants used to prepare a series of mesostructured NH₄-Y zeolites under the same reaction conditions. C8 (octyltrimethylammonium bromide), C10

(decyltrimethylammonium bromide), C12 (dodecyltrimethyl-ammonium bromide), C14 (tetradecyltrimethylammonium bromide), C16 (cetyltrimethylammonium bromide), and C18 (octadecyltrimethylammonium bromide). All chemicals are from Aldrich.

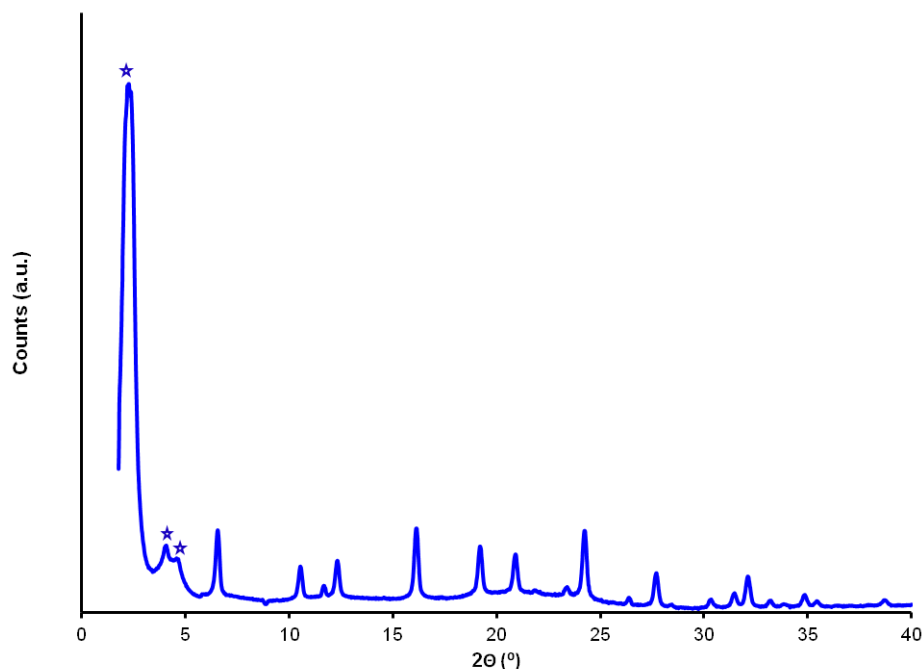


Figure S3. XRD pattern of mesostructured CBV720 showing the (100), (110) and (210) peaks (asterisked) due to the hexagonal ordering ($a_0=44.7$ Å, determined by $a_0=2d_{100}/\sqrt{3}$) of the mesopores ($2\theta < 5^\circ$) and peaks that are characteristic of zeolite Y ($2\theta > 5^\circ$). Additional XRD patterns showing hexagonal ordering of the mesopores are available in reference 50.

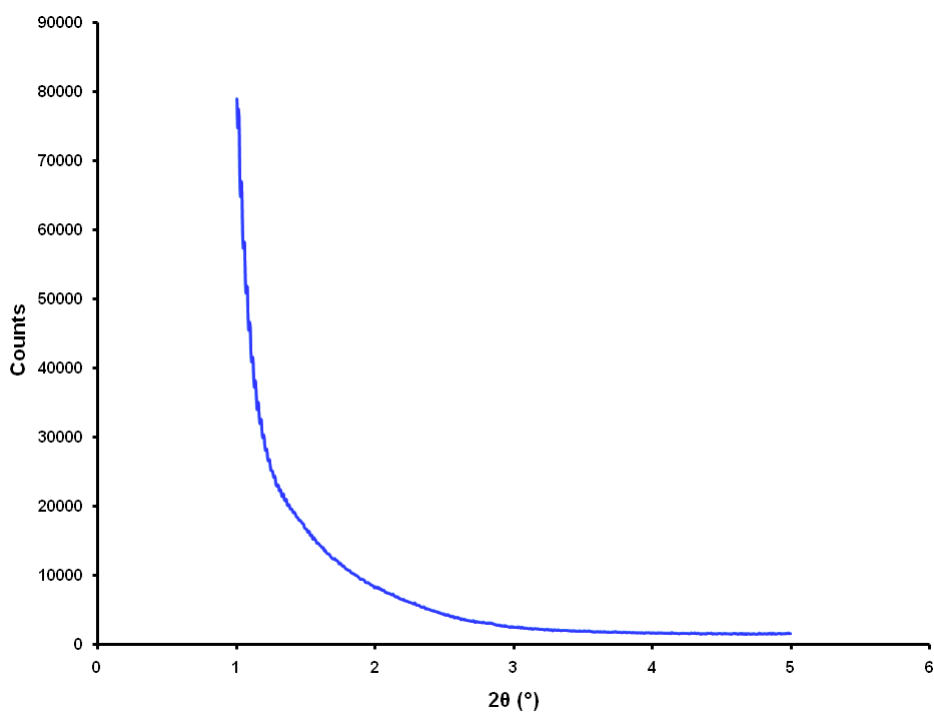


Figure S4. Low angle ($2\theta = 1-5^\circ$) XRD scan of the mesostructured Y described in Figure 8 and 9 showing no diffraction peaks, suggesting the mesopore are not ordered.

