Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Characterization of Fe^{2+} Ions in Fe,H/SSZ-13 Zeolites: FTIR Spectroscopy of CO and NO Probe Molecules

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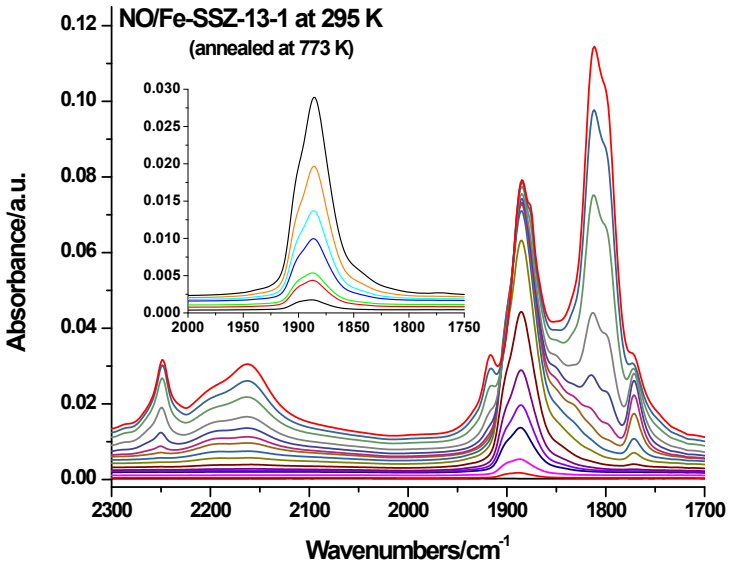
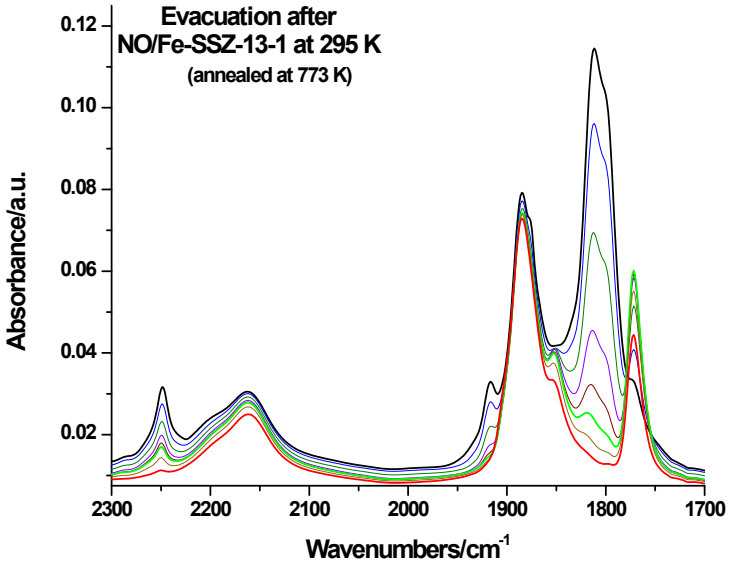
Figure S1. Selected IR spectra collected during the step-wise adsorption of NO on the annealed (773 K) Fe/SSZ-13-1 and -5 samples at 295 K: panels **a** and **c** adsorption, panels **b** and **d** desorption. (insets in panels **a** and **c** highlight the IR spectra recorded at the lowest NO dosages).

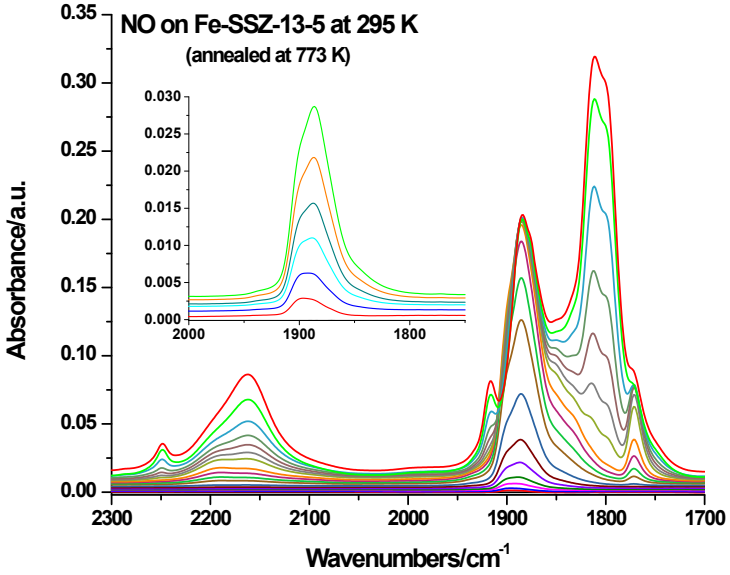
a.



