Supporting information for

Constructing the direct relations between various structure-directing agents and low-temperature hydrothermal durability over Cu-SAPO-34 during NH_3-SCR reaction

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Catalysts preparation details

$CuSO_4 \cdot 5H_2O$ (99 wt%), tetraethylenepentamine (TEPA, 99 wt%), DEA (99.5 wt%,), TEA (99.5 wt%), PA (99.5 wt%), and TEAOH (35 wt% in H_2O) were purchased from Sinopharm Chemical Reagent Co. Ltd, China. The Al source, Si source, and P source were boehmite (75 wt% Al_2O_3, Zibo Baida Chem. Ind. Co. Ltd, China), silica sol (30 wt%, Qingdao Haiyang Chem. Co. Ltd, China), H_3PO_4 (85 wt%, Sinopharm Chemical Reagent Co. Ltd, China), respectively.

In a typical synthesis: (1) phosphoric acid and deionized water were first mixed and stirred to obtain a homogeneous solution. (2) boehmite was then slowly added and stirred for 1h. (3) silica sol was added within 10 min and the slurry was stirred for 1 h. (4) SDAs was added drop by drop under stirring and the slurry was then stirred for 2 h. (5) The Cu-TEPA solution, measured to contain the desired amount of Cu, was slowly added to the slurry under stirring for 3 h. (6) The resulting gel was transferred to an autoclave with a Teflon liner, and heated at 200 ℃ for 48 h under static conditions. (7) The solid product was separated with centrifugation, washed twice with deionized water, and dried at 110 ℃ for 12 h, and the resulting samples were calcined at 600 ℃ for 5 h in air to properly remove the occluded organic species.

Characterization protocols

For NH_3-TPD, 0.05 g sample was pretreated under Ar gas (25 mL min^{-1}) at 550 °C for 1 h, then, cooled to 100 °C and saturated with 10% NH_3/N_2 gas for 45 min. After being purged by Ar gas for 1h to remove the physically adsorbed NH_3, desorption of NH_3 was carried out from 100 to 700 °C at 20 °C min^{-1}. For H_2-TPR, the sample (0.05 g) was pretreated under Ar gas

(25 mL min^{-1}) at 550 °C for 1 h, then cooled down to 40 °C. Finally, the reduction process was carried out from 40 to 850 °C at 10 °C min^{-1} in 10% H_2/Ar flow (10 mL min^{-1}).

For *in-situ* DRIFTS experiments, about 25 mg powder catalyst was packed into in situ diffuse-reflectance cell (Harrick) covered with a ZnSe window. Before each test, the sample was pretreated at 350 °C for 1 h in N_2 atmosphere (50 mL min^{-1}), then cooled to 200 °C to obtain the background spectrum. First, the catalytic powder was exposed to a flow of 1000 ppm NH_3/N_2 (or 1000 ppm NO + 5% O_2/N_2) at 200 °C for 40 min, then purged with N_2 for 30 min, whereafter, exchanging to 1000 ppm NO + 5% O_2/N_2 (1000 ppm NH_3/N_2) for 1h.

