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

SUPPLEMENTARY INFORMATION

Local anisotropy in single crystals of zeotypes with the MFI framework structure evidenced by polarised Raman spectroscopy

Anna Martinelli, Simone Creci, Szilvia Vavra,
Per-Anders Carlsson and Magnus Skoglundh

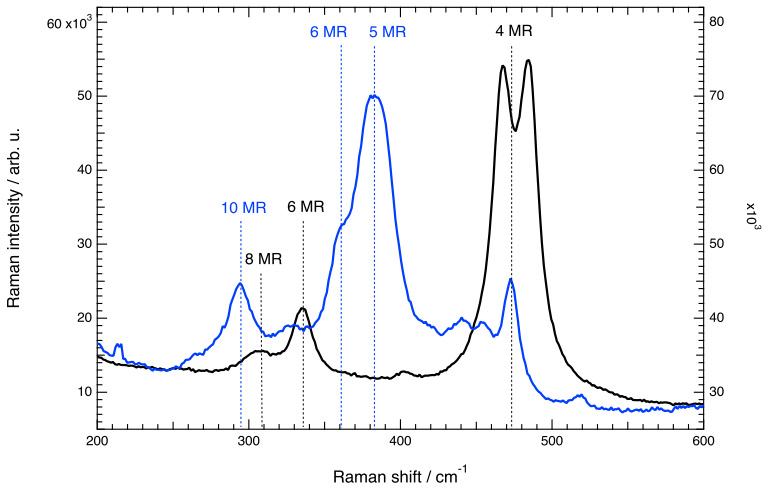

FIGURE 1. Figure S1. Raman spectra of the zeolites ZSM-5 (blue, MFI framework structure) and SSZ-13 (black, CHA framework structure) collected at room temperature. The assignment that we propose, based on the dependence of the frequency of the O-bending modes on the ring size, is indicated.

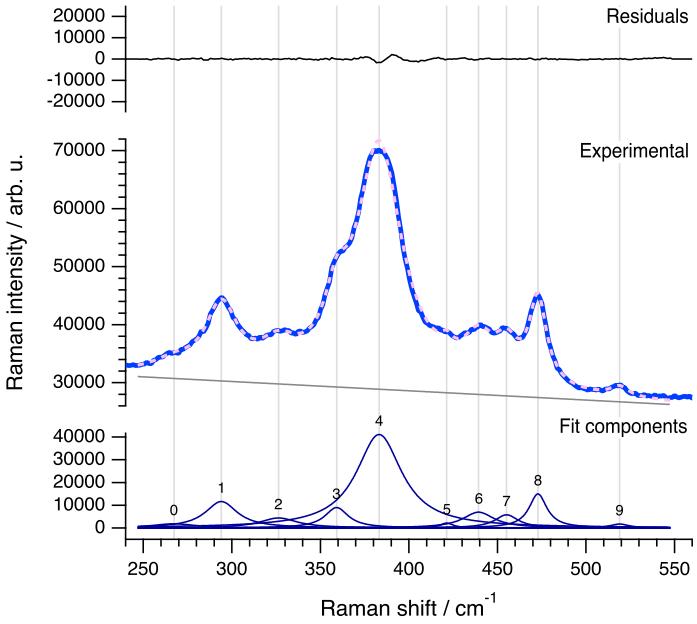

FIGURE 2. Figure S2. Details of the peak fit model used to estimate Raman intensities as the area under each peak. The model consists in the sum of a linear background and a number of Lorentzian functions. The spectrum shown is for a single crystal of Silicalite-1.

The Raman tensor of all investigated peaks resulted to be, after internal normalisation, as follows:

$$294cm^{-1}: \begin{pmatrix} 1.00 & 0.34 \\ 0.34 & 0.90 \end{pmatrix} \qquad 360cm^{-1}: \begin{pmatrix} 0.92 & 0.32 \\ 0.33 & 1.00 \end{pmatrix}$$

$$383cm^{-1}: \begin{pmatrix} 0.95 & 0.32 \\ 0.31 & 1.00 \end{pmatrix} \qquad 472cm^{-1}: \begin{pmatrix} 1.00 & 0.22 \\ 0.23 & 0.50 \end{pmatrix}$$

$$795cm^{-1}: \begin{pmatrix} 1.00 & 0.33 \\ 0.34 & 0.70 \end{pmatrix} \qquad 803cm^{-1}: \begin{pmatrix} 0.83 & 0.97 \\ 1.02 & 1.00 \end{pmatrix}$$

$$818cm^{-1}: \begin{pmatrix} 0.90 & 0.52 \\ 0.50 & 1.00 \end{pmatrix} \qquad 832cm^{-1}: \begin{pmatrix} 0.74 & 0.26 \\ 0.28 & 1.00 \end{pmatrix}$$

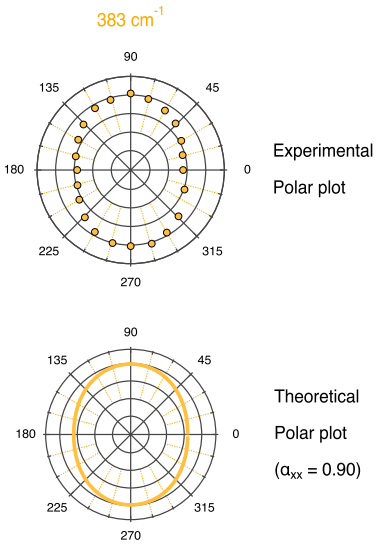

FIGURE 3. Figure S3. Experimental (top) and theoretical (bottom) plots of the angular dependence of the Raman active vibrational mode observed at 383 cm^{-1}.