b.


Evacuation after
NO/Fe-SSZ-13-1 at 295 K
(annealed at 773 K)
Absorbance/a.u.
0.12
0.10
0.08
0.06
0.04
0.02
2300
2200
2100
2000
1900
1800
1700
Wavenumbers/cm-1

c.


NO on Fe-SSZ-13-5 at 295 K
(annealed at 773 K)
Absorbance/a.u.
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.030
0.025
0.020
0.015
0.010
0.005
0.000
2000
1900
1800
2300
2200
2100
2000
1900
1800
1700
Wavenumbers/cm-1

d.

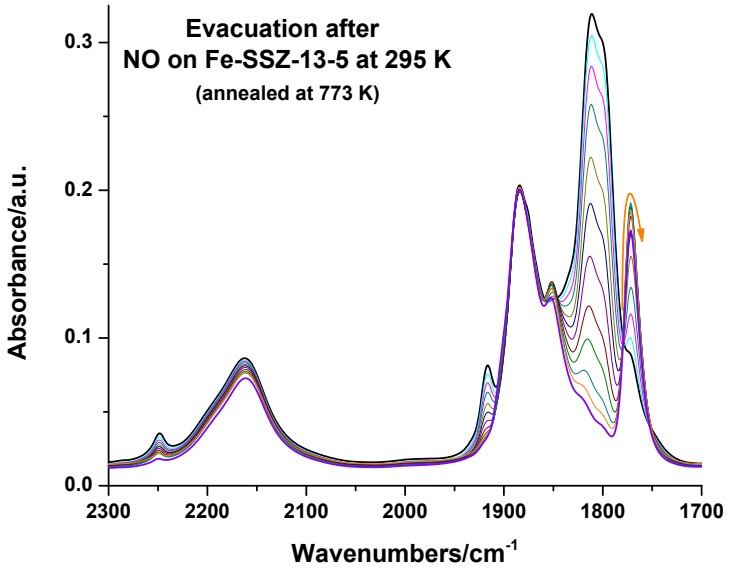
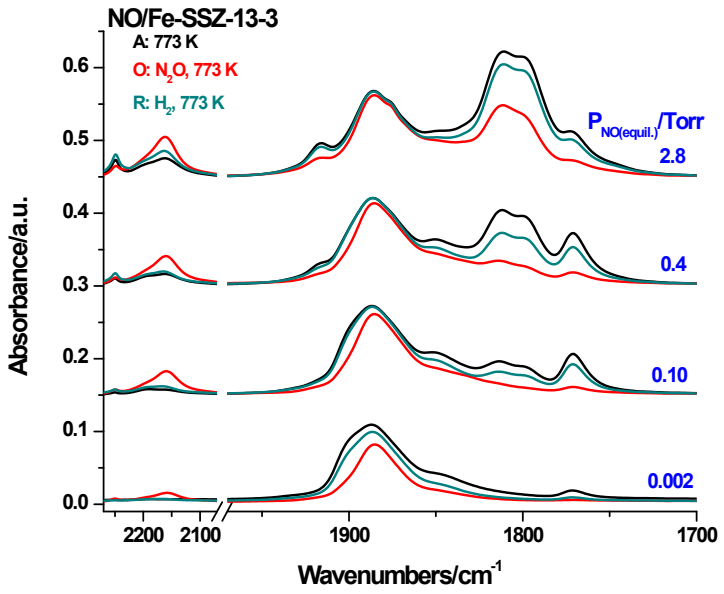


Figure S2. IR spectra obtained during step-wise NO adsorption on the annealed, oxidized and reduced Fe/SSZ-13 samples (**a:** Fe/SSZ-13-3, **b**: -5) at selected NO equilibrium pressures at 295 K. (annealing: at 773 K, 2h, in vacuum; oxidation: at 773 K in N_2O; reduction: at 773 K in H_2)

a.



b.