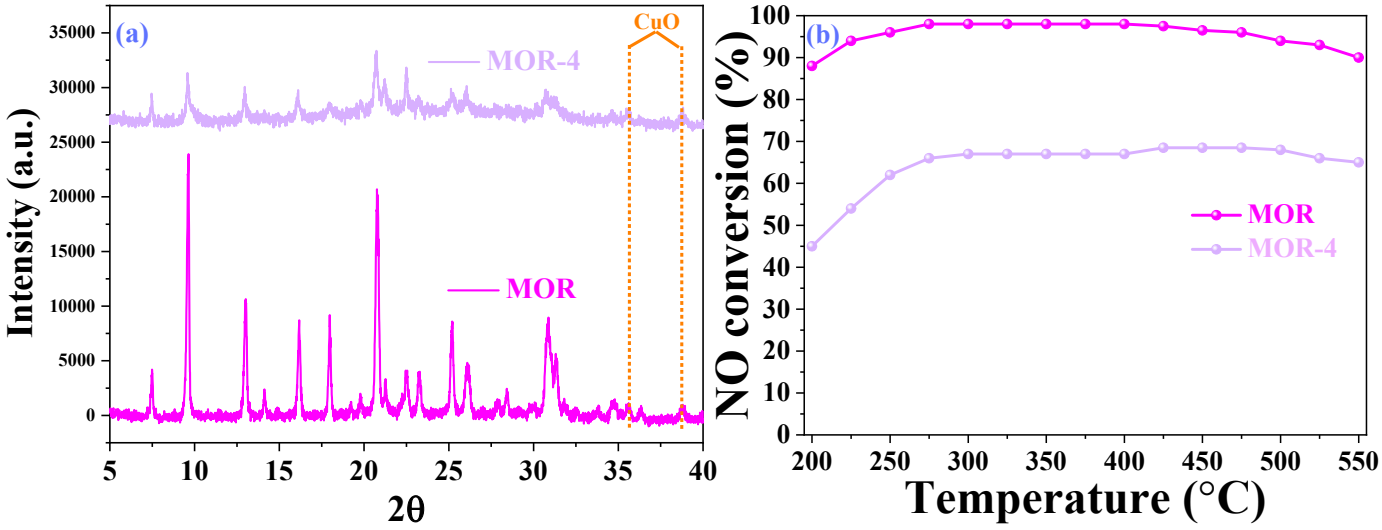


Fig. S1. XRD profiles (a) and NH_3-SCR performance (b) of fresh and LHAT catalysts synthesized with MOR.

