Supplementary Information

Modulated Excitation DRIFTS and Steady-State Isotopic Transient Kinetic Analysis (SSITKA) of NH_3-SCR-DeNO$_x$ on Cu-Containing Zeolite Y

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1. Experimental

1.1 Catalyst physico-chemical characterization

The XRD patterns were recorded using a HUBER G670 (Rimsting, Germany) diffractometer applying Cu-Kα radiation (wavelength: 0.154 nm). The samples were measured with a scanning range of the diffraction angle 2θ between 4° and 90° in intervals of 0.005°. The CRYSTAL IMPACT software version 3.6.2.121 was used to analyze the results.

Nitrogen sorption isotherms were recorded at -196 °C using a MicrotracBEL Corp., BELSORP-miniX (Haan/Duesseldorf, Germany). Before measurement, ca. 0.1-0.2 g of the sample was activated at 250 °C and 1 Pa. The total pore volume was taken from the point p p_0^{-1} = 0.99. The specific surface area was calculated using the Brunauer-Emmett-Teller (BET) method, and the pore width distribution was obtained using the Barret-Joyner-Halenda (BJH) method. The micropore volume was calculated using the Harkins and Jura model (t-plot analysis).

SEM images were acquired using a scanning electron microscope (SEM) LEO Gemini 1530 SEM from Zeiss (Oberkochen, Germany) operated at an acceleration voltage of 5 kV. The samples were gently crushed using a ceramic pestle and mortar. Before taking the images, the samples were placed on carbon conductive tabs. To improve the conductivity, the samples were sputtered with Au. ImageJ software version 1.53t was used to derive the average particle sizes from the SEM images.

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) experiments were performed using a TOF-SIMS IV instrument (ION-TOF GmbH, Münster, Germany) equipped with a 25 kV pulsed Bi^{3+} primary ion gun. For each sample, at least three spectra were collected from different locations. In the case of mass spectra collecting

the analyzed area corresponded to a square of size 500 µm × 500 µm, while for imaging it varied between 500 µm × 500 µm and 5 µm × 5 µm. A pulsed electron flood gun was used for the charge compensation.

The Al, Si, Na, and Cu content in the samples was analysed by inductively coupled plasma optical emission spectroscopy (ICP-OES) on a Perkin Elmer, Optima 8000 instrument (Rodgau, Germany). The samples (ca. 0.1 g) were dissolved in a mixture of hydrofluoric acid (2 ml, 48 wt.-%, Sigma-Aldrich), nitric acid (2 ml, 69 wt.-%, Sigma-Aldrich), and hydrochloric acid (3 ml, 35 wt.-%, Sigma-Aldrich) with microwave radiation (1 h, 200 °C). Before measurement, HF was removed by complexing with H_3BO_3 (12 ml, 99.99 wt.-%, Sigma-Aldrich) under microwave radiation (5 min, 200 °C).

^{27}Al and ^{29}Si solid-state nuclear magnetic resonance (NMR) spectra were acquired using a Bruker Avance 750 spectrometer (Rheinstetten, Germany; magnetic field strength 17.6 T) at frequencies of 195.06 MHz and 148.67 MHz, respectively. The spinning frequency was 7 kHz. Direct excitation was used for both nuclei. To obtain ^{27}Al spectra a 1 µs pulse length, equivalent to approximately a 30° flip angle, and a recycle delay of 0.1 s was used. ^{29}Si spectra were recorded with a 2.5 µs 90° pulse and a 10-second recycle delay. Spectra were referenced to a 1 M $Al(NO_3)_3$ solution and tetramethylsilane (TMS) for ^{27}Al and ^{29}Si, respectively. The analysis of NMR spectra was carried out using the dmfit program [1]. In all instances, Gaussian lines were used to deconvolute NMR spectra. In specific cases, the deconvolution of ^{27}Al spectra showed enhancement when employing a distribution of chemical shifts with the Czjzek model in dmfit [1].

Diffuse reflectance (DR) UV-Vis spectra of the samples were recorded at room temperature using a Perkin Elmer Lambda 650S UV-Vis spectrometer (Rodgau,

Germany) equipped with a 150 mm integrating sphere using spectralon® (PTFE, reflective value 99 %, Rodgau, Germany) as a reference. The experiments were carried out in the wavelength range of 200-900 nm with a step width of 1 nm and a slit width of 2 nm.

Hydrogen temperature programmed reduction (TPR-H_2) measurements were carried out by MicrotracBel Corp., BELCAT II (Haan/Duesseldorf, Germany). The samples were pressed and sieved to 100-300 µm. Approximately a 0.05 g sample was used for the measurement. For each sample, 20 vol.-% O_2 in Ar was used for pretreatment at 300 °C, and reduction was done with 5 vol.-% H_2 in Ar at a total flow rate of 30 ml min^{-1} to 800 °C.

The EPR measurements were carried out with a Bruker EMX micro (the X-band frequency corresponds to 9.4 GHz) spectrometer equipped with an Oxford Instruments He cryostat ESR 900 to allow low-temperature measurements. The spectrometer was fitted with an ER 4119 HS cylindrical cavity. The microwave power was adjusted between 0.063 and 2 mW to avoid a saturation effect. The frequency and amplitude of the modulation were kept at 100 kHz and 0.5 mT, respectively. The samples as a powder (ca. 20 mg) were put into a quartz tube with a 3.8 mm inner diameter and then sealed to avoid contact with the air. The activation procedure was carried out on all samples at 200 °C for 2 h under vacuum conditions (at least 10^{-2} mbar pressure). EPR measurements for hydrated and dehydrated samples were conducted at room temperature and -196 °C, respectively.

1.2 NH_3-SCR-DeNO$_x$

Catalytic experiments were achieved using a QMS MKS Cirrus 3 detector directly connected to the reactor (ID: 6 mm, L: 200 mm) outlet using a heated capillary.