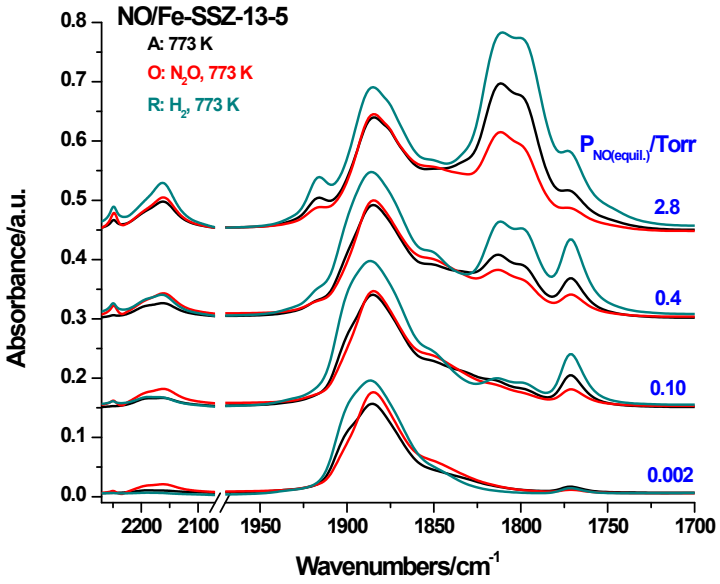


Figure S3. Series of IR spectra obtained during stepwise CO adsorption from the annealed Fe/SSZ-13- 1 sample at 150 K. (The inset in the figure shows the IR spectra at low CO dosages.)

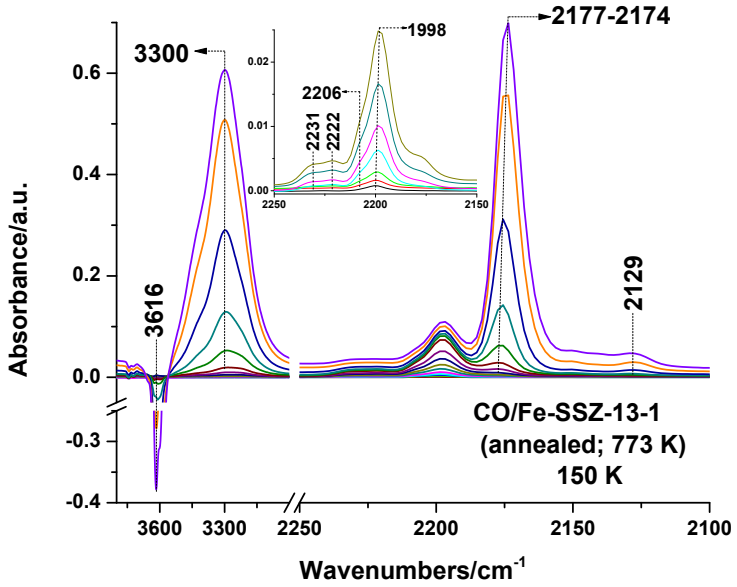


Figure S4. Series of IR spectra obtained under dynamic vacuum following stepwise CO adsorption from the annealed Fe/SSZ-13-1 sample at 150 K. (The inset in the figure shows the IR spectra recorded at low CO coverages.)