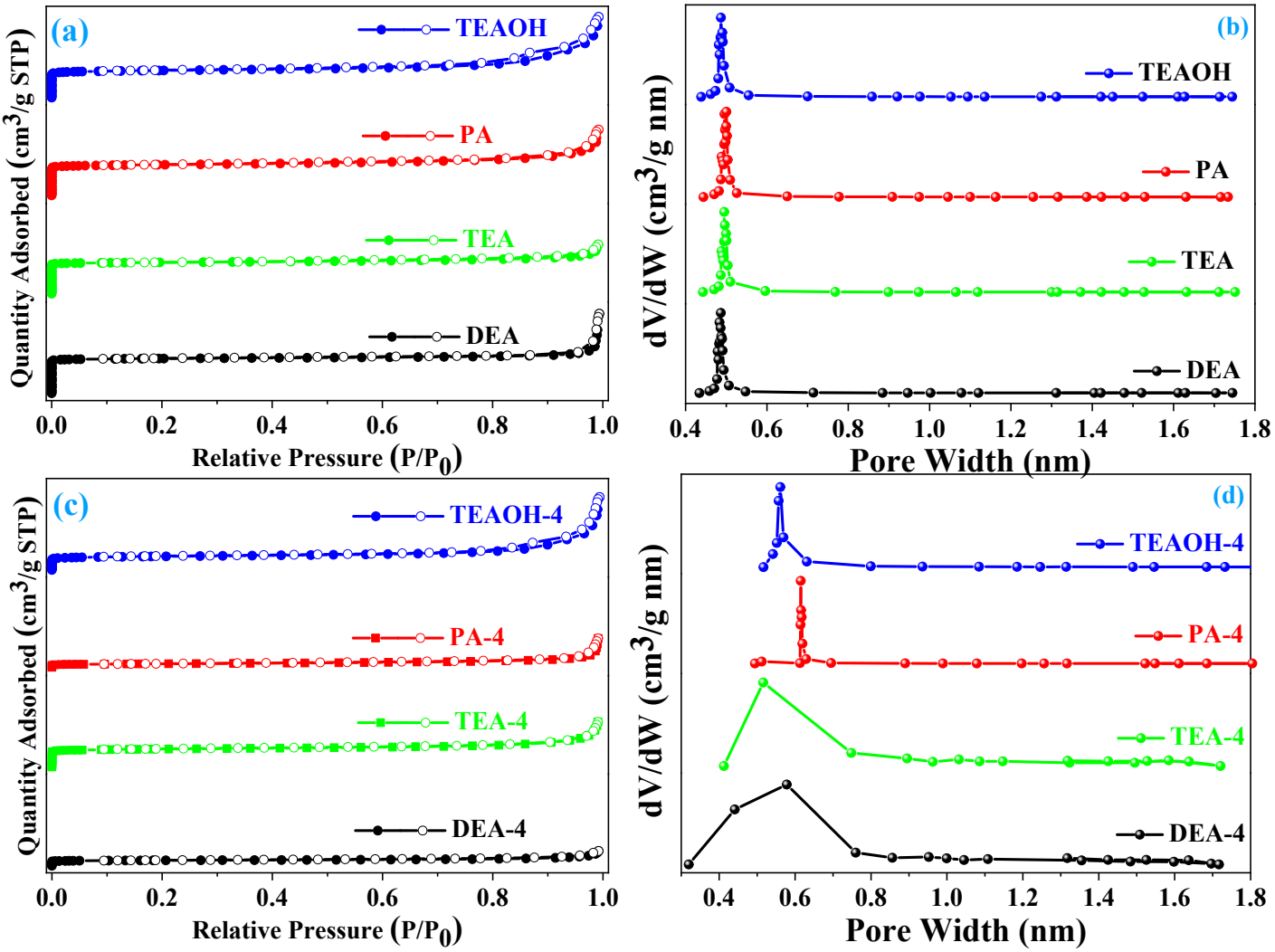
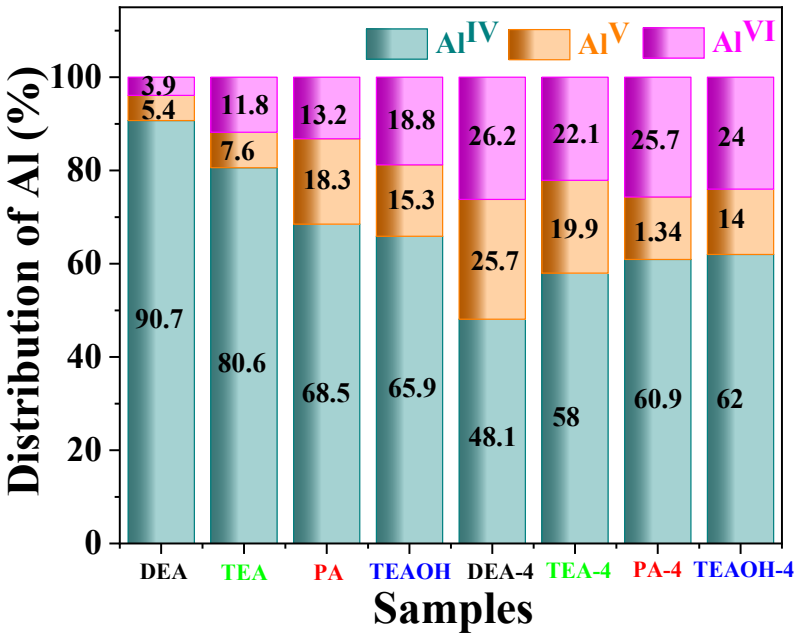
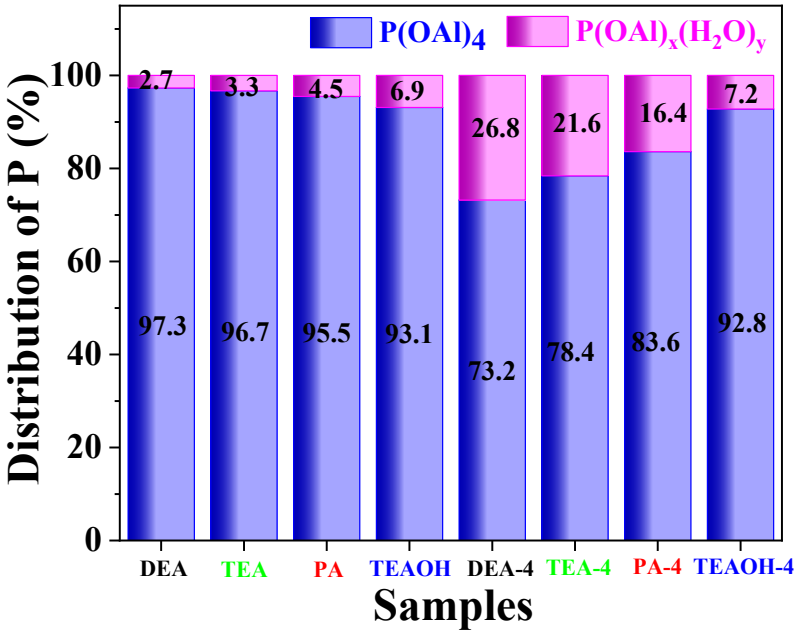


Fig. S2. (a) N_2 adsorption desorption isotherms of fresh (a) and LHAT (c) samples, and the corresponding pore size distributions of the fresh (b) and LHAT (d) samples.



69 **Fig. S3**. The proportion of various Al species calculated from ^{27}Al NMR



70 spectra of the samples.

71 **Fig. S4**. The proportion of various P species calculated from ^{31}P NMR

72 spectra of the samples.

