

Supplementary information

Sorption Modeling.

The atomic positions for the zeolite frameworks were obtained from previous X-ray and neutron diffraction determinations of the structures.¹⁻⁴ The structural parameters of PTZ derived from previous structural and theoretical works.⁵⁻⁷ In the Monte Carlo (MC) calculations, the Si, Al, O and H positions were fixed and the PTZ structure was taken to be rigid. The MC simulations at fixed loading were carried out at 300 K using the conventional Metropolis algorithm taking into account the non bonding interactions (E_{ZS}). The non bonding interactions were modeled by Lennard-Jones (L-J) and coulombic forces. The non bonding L-J force field values and partial charges of Si, Al, O (q_i) and C, H (q_j) atoms were taken from previous works^{1, 8, 9}. The long-range electrostatic interactions were calculated using the Ewald summation technique. One typical MC run took 1500000 steps. From each sorption trajectory, a histogram of the energy distribution for PTZ was generated. In the subsequent molecular mechanics (MM) simulations, the zeolite framework was taken to be rigid and PTZ was taken to be mobile and flexible. The MM calculations take into account the non bonding interactions (E_{ZS}) and the bond interaction (E_S) between PTZ atoms. We employ a bonding interaction force field with harmonic terms for bond stretching, bond angle bonding and torsional rotation. The energy minimization of sorbate-zeolite energy ($E_S + E_{ZS}$) was performed using the conjugate gradient minimization procedure.

¹ E. Beerdsen, D. Dubbeldam, B. Smit, T. J. Vlugt, and S. Calero, *The Journal of Physical Chemistry B*, 2003, **107**, 12088.

² I. Bull, P. Lightfoot, L. A. Villaescusa, L. M. Bull, R. K. B. Gover, J. S. O. Evans, and R. E. Morris, *Journal of the American Chemical Society*, 2003, **125**, 4342.

³ A. Martucci, A. Alberti, G. Cruciani, P. Radaelli, P. Ciambelli, and M. Rapacciuolo, *Microporous and Mesoporous Materials*, 1999, **30**, 95.

⁴ A. Martucci, G. Cruciani, A. Alberti, C. Ritter, P. Ciambelli, and M. Rapacciuolo, *Microporous and Mesoporous Materials*, 2000, **35-36**, 405.

⁵ C. Baehtz and H. Fuess, *Physical Chemistry Chemical Physics*, 2002, **4**, 4543.

⁶ C. Morin, D. Simon, and P. Sautet, *The Journal of Physical Chemistry B*, 2004, **108**, 12084.

⁷ K. B. Wiberg, *Journal of Organic Chemistry*, 1997, **62**, 5720.

⁸ I. Gener, G. Buntinx, and C. Bremard, *Microporous and Mesoporous Materials*, 2000, **41**, 253.

9

D. H. Olson, N. Khosrovani, A. W. Peters, and B. H. Toby, The Journal of Physical Chemistry B, 2000, 104, 4844.

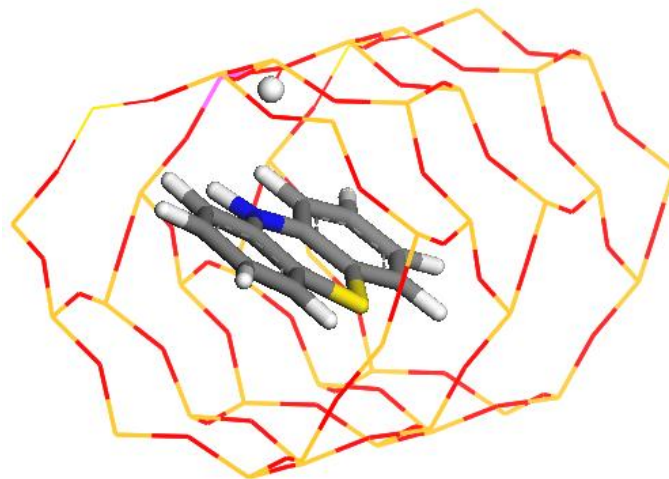


Figure S1 : Monte Carlo simulation of PTZ occluded in the straight channel of H-FER. Red, yellow and pink lines represent the O, Si and Al atoms of the framework, respectively. The white, shaded, blue and yellow cylinders represent the H, C, N and S atoms of the PTZ (C₁₂H₉NS) molecule, respectively. The white sphere represents the charge balancing H⁺ cation.

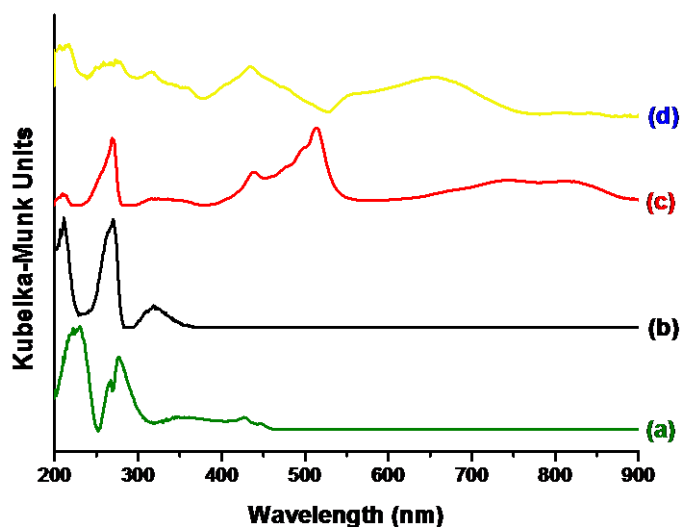


Figure S2 : UV-visible absorption spectra of pure species resolved by a MCR-ALS chemometric analysis of the spectra recorded during several months after the mixing of solid PTZ and dehydrated H_{6,6}ZSM-5. (a) solid PTZ; (b) PTZ@H-ZSM-5; (c) PTZ^{•+}@H-ZSM-5^{•-}; (d) PTZ²⁺@H-ZSM-5²⁻.

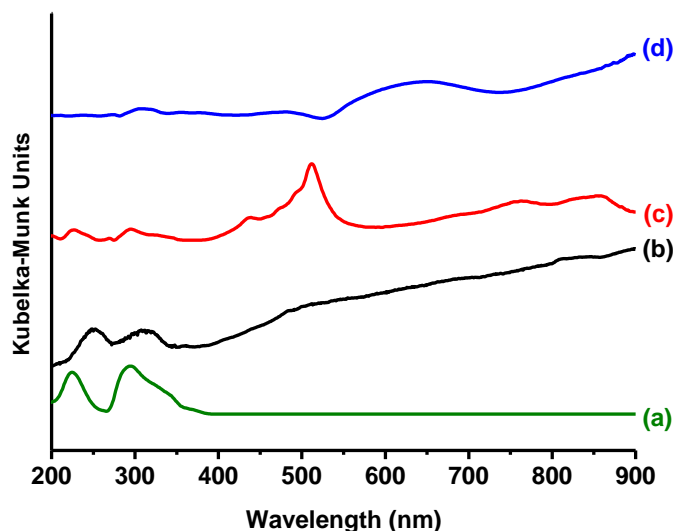


Figure S3 : UV-visible absorption spectra of pure species resolved by a MCR-ALS chemometric analysis of the spectra recorded during several months after the mixing of solid PTZ and dehydrated H-MOR. (a) solid PTZ; (b) PTZ@H-MOR; (c) PTZ^{•+}@H-MOR^{•-}, (d) PTZ²⁺@H-MOR²⁻.