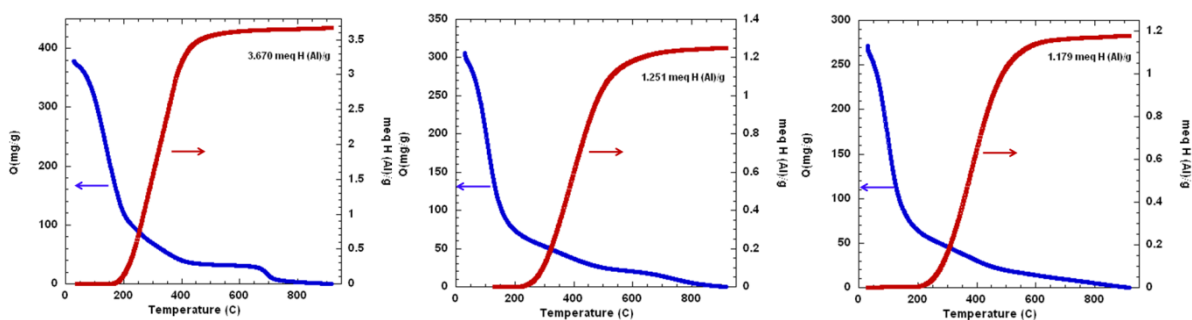


Figure S5. TPD) results of the starting $\text{NH}_4\text{-Y}$ (CBV300, left), a conventional USY (CBV500, center) and a mesostructured USY (right).

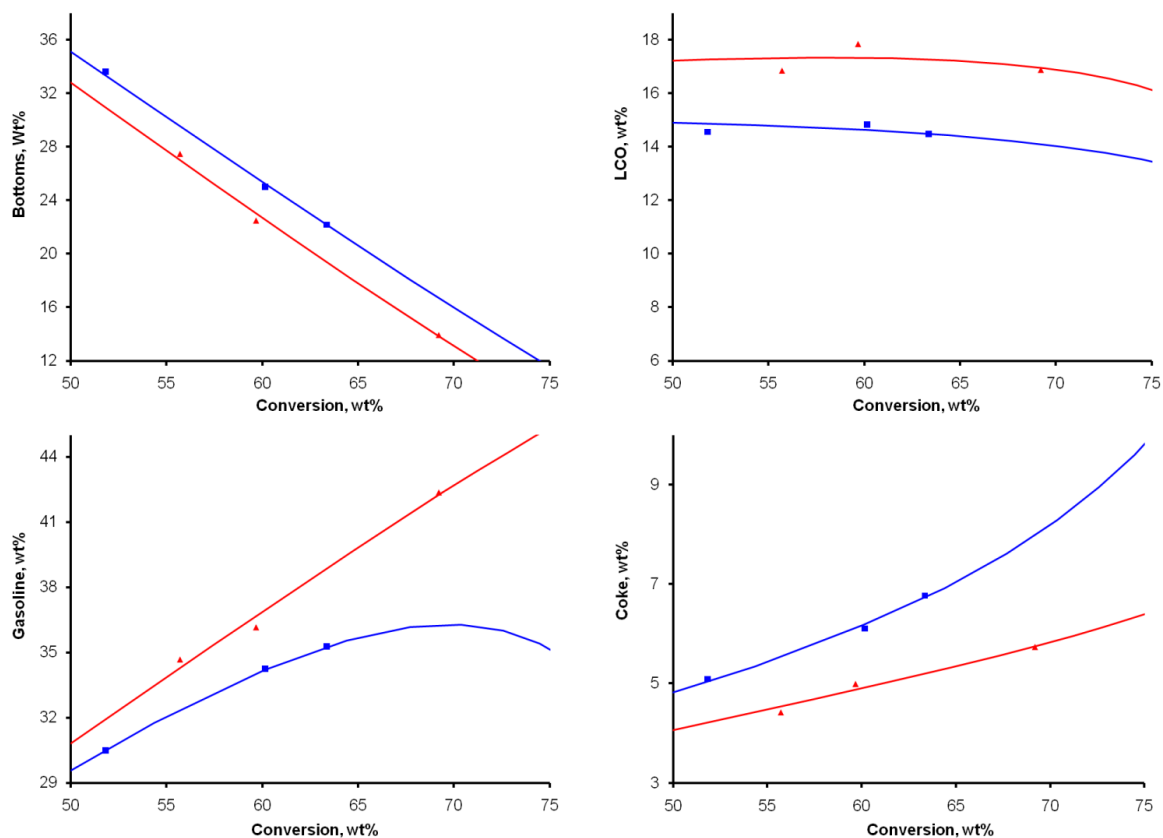


Figure S6. The MAT test results of (red triangle) mesostructured zeolite USY and (blue square) conventional zeolite USY. The zeolites were ultrastabilized, and then deactivated at 1450°F in 100% steam for 4 h before being tested. The curves were fitted by a kinetic lump model.