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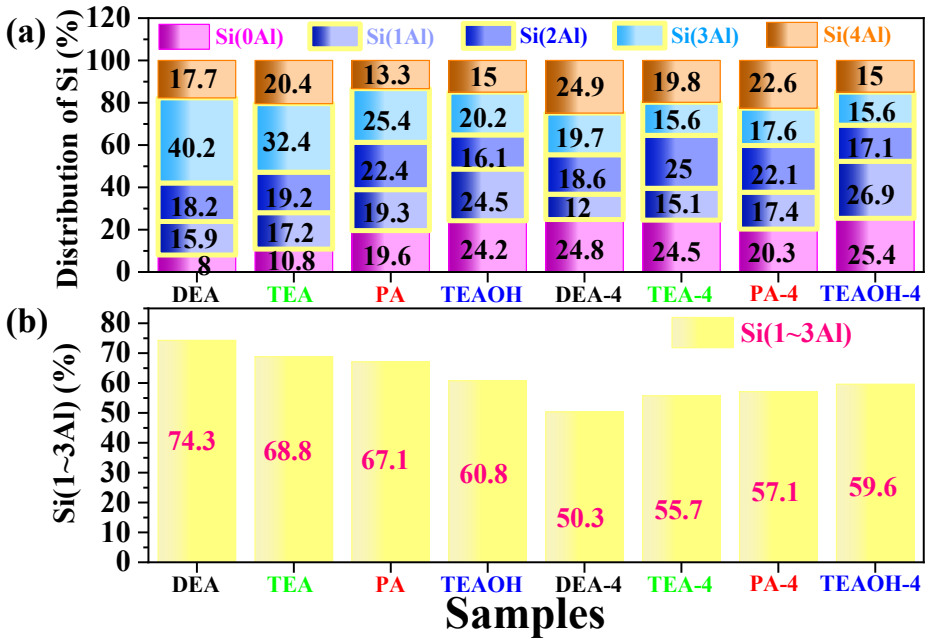
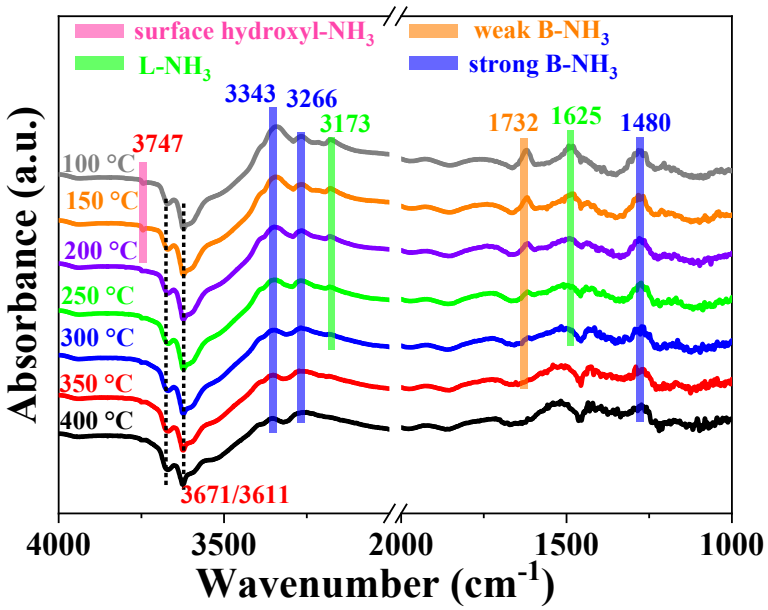


77 **Fig. S5**. The proportion of various Si species (a) and the Si(1-3Al) (b)

78 calculated from ^{32}Si NMR spectra of the samples.



79 **Fig. S6**. DRIFTS spectra of NH_3 desorption collected at different temperatures over fresh