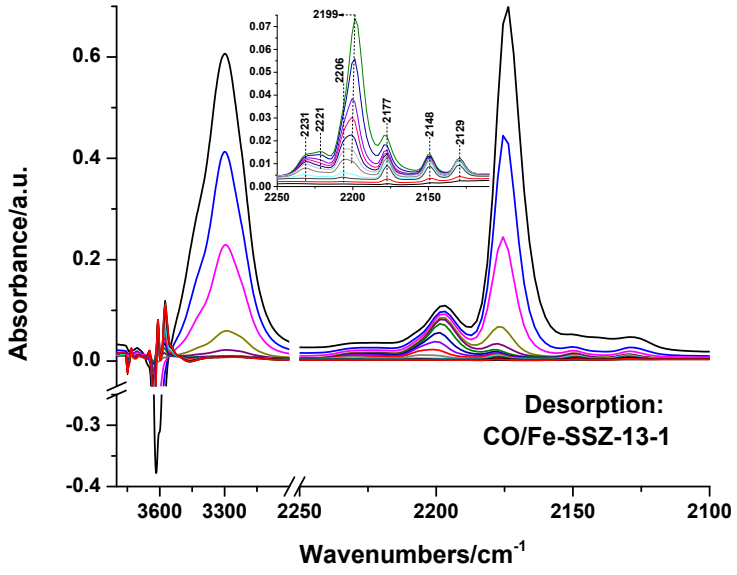
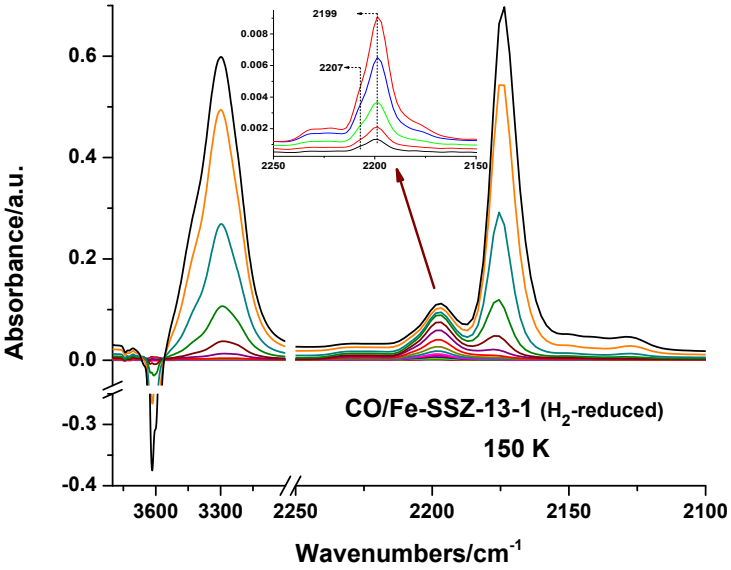


Figure S5. Series of IR spectra recorded during CO adsorption on the reduced Fe/SSZ-13-1 (***a***) and -5 (***b***) samples at 150 K. (Reduction: 773 K in H_2)

a.



b.

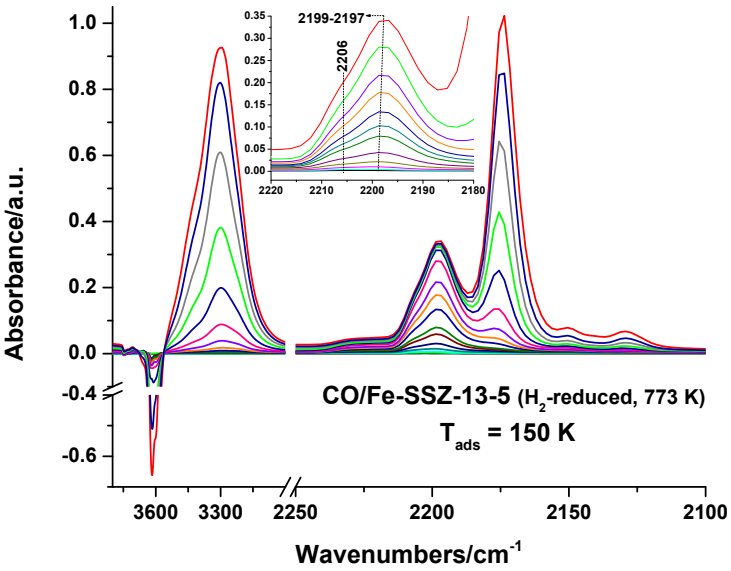
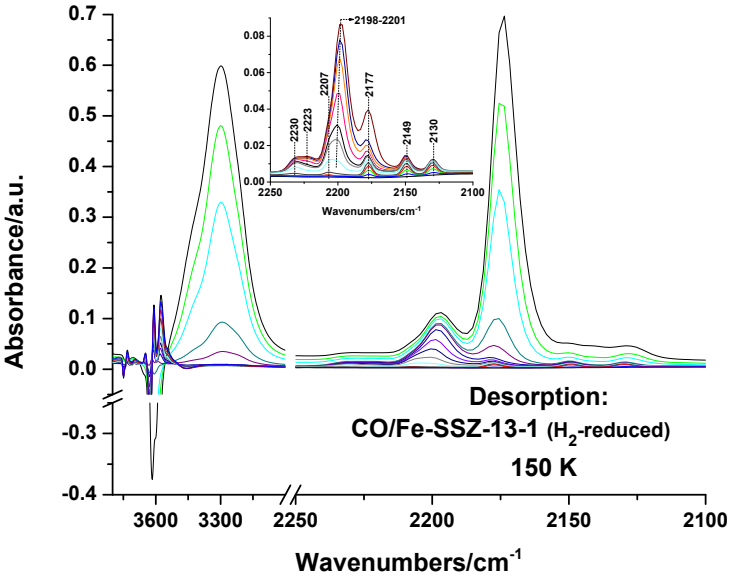