Before each experiment, the catalysts (0.1 g, sieved with a fraction of 200-400 µm) were activated at 500 °C for 1.5 h under a flow of 50 ml min^{-1} of He and then cooled down below 75 °C. After that, the simulated flue gas, composed of c(NO) = 0.1 vol.-%, c(NH_3) = 0.1 vol.-%, c(O_2) = 10 vol.-% diluted in He with a total flow rate (F_{TOT}) of 120 ml min^{-1}, was switched on to pass through the catalyst bed. In the case of NH_3-SCO, the feed gas was composed of c(NH_3) = 0.1 vol.-%, c(O_2) = 10 vol.-% diluted in He with a total flow rate (F_{TOT}) of 120 ml min^{-1}. The gas hourly space velocity (GHSV) was determined to be ca. 30,000 h^{-1}. The reaction was carried out at atmospheric pressure and in a range of temperatures from 75 to 500 °C with an interval of 25-50 °C. At each temperature, the reaction was stabilized for 70 min before the quantitative analysis of respective concentrations. The individual flow rates were controlled by Bronkhorst mass flow controllers. The total flow rate of the reaction mixture was 120 ml min^{-1}. The signal of the helium line served as the internal standard to compensate for small fluctuations in the operating pressure. The conversion of NO (X(NO)) was determined according to $X(NO) = ([c(NO)_{in} - c(NO)_{out}]/c(NO)_{in}) \times 100\%$, where: $c(NO)_{in}$ and $c(NO)_{out}$ are concentrations of NO in the inlet and the outlet gas, respectively. During the NH_3-SCR-DeNO_x, among N-containing products N_2 and N_2O were detected. Therefore, for calculation of the N_2 selectivity the following equation was applied: $S(N_2) = (c(N_2)_{out})/(c(N_2)_{out} + c(N_2O)_{out}) \times 100\%$, where: $c(N_2)$out, and $c(N_2O)_{out}$ are concentrations in outlet gases of N_2 and N_2O, respectively.

1.3 Temperature-programmed reaction studies

Temperature-programmed reaction desorption of NH_3 was recorded using a QMS MKS Cirrus 3 spectrometer (Munich, Germany) directly connected to the outlet of the

reactor. Before sorption, the sample (0.1 g, sieved with a fraction of 200-400 µm) placed in a fixed-bed quartz reactor (ID = 6 mm, L = 200 mm) was subjected to outgassing in a flow of pure He (50 ml min^{-1}) at 500 °C for 1.5 h. Following that, the reactor was gradually cooled down to 100 °C, during which the sample was saturated for a period of 2 h with the gas mixtures, flowing at a rate of 50 ml min^{-1} of the following compositions: $c(NH_3)$ = 0.3 vol.-% diluted in He, for a duration of 2 h. The individual flow rates were controlled by Bronkhorst mass flow controllers. Subsequently, the catalyst was purged at 100 °C in a flow of pure He for 3 h. For the desorption step, the reactor was heated up to 500 °C with a linear heating rate of 10 °C min^{-1} in a flow of pure He. Among reactants and products, such components as NH_3 (*m/z* 17), H_2O (*m/z* 18) N_2 (*m/z* 28), NO (*m/z* 30), N_2O (*m/z* 44), and NO_2 (*m/z* 46) were monitored.

Similarly to the temperature-programmed desorption investigations, a series of stop-flow experiments were conducted to study NH3-SCR-DeNOx. Before the experiment, a 0.1 g catalyst was activated at 500 °C for a duration of 1.5 h, using a pure He flow (50 ml min^{-1}). Subsequently, the catalyst was cooled down to 100 °C. Following the cooling phase, a gas mixture comprising $c(NO)$ = 0.1 vol.-%, $c(NH_3)$ = 0.1 vol.-%, and $c(O_2)$ = 5 vol.-%, which was diluted in He, was introduced over Cu-containing zeolite Y samples for a period of 2 h. This process was carried out at 125 °C. Subsequently, the catalyst was purged at the same temperature using a pure He flow rate of 50 ml min^{-1} until a consistent baseline level was established, which typically took approximately 3 h. Afterwards, the reactor temperature was increased from 100 °C to 500 °C at a heating rate of 10 °C min^{-1}. This heating process was carried out using a pure He flow. Simultaneously, the gases released from the reactor outlet, including

NH_3 (m/z 17), H_2O (*m/z* 18), N_2 (*m/z* 28), NO (*m/z* 30), N_2O (*m/z* 44), and NO_2 (*m/z* 46), were analyzed using the QMS MKS Cirrus 3 spectrometer (Munich, Germany).

1.4 *In situ* / *operando* DRIFTS experiments

DRIFTS spectra were measured using a Thermo Nicolet iS50 spectrometer at a resolution of 4 cm^{-1}. Prior to each experiment, the samples were first dried in 10 vol.-% O_2, total flow rate of 50 ml min^{-1}, at 450 °C for 1 h. For all IR experiments, the total flow rate was maintained at 50 ml min^{-1}. The background spectrum was collected at 125 °C. Ar was used as a balance.

For a transient experiment, the following sequence of treatments was applied:

1 NH_3 + O_2 (20 min; 15 min IR record) → O_2 (20 min) → 2 NO + O_2 (20 min; 15 min IR record) → O_2 (20 min) → 3 NH_3 + O_2 (20 min; 15 min IR record) → SCR (30 min) → 4 NO ME in NH_3 + O_2 (60 s NH_3 + O_2 *vs* 60 s NO + NH_3 + O_2, 10 circles)

1.5 Steady-state isotopic transient kinetic analysis (SSITKA)

Similarly, to the catalytic studies, a series of steady-state isotopic transient kinetic analysis (SSITKA) were conducted. Before the experiment, a 0.1 g catalyst was activated at 500 °C for 1.5 h, using a pure He flow (50 ml min^{-1}). Subsequently, the catalyst was cooled down to 75 °C. Following the cooling phase, a gas mixture comprising *c*(NO) = 0.1 vol.-%, *c*(NH_3) = 1 vol.-%, *c*(Ar) = 1 vol.-%, and *c*(O_2) = 10 vol.-%, which was diluted in He, was introduced over Cu-containing zeolite Y samples for a period of 1 h. Subsequently, the NH_3 was exchanged with isotope-labelled $^{15}NH_3$ (*c*(NH_3) = 1 vol.-%, *c*(Kr) = 1 vol.-%) for 5 or 10 min, followed by switch-back for 5, 7 or 10 min. This process was carried out at three different

temperatures, including 100 °C, 125 °C and 150 °C. The reactants and products were analyzed using the QMS MKS Cirrus 3 spectrometer (Munich, Germany). Based on the signal response of $^{14}NH_3$ and Ar (or $^{15}NH_3$ and Kr), as well as $^{14}N_2$ and Ar (or $^{14}N^{15}N$ and Kr) obtained after switching from $^{14}NH_3$/Ar to $^{15}NH_3$/Kr, the average-surface life-time and surface concentration of reversible adsorbed ammonia molecules, adsorbed nitrogen molecules and intermediates leading to the formation of nitrogen were calculated.