80 DEA catalyst.

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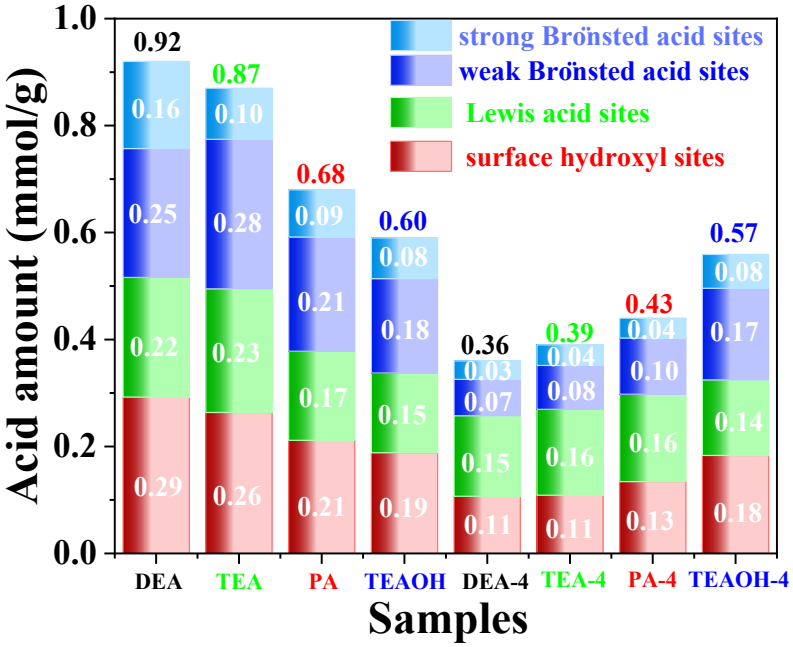
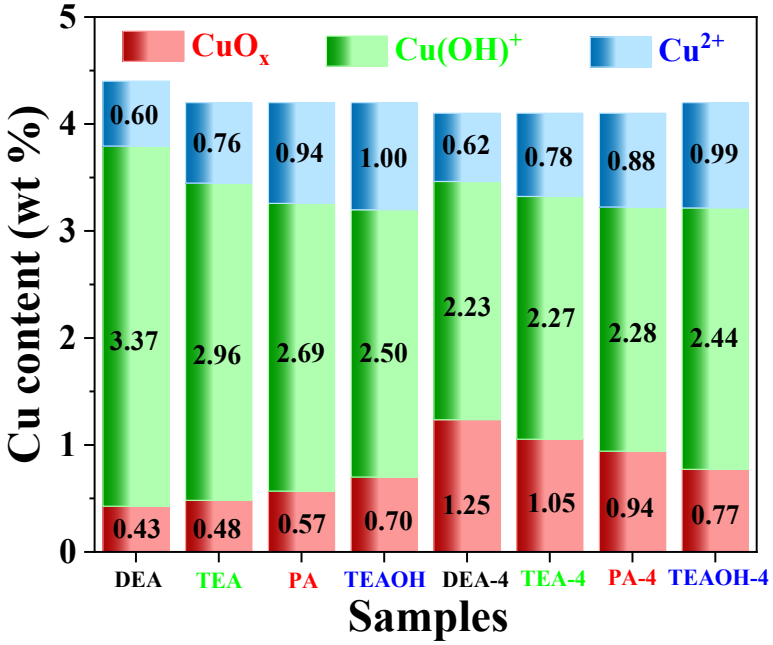


84 **Fig. S7**. Integrated NH_3 desorption amounts calculated from NH_3-TPD results.



85 **Fig. S8**. The CuO_x, $Cu(OH)^+$, and isolated Cu^{2+} contents calculated from H_2-TPR results.

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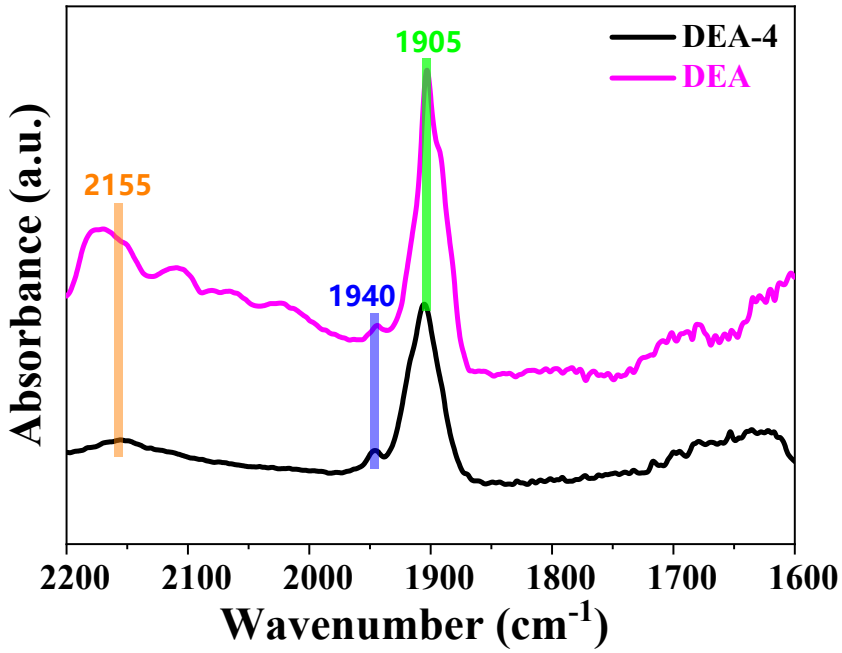