Figure S6. Series of IR spectra recorded during evacuation following CO adsorption on the reduced Fe/SSZ-13-1 (***a***) and -5 (***b***) samples at 150 K.

a.



b.

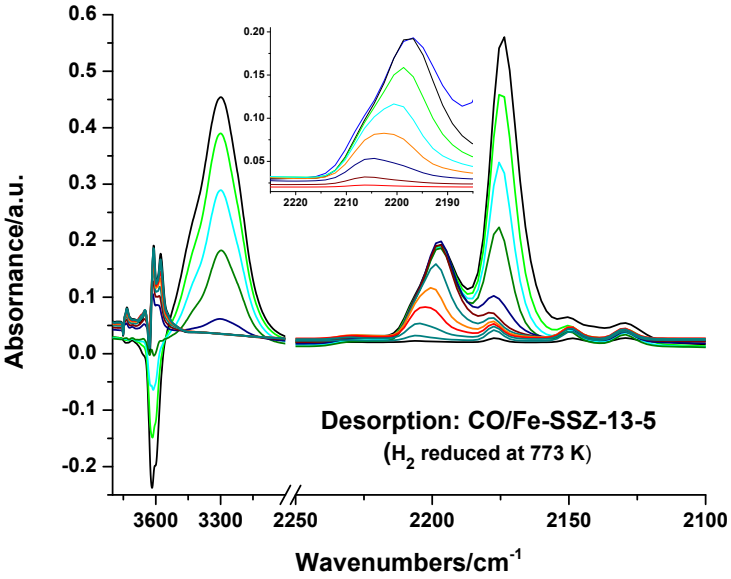


Figure S7. Total pressure vs. time-on-stream during N_2O decomposition over Fe/SSZ-13-1 and -5 samples at 773 K.