The values of the average-surface life-time of adsorbed nitrogen molecules and intermediates leading to the formation of nitrogen ($^{\tau_{N_2}}/_{sec}$) were determined based on the magnitude of the delay time between the signal of $^{14}N_2$ (the response of $^{14}N_2$ – F_{N_2}) and Ar (the response of Ar – F_{Ar}), according to the equation (Eq. 1):

$$\tau_{N_2} = \int_0^t F_{N_2} dt - \int_0^t F_{Ar} dt \quad (1)$$

The values of the average-surface life-time of reversible adsorbed ammonia molecules ($^{\tau_{NH_3}}/_{sec}$) were determined based on the magnitude of the delay time between the signal of $^{14}NH_3$ (the response of $^{14}NH_3$ – F_{NH_3}) and Ar (the response of Ar – F_{Ar}), according to the equation (Eq. 2):

$$\tau_{NH_3} = \int_0^t F_{NH_3} dt - \int_0^t F_{Ar} dt \quad (2)$$

The surface concentration of adsorbed nitrogen molecules and intermediates leading to the formation of nitrogen ($^{N_{N_2}}/_{mmol\, g^{-1}}$) were calculated according to the equation (Eq. 3):

$$N_{N_2} = \tau_{N_2} \cdot r_{N_2} \quad (3)$$

where: r_{N_2} – the formation rate of N_2 (mmol s^{-1} g_{cat}^{-1}).

The surface concentration of reversible adsorbed ammonia molecules (N_{NH_3}) were calculated according to the equation (Eq. 4):

$$N_{NH_3} = \tau_{NH_3} \cdot \left(r_{NH_3} - r_{N_2}\right) \quad (4)$$

where: r_{NH_3} – the feed rate of NH_3 (mmol s^{-1} g_{cat}^{-1}).

2. Results

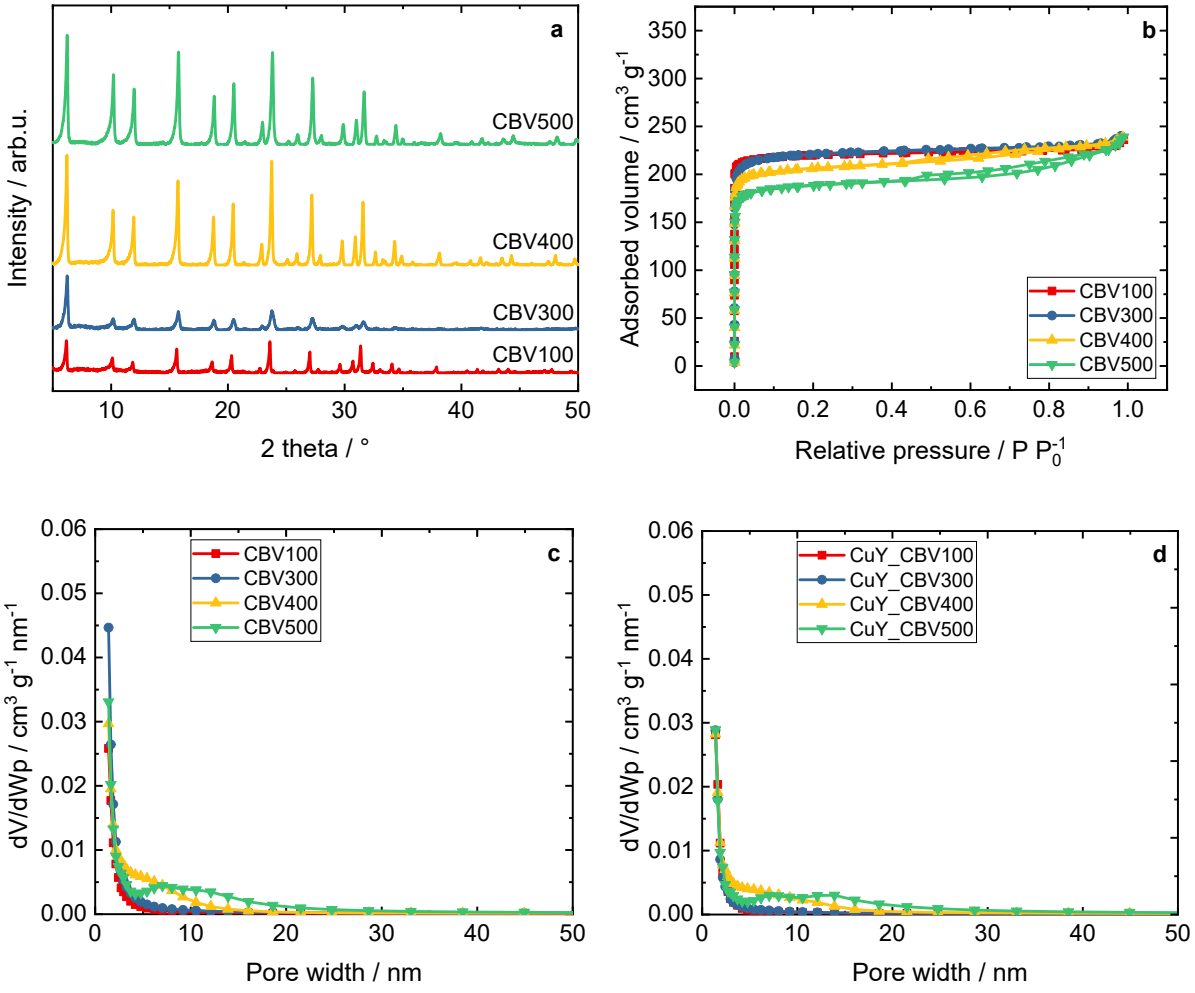

Fig. SI1: a) XRD patterns and b) N_2 sorption isotherms of calcined zeolite Y samples as well as c-d) pore width of the calcined zeolite Y samples and their Cu-containing forms.

Tab. SI1: Textural properties determined from the N_2 sorption isotherms: specific surface area ($A_{S(BET)}$), specific total pore volume ($V_{(TOT)}$), micropore ($V_{(MIC)}$), and mesopore volume ($V_{(MES)}$) of calcined zeolite Y samples and their Cu-containing forms.