Fig. S9. The NO-DRIFT spectra of DEA and DEA-4 at 200 °C for 30 min

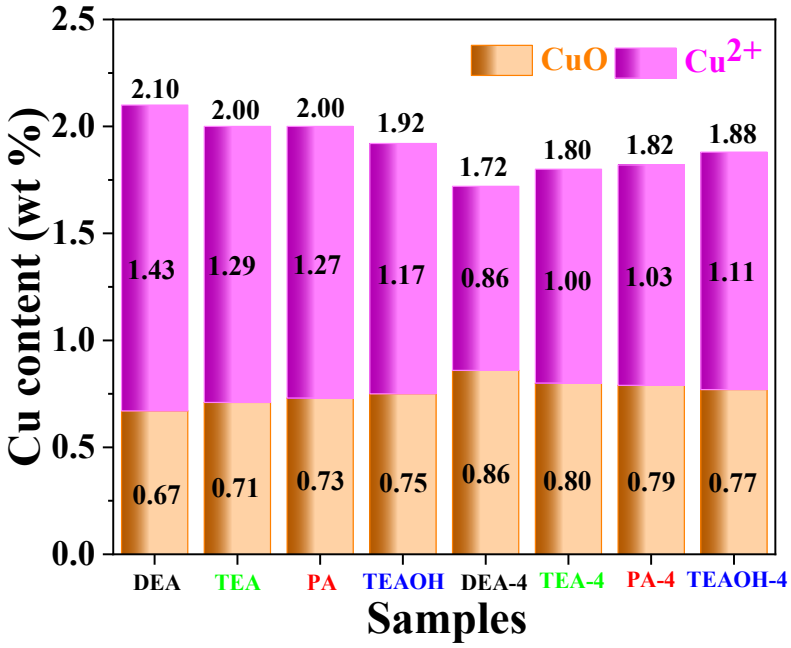


Fig. S10. The Cu^{2+} and CuO contents calculated from XPS results.