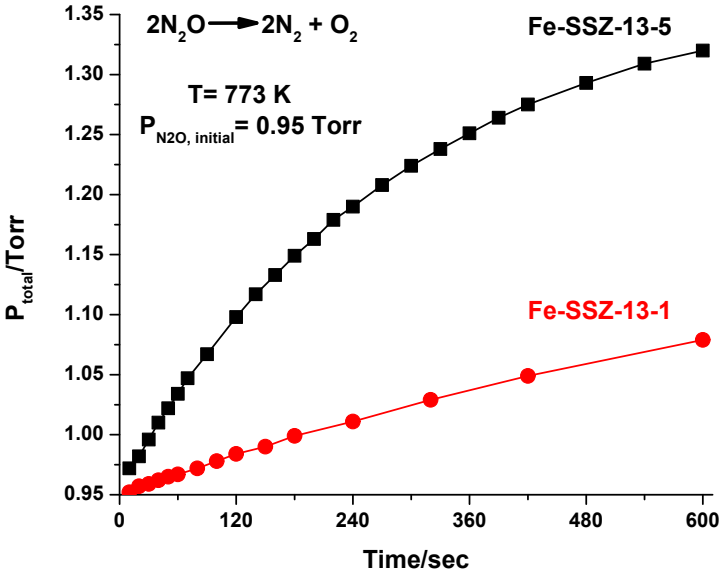


Figure S8. Variation in the 28, 30 and 32 amu mass fragments as a function of time-on-stream during N_2O decomposition over Fe/SSZ-13-1 and -5 samples at 773 K.

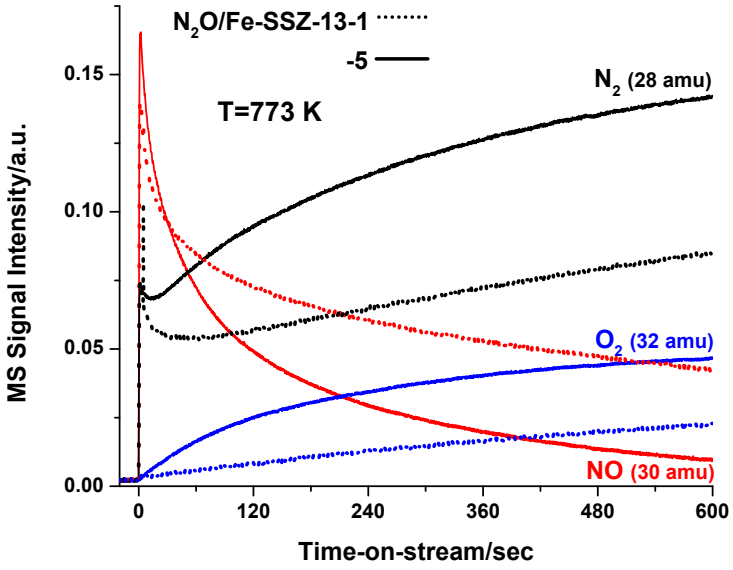


Figure S9. Series of IR spectra obtained during stepwise CO adsorption from the N_2O-oxidized (at 573 K) Fe/SSZ-13-1 sample at 150 K. (The inset shows the IR spectra collected at low CO dosages.)

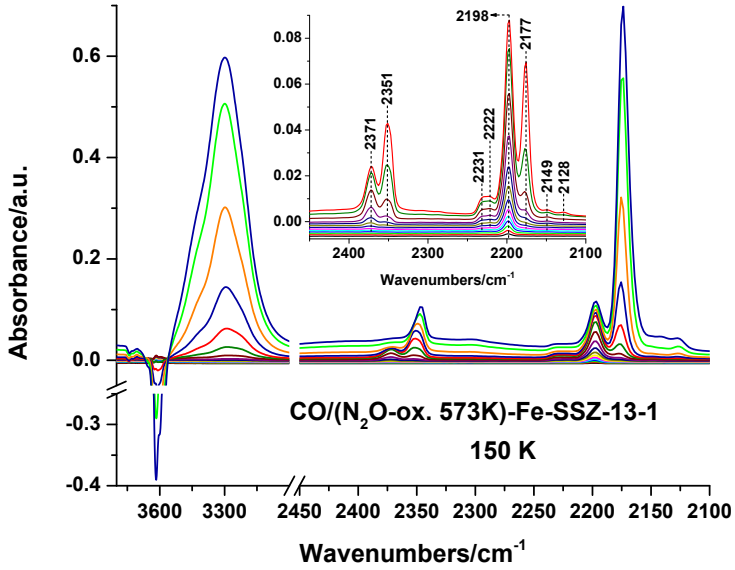


Figure S10. Series of IR spectra obtained during the repeated (2nd) stepwise CO adsorption from the N_2O-oxidized (at 573 K) Fe/SSZ-13-1 sample at 150 K. Following the first CO adsorption experiment (see Fig. S9) the sample was annealed to 373 K to remove all the CO_x species. (The inset shows the IR spectra collected at low CO dosages.)