Sample	$A_{S(BET)}$ / $m^2\,g^{-1}$	$V_{(TOT)}$ / $cm^3\,g^{-1}$	$V_{(MIC)}$ / $cm^3\,g^{-1}$	$V_{(MES)}$ / $cm^3\,g^{-1}$
CBV100	927	0.37	0.35	0.02
CBV300	890	0.37	0.35	0.02
CBV400	907	0.37	0.35	0.02
CBV500	808	0.37	0.33	0.04
CuY_CBV100	795	0.32	0.30	0.02
CuY_CBV300	358	0.16	0.14	0.02
CuY_CBV400	745	0.33	0.31	0.02
CuY_CBV500	674	0.33	0.29	0.04

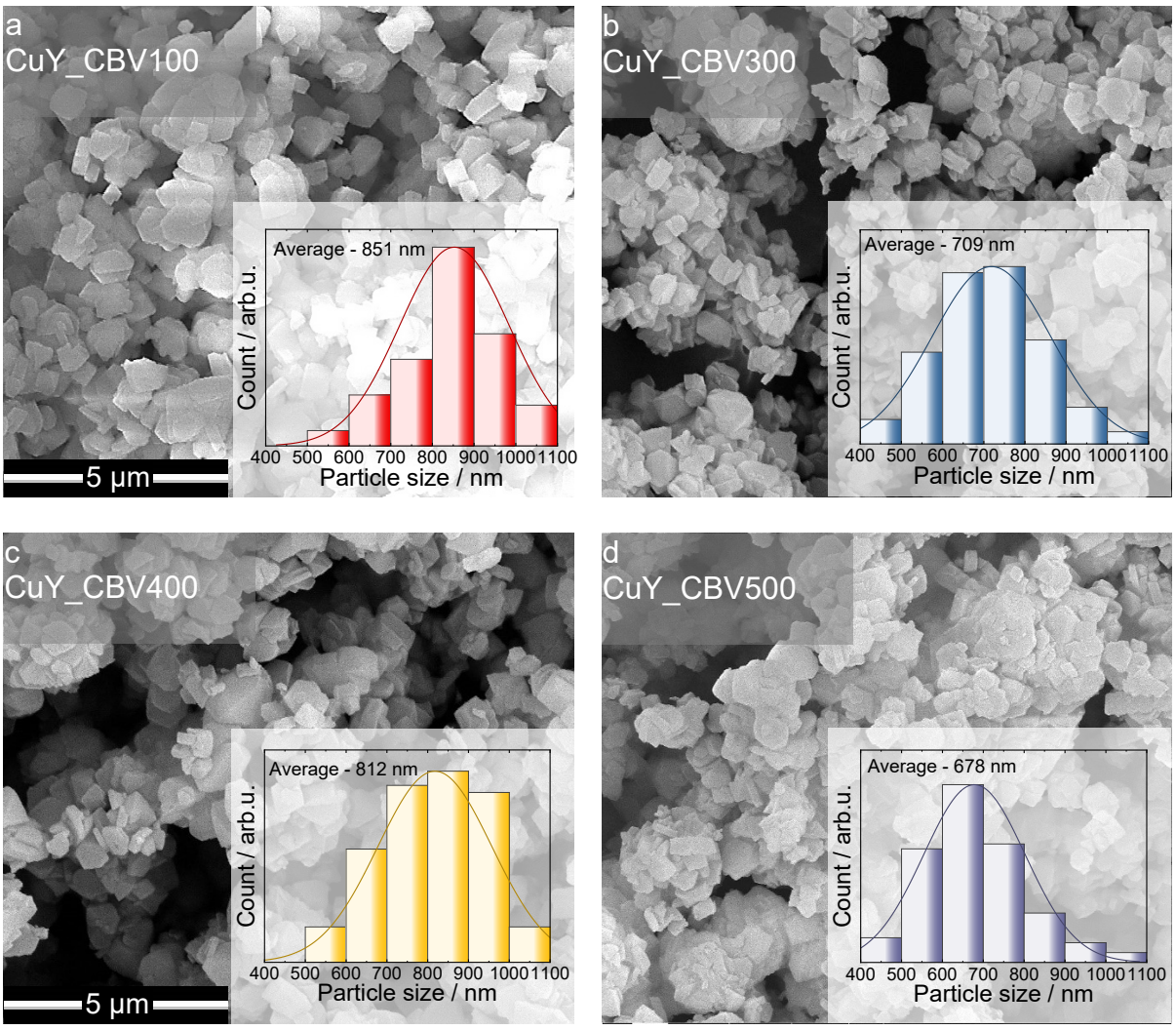

Fig. SI2: a-d) SEM images of the Cu-containing zeolite Y samples. The particle size distribution was obtained by measuring 100 particles from SEM images.

Tab. SI2: Intensity ratios of selected ions calculated based on ToF-SIMS spectra collected from the surface of the calcined zeolite Y samples.

	CBV100	CBV300	CBV400	CBV500
Al^+/Si^+	2.99	0.75	4.69	3.33
Al^+/total ion^+	0.054	0.027	0.069	0.067
Si^+/total ion^+	0.018	0.036	0.015	0.020

Tab. SI3: Intensity ratios of selected ions calculated based on ToF-SIMS spectra collected from the surface of the Cu-containing zeolite Y samples.

	CuY_CBV100	CuY_CBV300	CuY_CBV400	CuY_CBV500
Al^+/Si^+	1.31	1.14	3.47	3.51
Cu^+/Al^+	0.66	0.54	0.27	0.21
Cu^+/Si^+	0.87	0.62	0.93	0.73
Cu^+/total ion^+	0.019	0.015	0.009	0.008

