Supporting Information

Insights into structure-function relationships of mesoporous H-ZSM-5 zeolite catalysts for direct amination of cyclohexene with NH_3

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$$\text{Conversion of cyclohexene}(\%) = \frac{[\text{the amount (mol) of starting cyclohexene}] - [\text{the amount (mol) of cyclohexene recovered}]}{[\text{the amount (mol) of starting cyclohexene}]} \times 100\%$$

$$\text{Selectivity of cyclohexylamine}\ (\%) = \frac{[\text{the amount (mol) of cyclohexylamine}]}{[\text{the amount (mol) of starting cyclohexane}] - [\text{the amount (mol) of cyclohexane recovered}]} \times 100\%$$

Scheme S1 The formulas for the calculations of cyclohexene conversion and cyclohexylamine selectivity

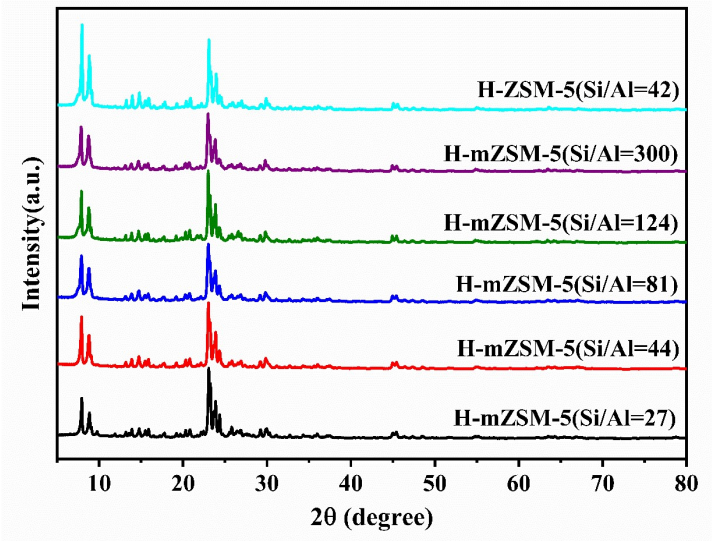

Figure S1 XRD of synthesized ZSM-5 zeolites.

