

Fig. S1. FTIR spectra of H–ZSM-5 (panel A) and D–ZSM-5 samples (panel B) in the region of OH (A) and OD (B) combination modes. The spectra are automatically corrected for baseline and smoothed.

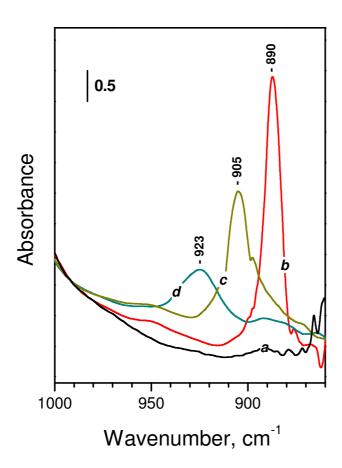


Fig. S2. FTIR spectra ( $1000-860~\text{cm}^{-1}$  region) of H–ZSM-5 (a), H–D–ZSM-5 (b) and after saturation of H–D–ZSM-5 with  $^{15}N_2$  (c) and CO (d). The spectra are smoothed.

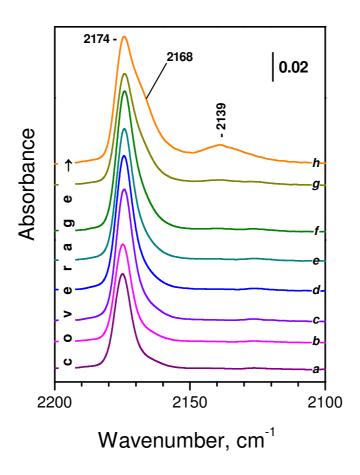


Fig. S3. Changes in the FTIR spectra of H–D–ZSM-5 in the carbonyl region during small changes of the CO coverage (for details see text). The coverage increases in the sequence (a)-(h). The Figure corresponds to low and medium CO coverages. The same set of spectra as for Fig. 7 from the main text is used.

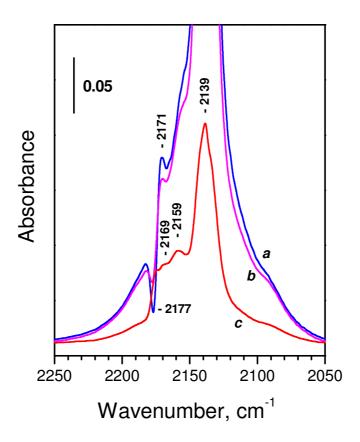


Fig. S4. Changes in the FTIR spectra of H–D–ZSM-5 in the carbonyl region during small changes of the CO coverage (for details see text). The coverage increases in the sequence (a)-(c). The Figure corresponds to high CO coverages. The same set of spectra as for Fig. 8 from the main text is used.

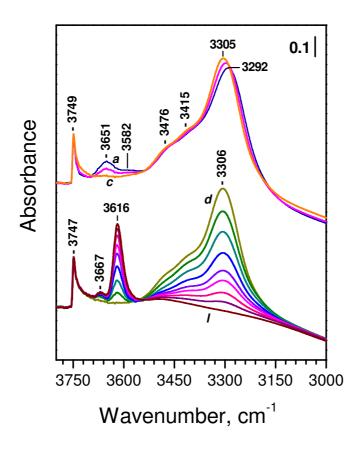


Fig. S5. FTIR spectra of <sup>13</sup>CO adsorbed at 100 K on H–ZSM-5. Equilibrium CO pressure of 500 Pa (a) and evolution of the spectra under dynamic vacuum at 100 K (b-l).

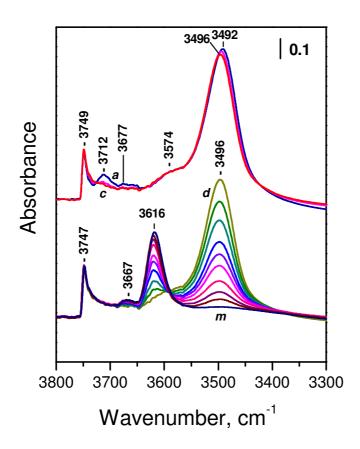


Fig. S6. FTIR spectra of  $^{14}N_2$  adsorbed at 100 K on H–ZSM-5. Equilibrium  $^{14}N_2$  pressure of 1 kPa (a) and evolution of the spectra under dynamic vacuum at 100 K (b-m).

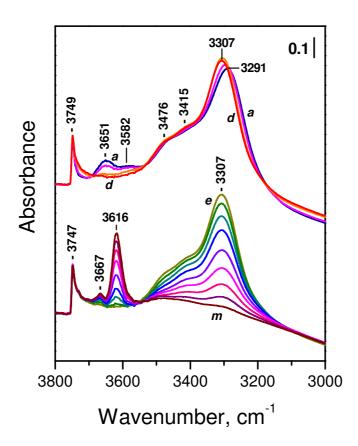


Fig. S7. FTIR spectra of CO adsorbed at 100 K on H–ZSM-5. Equilibrium CO pressure of 500 Pa (a) and evolution of the spectra under dynamic vacuum at 100 K (b-m).

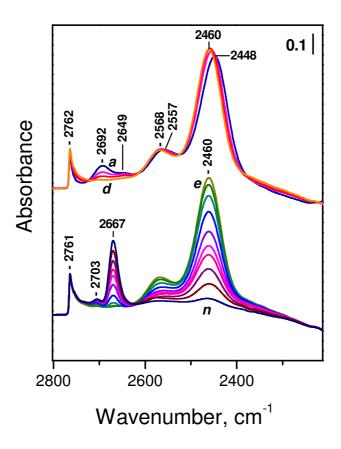


Fig. S8. FTIR spectra of CO (500 Pa equilibrium pressure) adsorbed at 100 K on D–ZSM-5 (a) and evolution of the spectra under dynamic vacuum at 100 K (b-n).