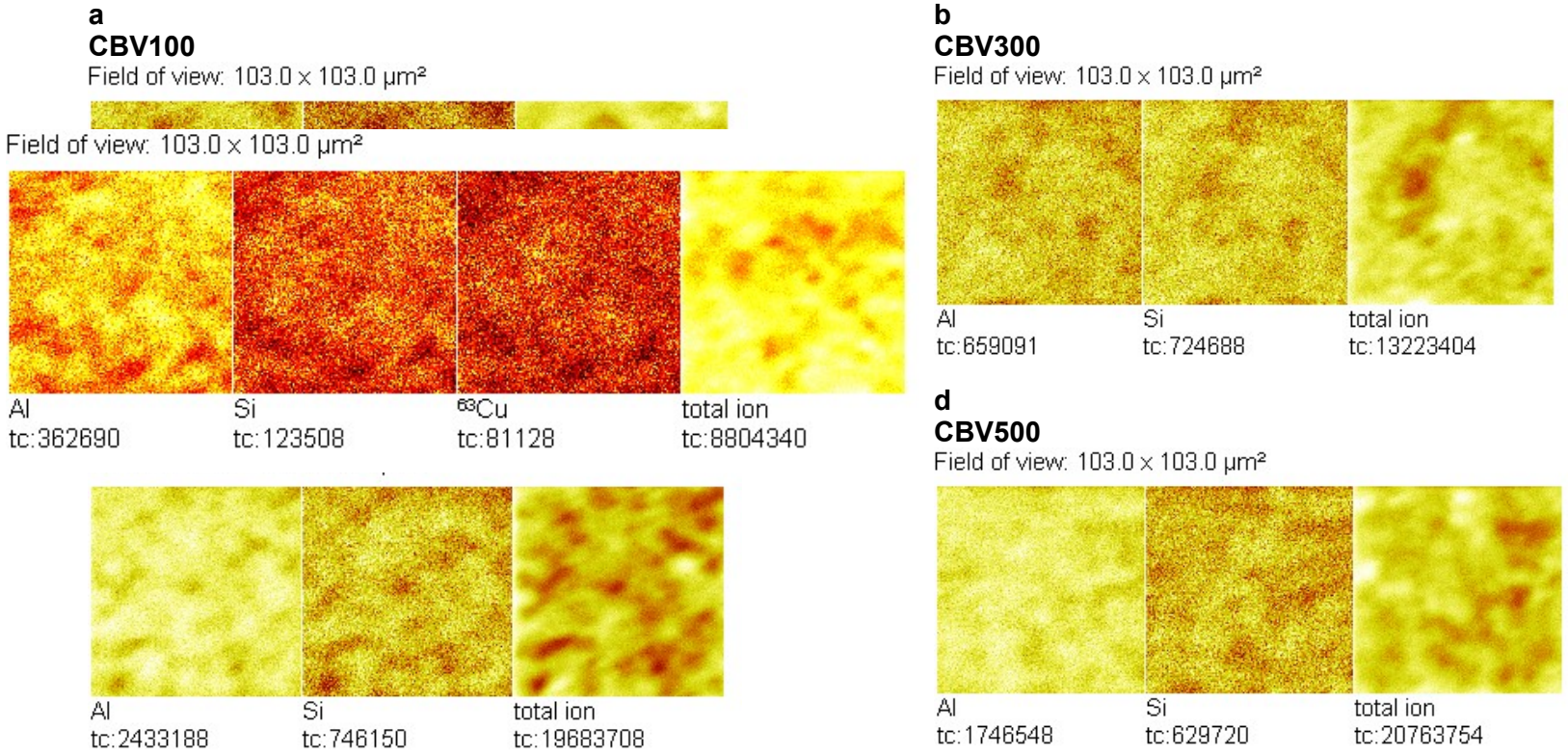

Fig. SI3: a-d) ToF-SIMS images collected from the surface of zeolite Y samples (tc - total counts).

Fig. SI4: a-c) ToF-SIMS images collected from the surface of the Cu-containing zeolite Y samples (tc - total counts).

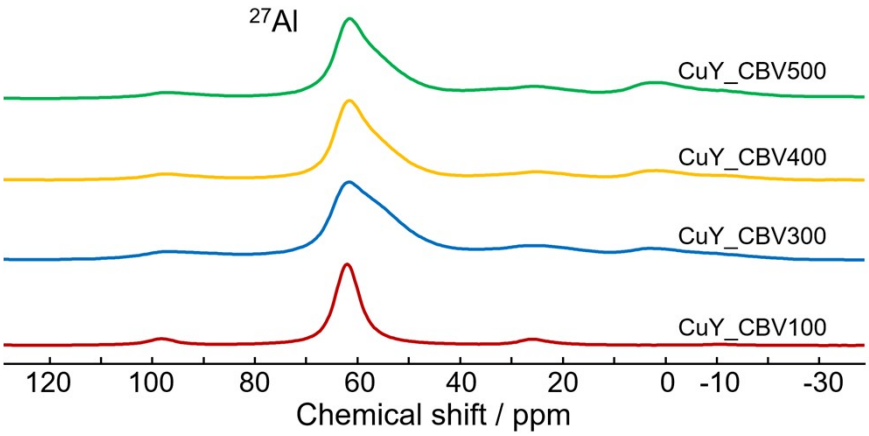

Fig. SI5: ^{27}Al MAS spectra of the Cu-containing zeolite Y samples.

Tab. SI4: Deconvolution of the ^{27}Al MAS NMR spectra.

Sample	Assignment	Chemical shift / ppm (Rel. area / %)
CuY_CBV100	Al(IV)	61.93 (100)
CuY_CBV300	Al(IV)	62.98 (93.1)
	Al(V)	31.84 (0.6)
	Al(VI)	1.14 (6.3)
CuY_CBV400	Al(IV)	63.69 (91.9)
	Al(V)	31.76 (2.7)
	Al(VI)	2.50 (5.4)
CuY_CBV500	Al(IV)	63.56 (85.2)
	Al(V)	37.56 (4.0)
	Al(VI)	3.87 (10.8)

Al^{IV} – four-coordinated aluminum

Al^{V} – five-coordinated aluminum

Al^{VI} – six-coordinated aluminum

Tab. SI5: Deconvolution of the ^{29}Si MAS NMR spectra.

Sample	-90 ppm	-95 ppm	-100 ppm	-105 ppm
CuY_CBV100	11.6 %	35.0 %	37.9%	18.5 %
CuY_CBV300*	4.5 %	25.7 %	19.5 %	50.3 %
CuY_CBV400	0.8 %	17.1 %	31.2 %	50.9 %
CuY_CBV500	1.5 %	6.7 %	33.9 %	57.9 %