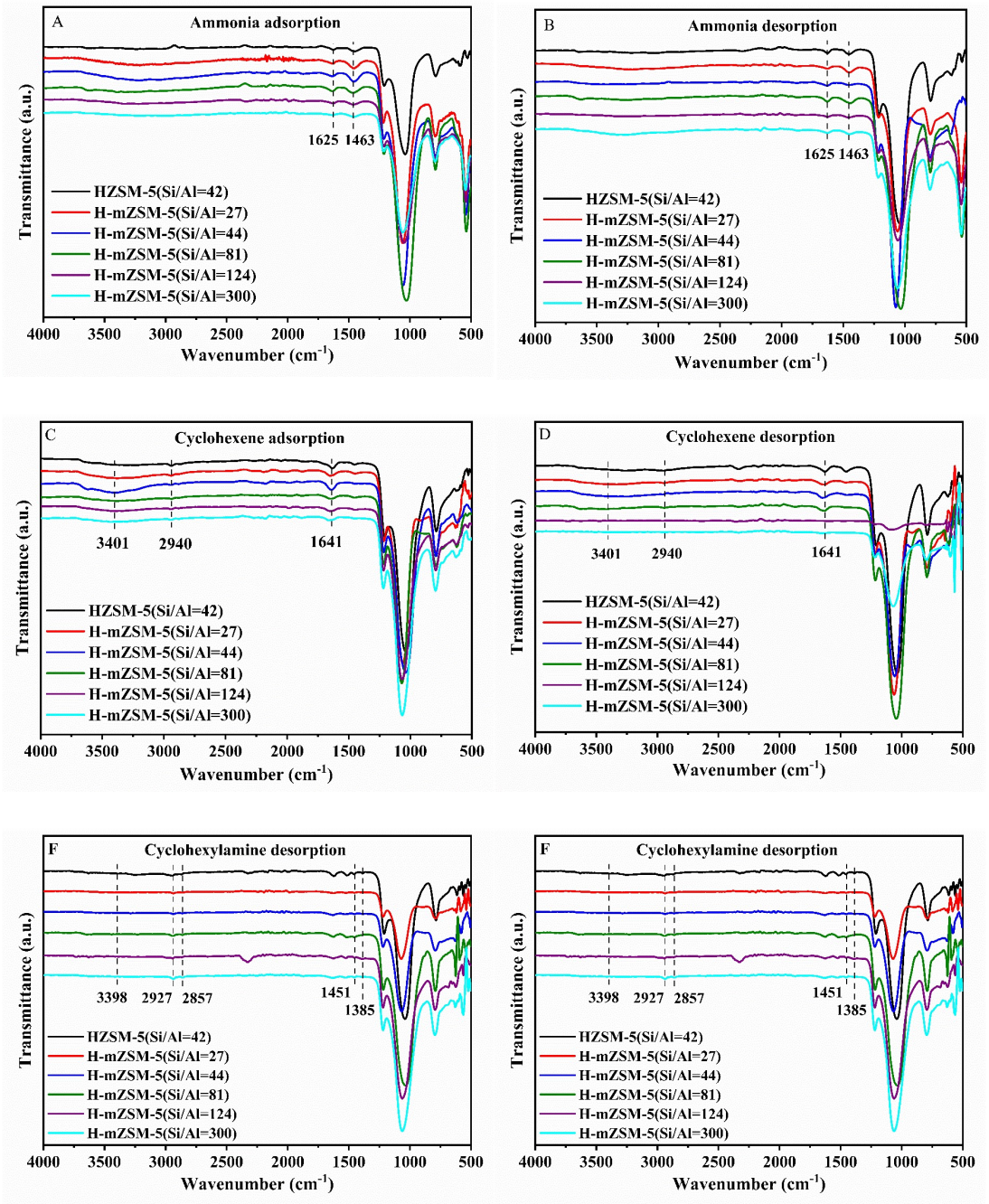

Figure S2 FT-IR spectroscopy measurements for NH_3 adsorption (A) and desorption (B), cyclohexene adsorption (C) and desorption (D), cyclohexylamine adsorption (E) and desorption (F) on ZSM-5 zeolites.

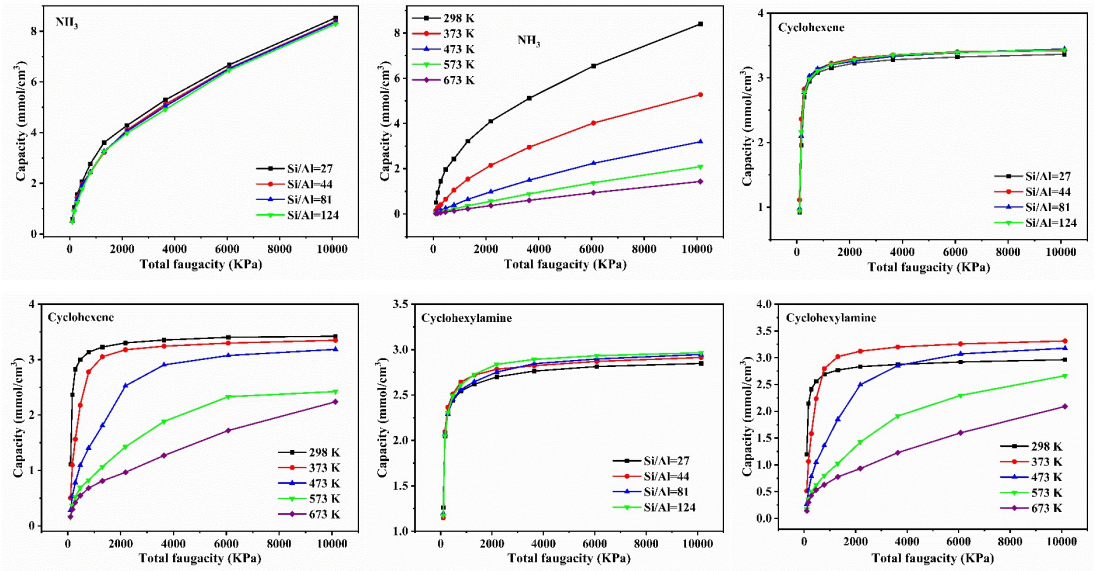

Figure S3 Adsorption capacities of pure NH_3, cyclohexene and cyclohexylamine on zeolite with different Si/Al ratios and temperatures.