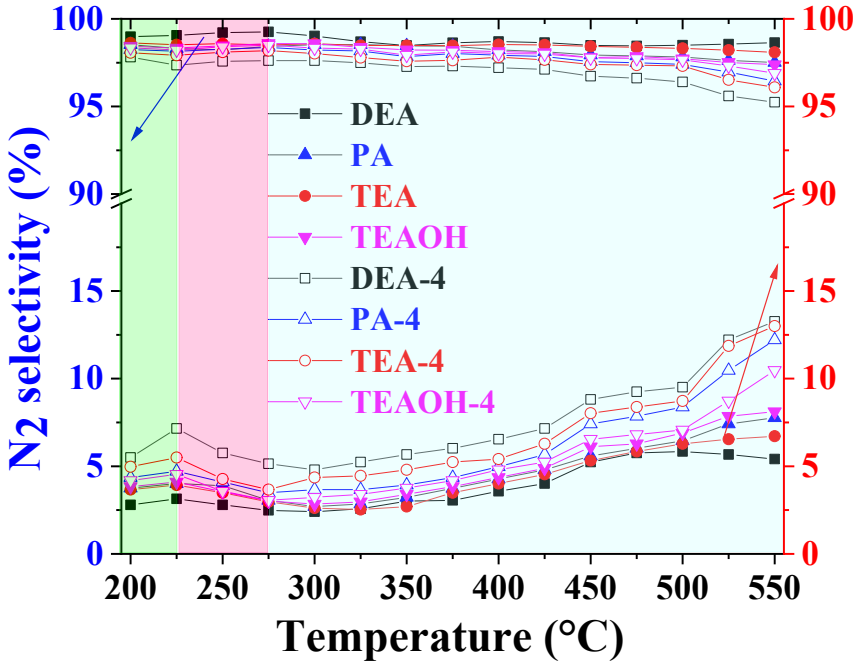
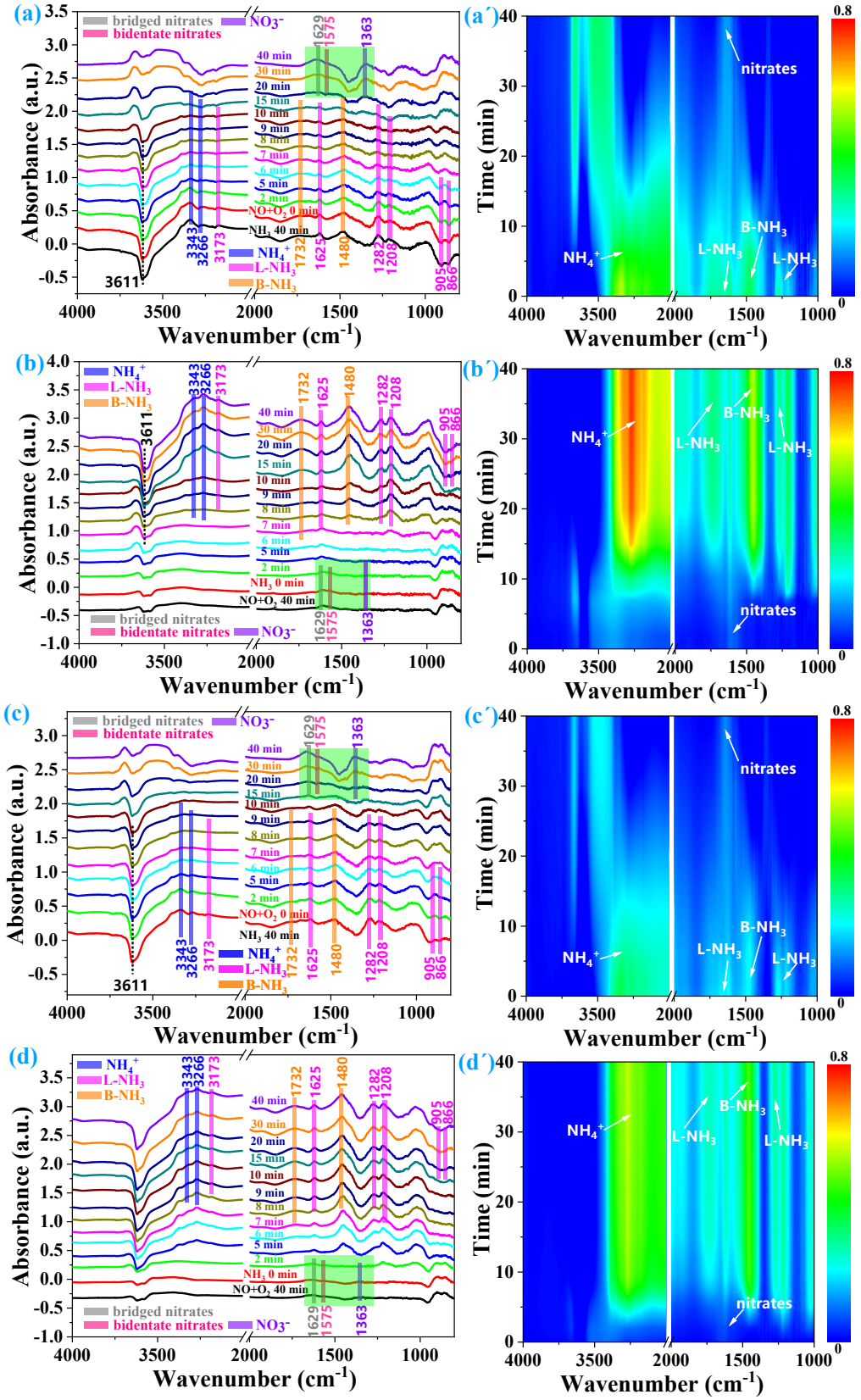