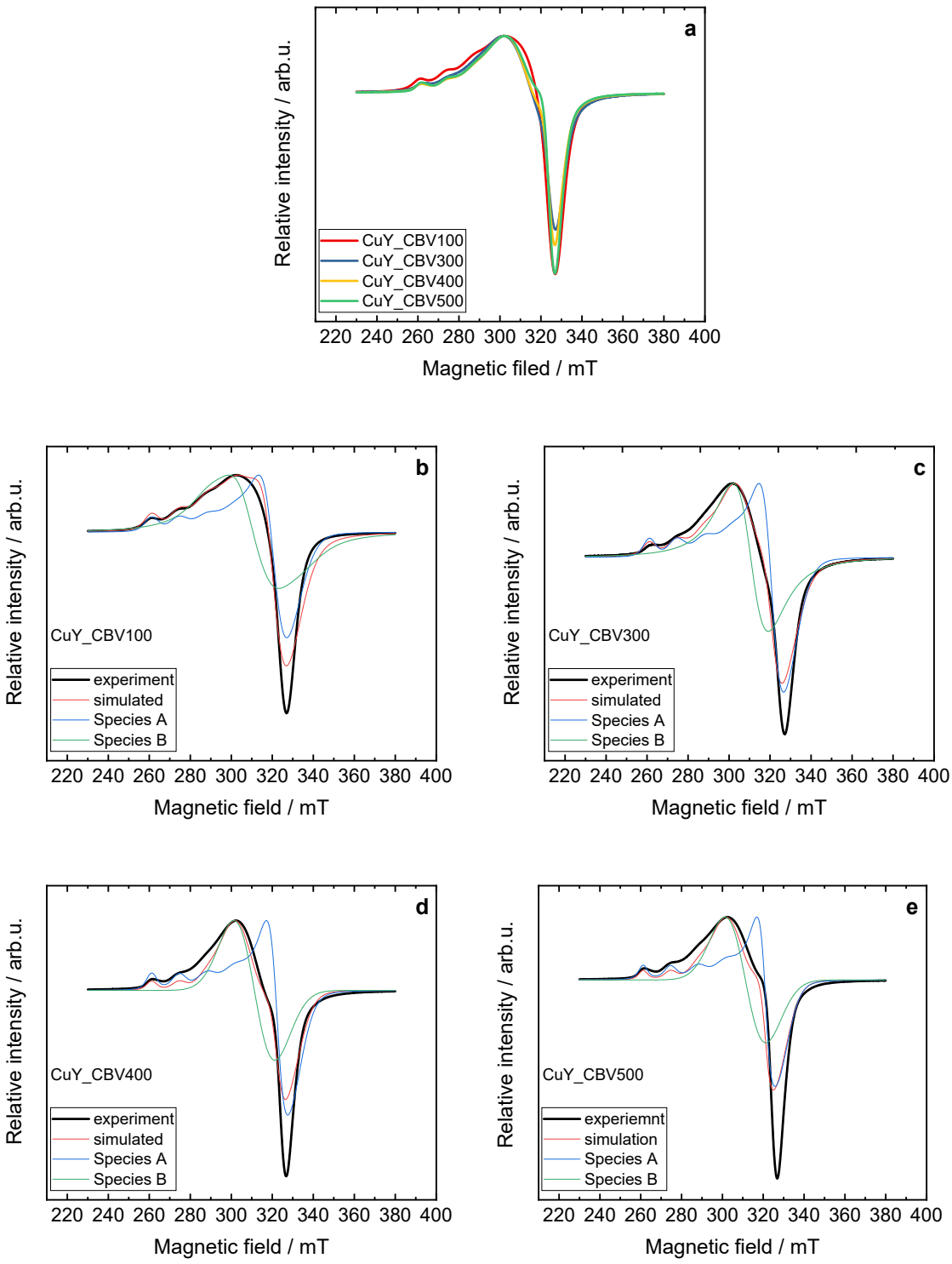

Fig. SI6: a) Weight normalised x-band EPR spectra of the as-made state recorded at a temperature of -196 °C, and b-e) show the simulated EPR spectra with species *A* and species *B* for the corresponding samples mentioned in the bottom left corner in every image.

Tab. SI6: Relative weight of Cu^{2+} species calculated from -196 °C spectra normalised to the content in Cu_CBV500.

Sample	Relative Cu^{2+} intensity
CuY_CBV100	1.99
CuY_CBV300	5.24
CuY_CBV400	1.15
CuY_CBV500	1.00

To get information about the contributing species to the EPR spectra, EasySpin 6.0.6 has been used for simulation using the following Hamiltonian (Eq. 1) [1]:

$$\hat{H} = \beta_e \vec{B} \vec{\vec{g}} \hat{\vec{S}} + \hat{\vec{S}} \vec{\vec{A}} \hat{\vec{I}} \quad (1)$$

Where $\beta_e$is Bohr magneton, $\vec{\vec{g}}$ is the g-tensor, $\vec{\vec{A}}$ is the hyperfine tensor, $\vec{B}$ is the external magnetic field and $\vec{S}$ is the spin operator for the spin doublet system. For the samples in the as-made state, we obtained the best fit (Fig. SI6) by involving two species, species A and species B, which have different EPR parameters. Species *A* comprise axially symmetric EPR parameters, $g_{xx} = g_{yy} = 2.07$ (1), $g_{zz} = 2.39$ (1) and $A_{xx} = A_{yy} = 30$ (8) MHz, A_{zz}= 440 (5) MHz; whereas species *B* comprise an isotropic EPR line centred at $g_{iso} = 2.16$ (1). Voigtian line shape is used for species A with Gaussian broadening of 1 mT and Lorentzian broadening of 2 mT. A Gaussian line shape is used for species B with 19 mT broadening. Species A can be assigned to Cu^{2+} ions, probably present at the centre of the hexagonal window between α and β cages with displacement towards the α cage of the zeolite. The ion is bound to three water molecules and three zeolitic oxygen ions [1]. It can be ruled out that species B arises from species *A* in high concentration, as the average g value from species A would be $g_{avg} = 2.18$ (1). So, species *B* is more consistent with Cu^{2+} bound to six water molecules, which could potentially be present in higher concentration in the sample [2]. For species *A*, g and *A* anticorrelated strain has been used, as we can

see that the EPR lines are getting broader with increasing m_s and for species *B*, only the g strain is used. The different weights of these two species are listed in Tab. SI3 (uncertainty 5 %):

Tab. SI7: Weight percentage of species *A* and *B*, and the g and *A* strain used for simulating the EPR spectra of -196 °C as-made samples with uncertainty 5 %.

Sample	Species *A*			Species *B*	
	g_{strain}	A_{strain}	weight	g_{strain}	weight
CuY_CBV100	0.08	80	80 %	0.08	20 %
CuY_CBV300	0.07	80	53 %	0.07	48 %
CuY_CBV400	0.05	80	54 %	0.05	46 %
CuY_CBV500	0.05	80	54 %	0.05	45 %

Tab. SI8: Weight percentage of species *A* and *B*, and the g and *A* strain used for simulating the EPR spectra of -196 °C activated samples with uncertainty 5 %.

Sample	Species *A*			Species *B*	
	g_{strain}	A_{strain}	weight	g_{strain}	weight
CuY_CBV100	0.02	0.02	12 %	0.05	88 %
CuY_CBV300	0.05	0.05	29 %	0.05	71 %
CuY_CBV400	0.03	0.06	29 %	0.05	71 %
CuY_CBV500	0.05	0.06	28 %	0.05	72 %