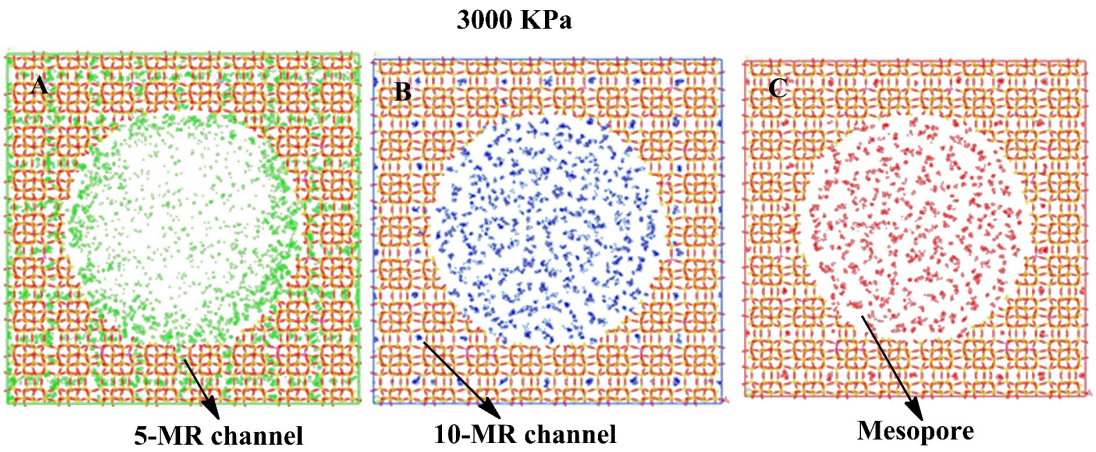

Figure S4 Configuration of adsorbed NH_3 (A), cyclohexene (B) and cyclohexylamine (C) with low energy over catalysts (373K) at 3000 KPa

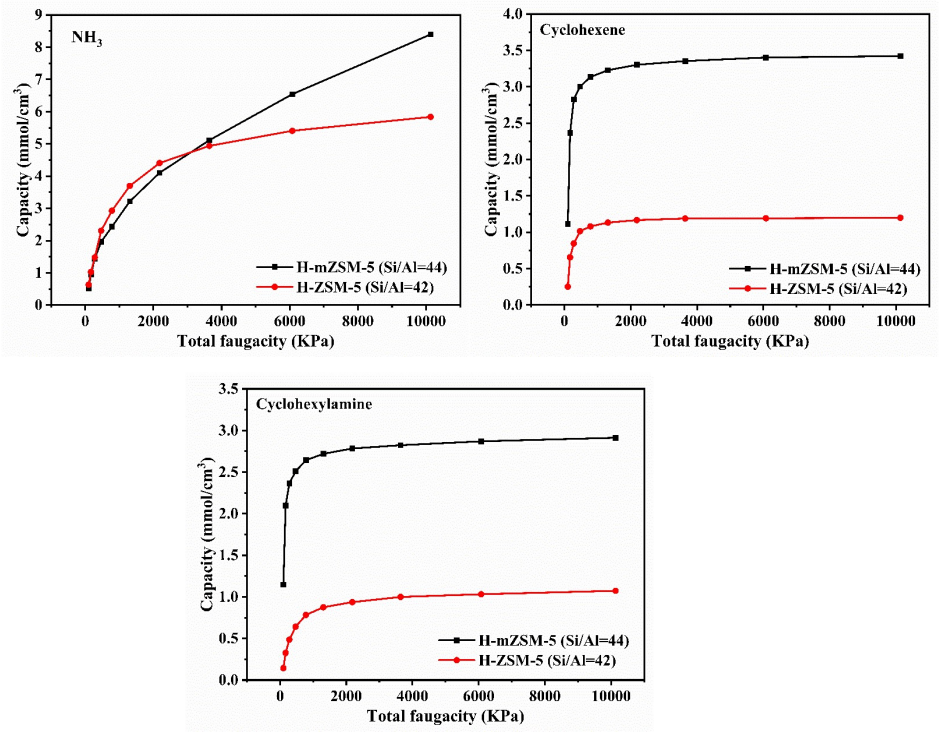

Figure S5 The comparison of the adsorption capacity between HM-ZSM-5 and HZSM-5, for NH_3, cyclohexene and cyclohexylamine.