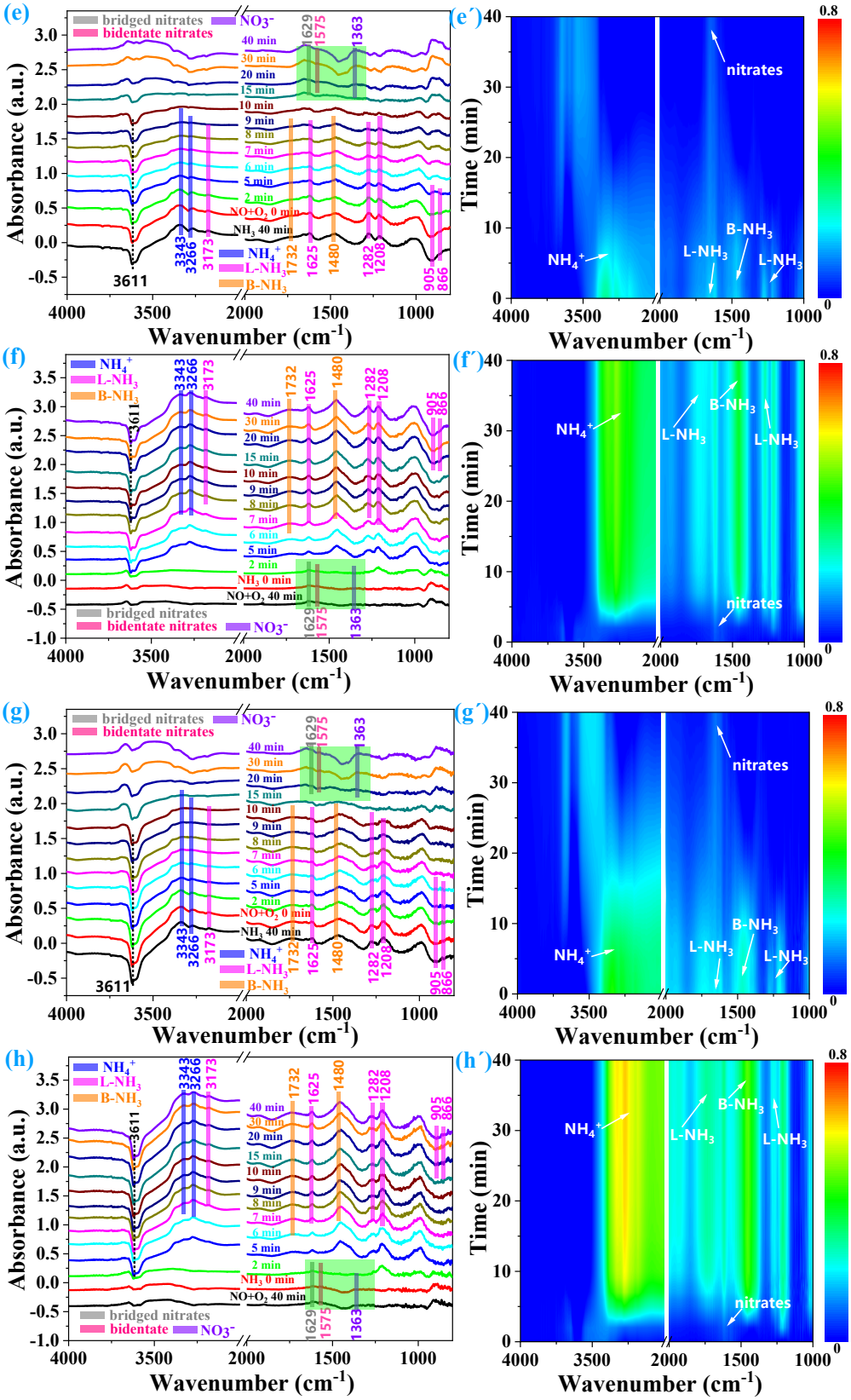
Fig. S11. The N_2 selectivity and N_2O formation of both fresh and LHAT samples synthesized with different SDAs as a function of temperature during standard SCR. Reactant feed contains 1000 ppm NO, 1100 ppm NH_3, 10% O_2 balanced with N_2 at a GHSV of 80,000 h^{-}



105 **Fig. S12.** In situ DRIFTs spectra with corresponding mapping results of pre-adsorbed NH_3

106 with NO/O_2 over DEA (a,a′) and TEA (c,c′); In situ DRIFTs spectra with corresponding

107 mapping results of pre-adsorbed NO/O_{22} with NH_3 over DEA (b,b′) and TEA (d,d′)



108 **Fig. S13**. In situ DRIFTs spectra with corresponding mapping results of pre-adsorbed NH_3

109 with NO/O_2 over PA (e,e′) and TEAOH (g,g′); In situ DRIFTs spectra with corresponding

110 mapping results of pre-adsorbed NO/O_2 with NH_3 over PA (f,f′) and TEAOH (h,h′)

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