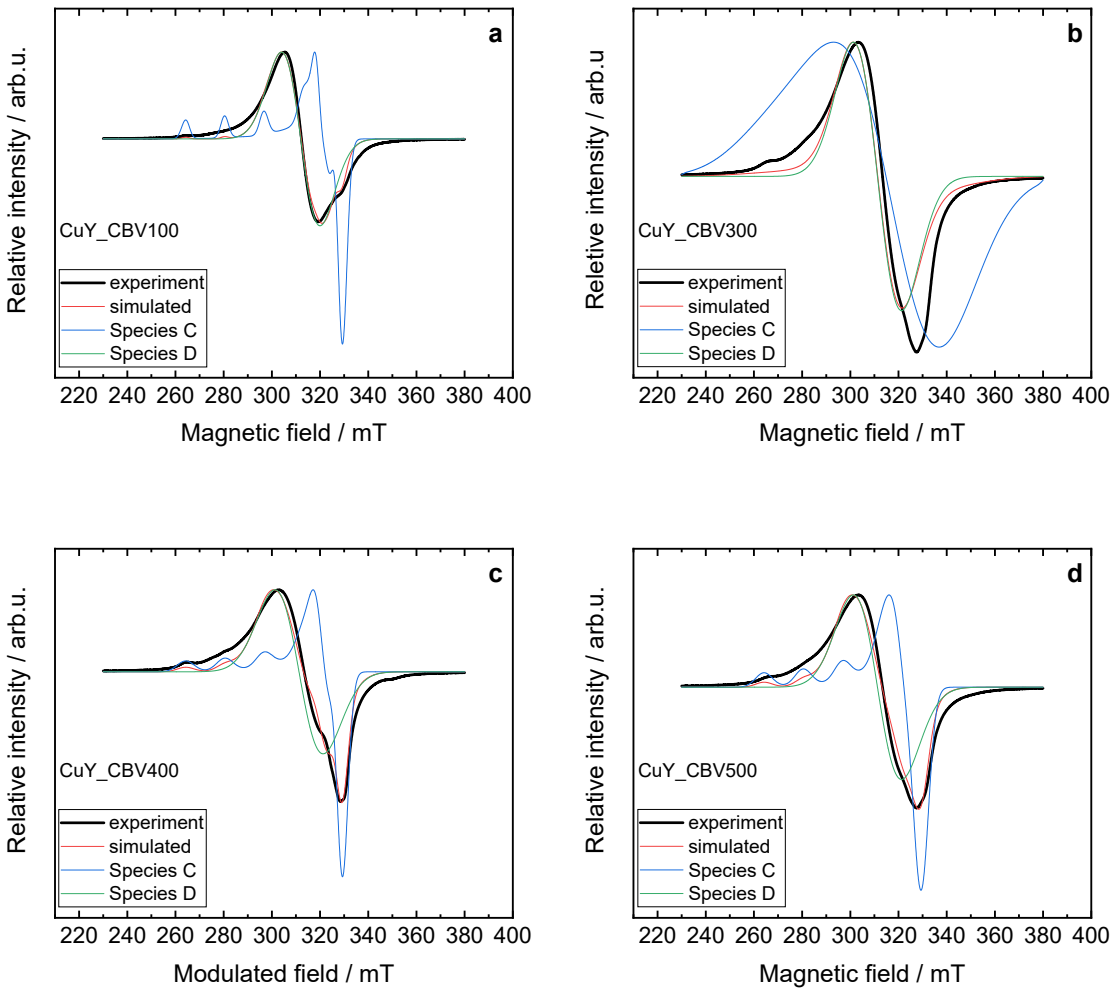

Fig. SI7: a-d) The weight normalised x-band EPR spectra of the activated samples recorded at a temperature of -196 C. The simulations are carried out with species *C* and species *D* for the corresponding samples mentioned in the bottom left corner in every image.

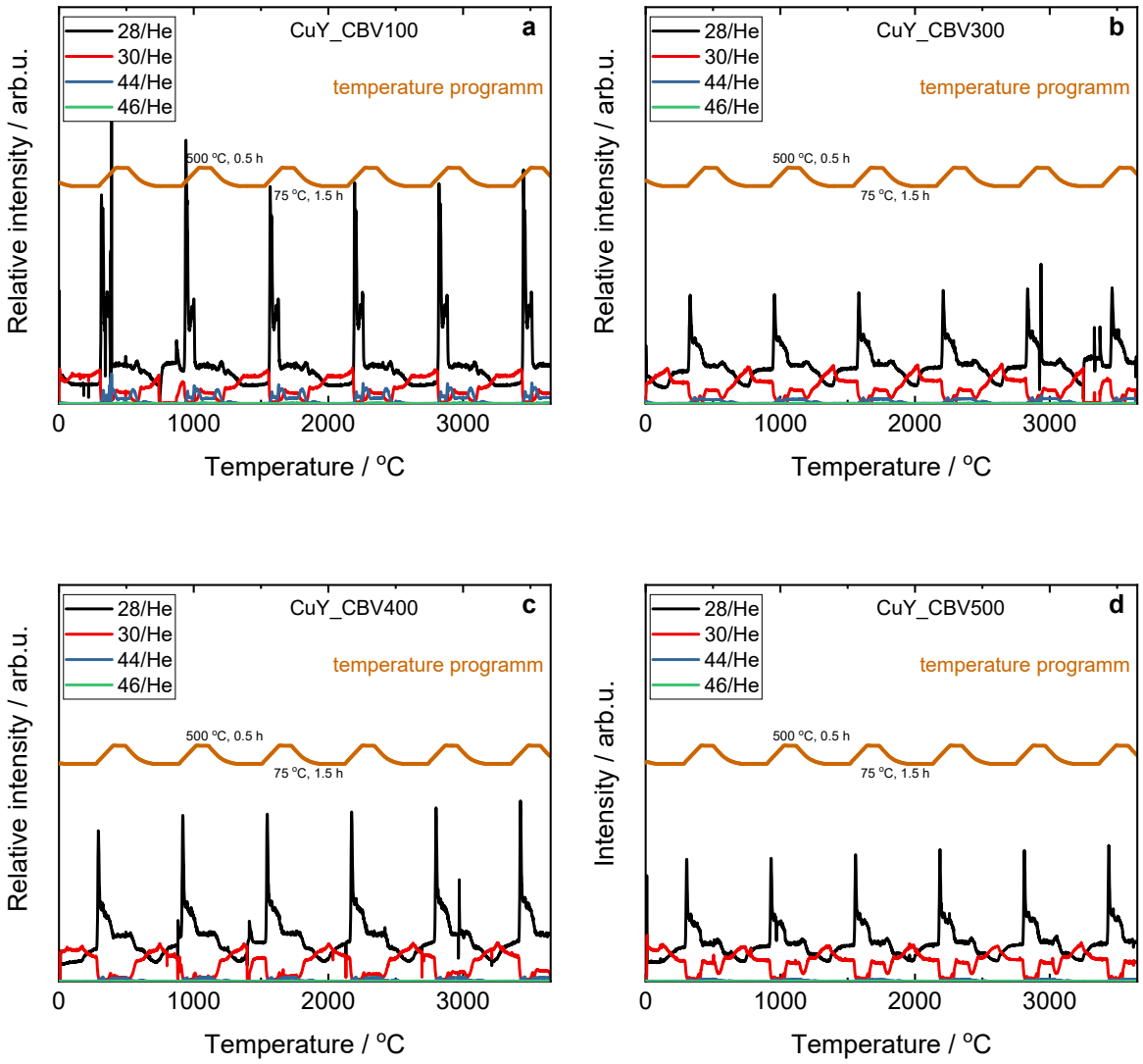

Fig. SI8: Comparison of the a-d) activity and selectivity of Cu-containing zeolite Y samples during the heating (75-500 °C) and cooling down (500-75 °C) in the NH_3-SCR-$DeNO_x$. Reaction conditions: m_K = 0.1 g, *c*(NO) = 0.1 vol.-%, *c*(NH_3) = 0.1 vol.-%, c(O_2) = 5 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}, linear heating rate of 10 °C min^{-1} (*m/z* – mass-to-charge ratio).