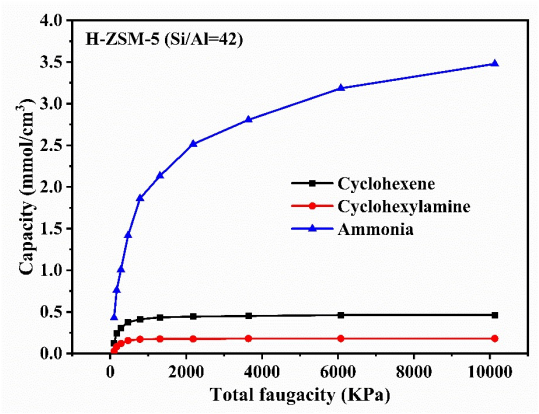

Figure S6 Adsorption capacities of NH_3, cyclohexene and cyclohexylamine in a mixture on HZSM-5 zeolite.

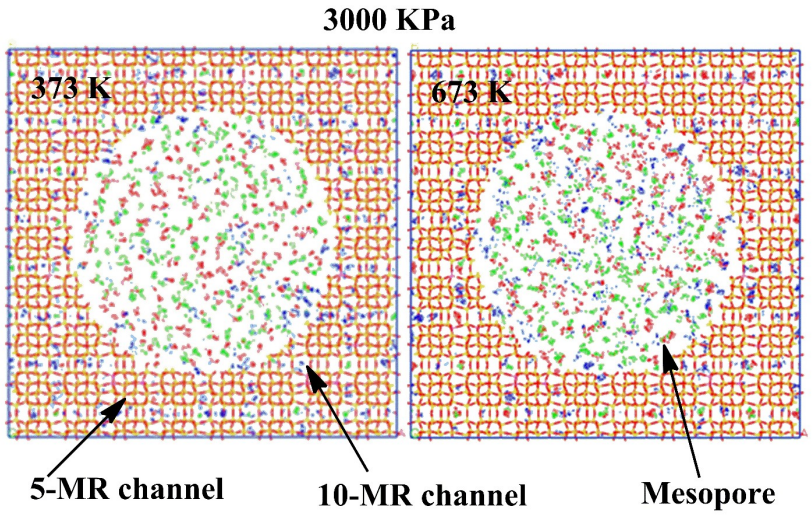

Figure S7 Configuration of adsorbed NH_3, cyclohexene and cyclohexylamine in a mixture for 573 K and 673 K with low energy over catalysts at 3000 KPa.