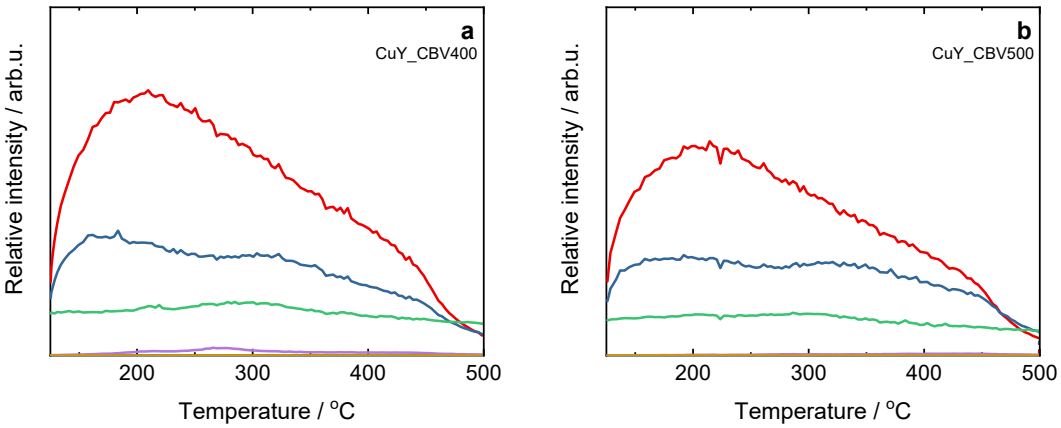

Fig. SI9: Stop-flow experiments over a) CuY_CBV400 and b) CuY_CBV500. Reaction conditions: m_K = 0.1 g, c(NO) = 0.1 vol.-%, c(NH_3) = 0.1 vol.-%, c(O_2) = 5 vol.-%, He balance, F_{TOT} = 120 ml min^{-1}, GHSV = 30,000 h^{-1}.

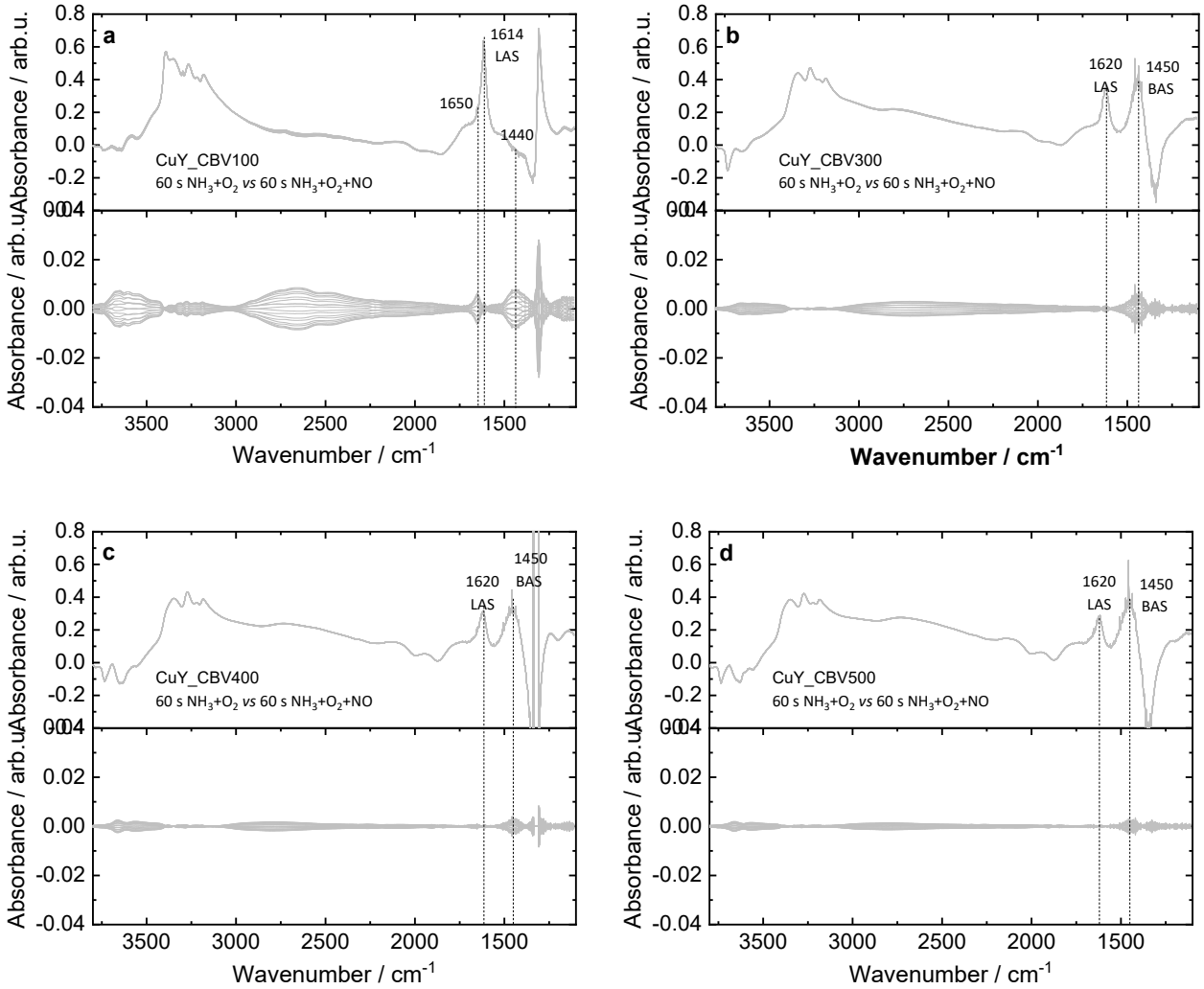

Fig. SI10: Time-resolved in situ IR spectra (top) and corresponding phase-resolved spectra (bottom) of a) CuY_CBV100, b) CuY_CBV300, c) CuY_CBV400, d) CuY_CBV500.

References

[1] D. Massiot, F. Fayon, M. Capron, I. King, S. Le Calvé, B. Alonso, J.-O. Durand, B. Bujoli, Z. Gan, G. Hoatson, Modelling One-and Two-Dimensional Solid-State NMR Spectra, *Magn. Reson. Chem.* 40 (2002) 70–76.