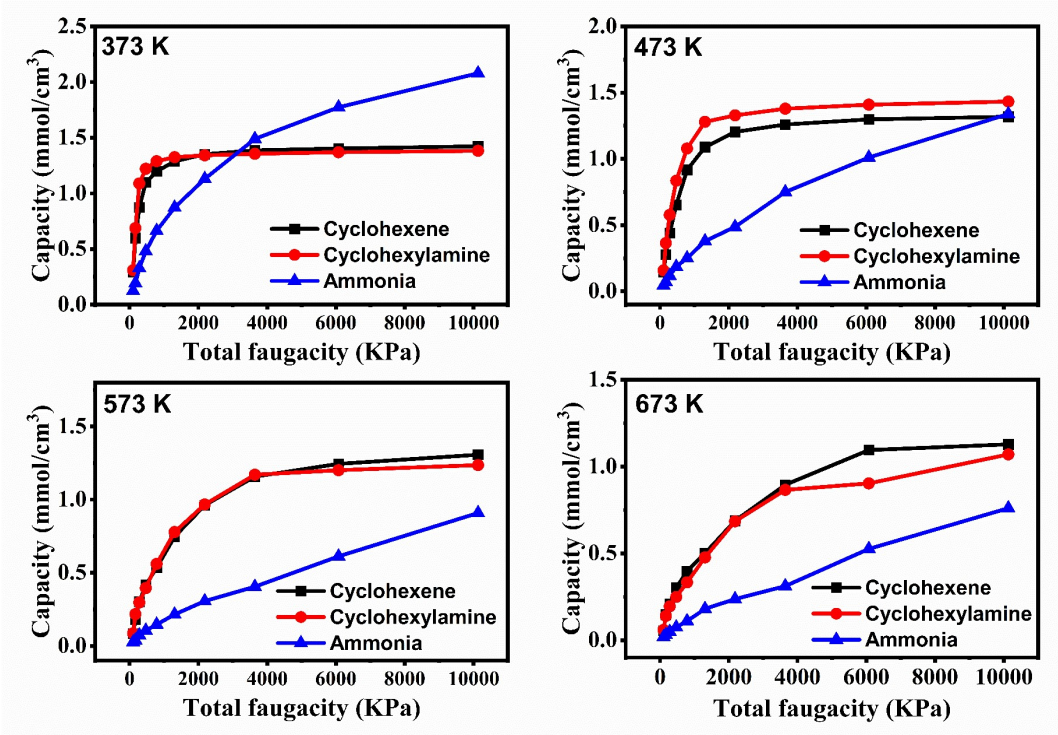

Figure S8 Adsorption capacities of NH_3, cyclohexene and cyclohexylamine in a mixture on HM-ZSM-5 zeolite with different temperatures.

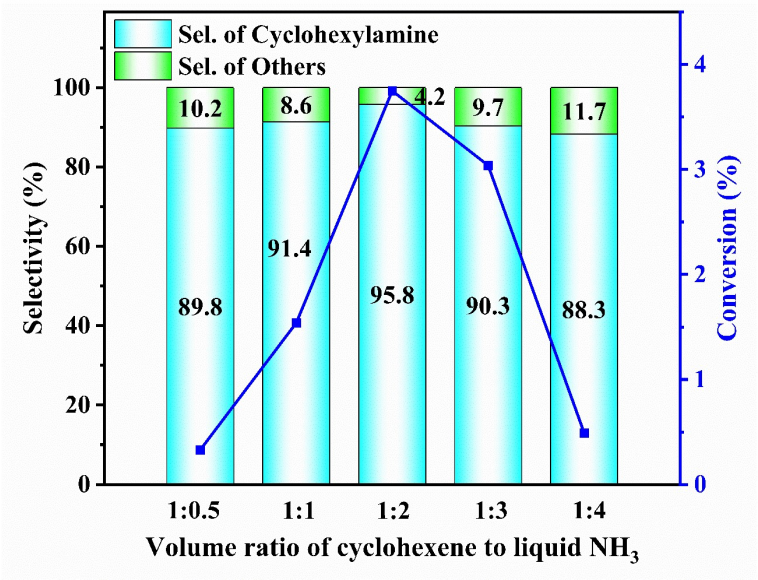

Figure S9 Effects of the volume ratio cyclohexene to ammonia on direct amination reaction

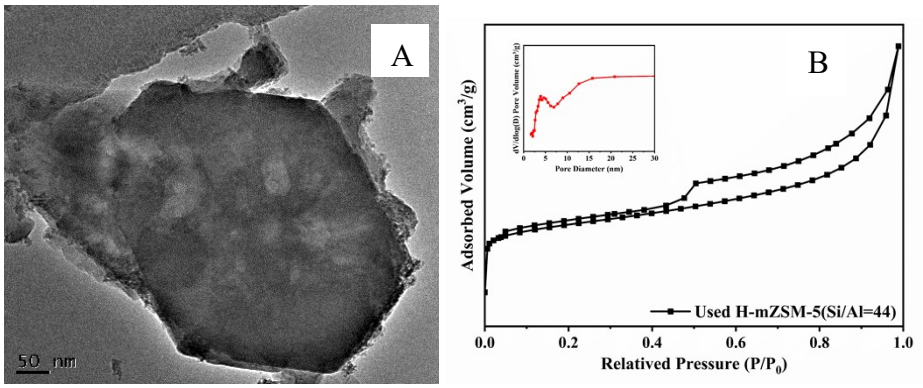

Figure S10 TEM images (A) and N_2 adsorption-desorption isotherms (B) of reused H-mZSM-5 zeolite.