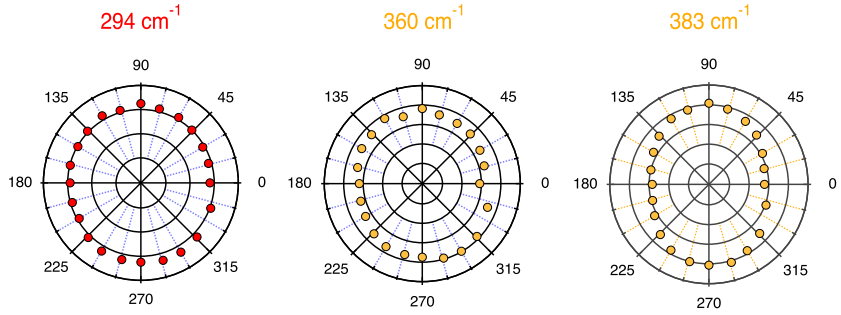

FIGURE 4. Figure S4. Polar plots of the experimentally measured Raman intensities for the vibrational modes observed at 294, 383 and 360 cm^{-1}.

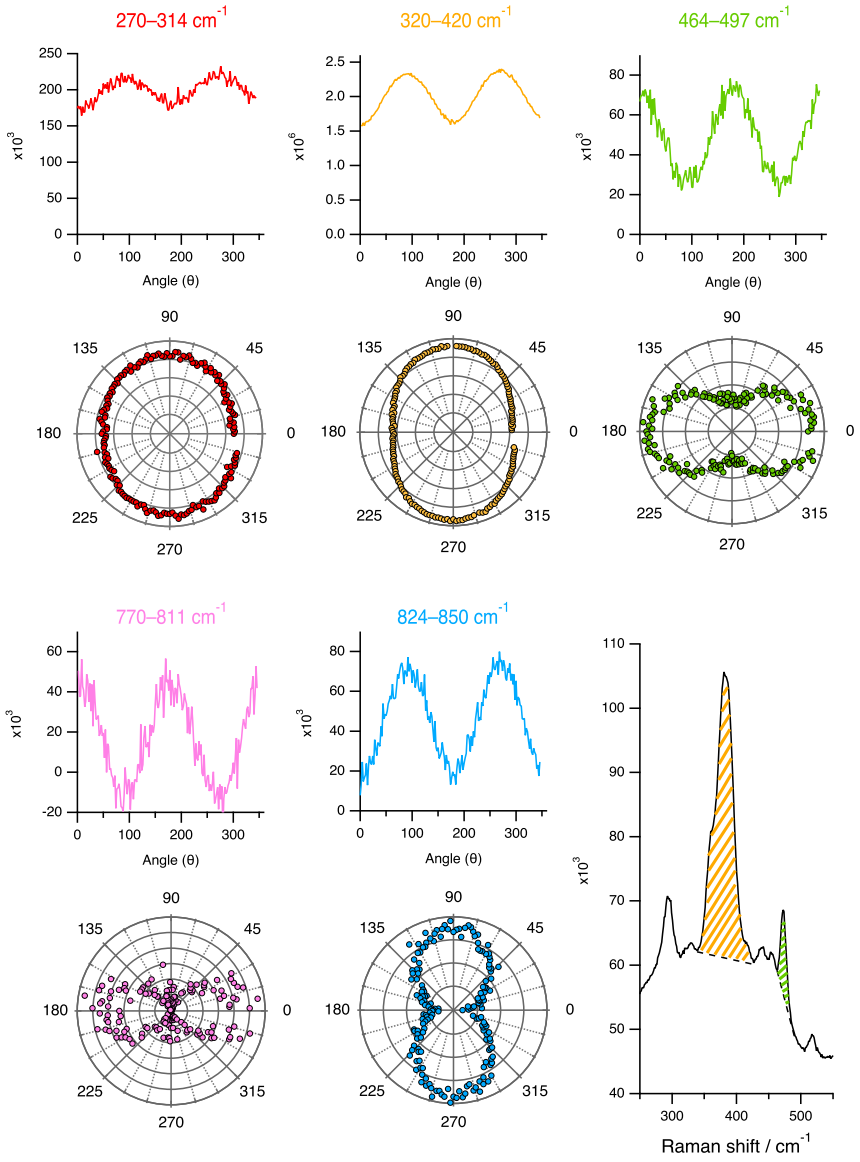

FIGURE 5. Figure S5. Angular dependence of the Raman intensity recorded without an analyser before the detector as a function of θ for a single crystal of Silicalite-1 with a MFI crystal structure. The plotted intensities are automatically achieved by the software as 'intensity-to-baseline' values, as also illustrated in the bottom-right spectrum. This is a less accurate procedure than the peak fit analysis but is as informative and appropriate for the purpose of comparison to the ZSM-5 case.

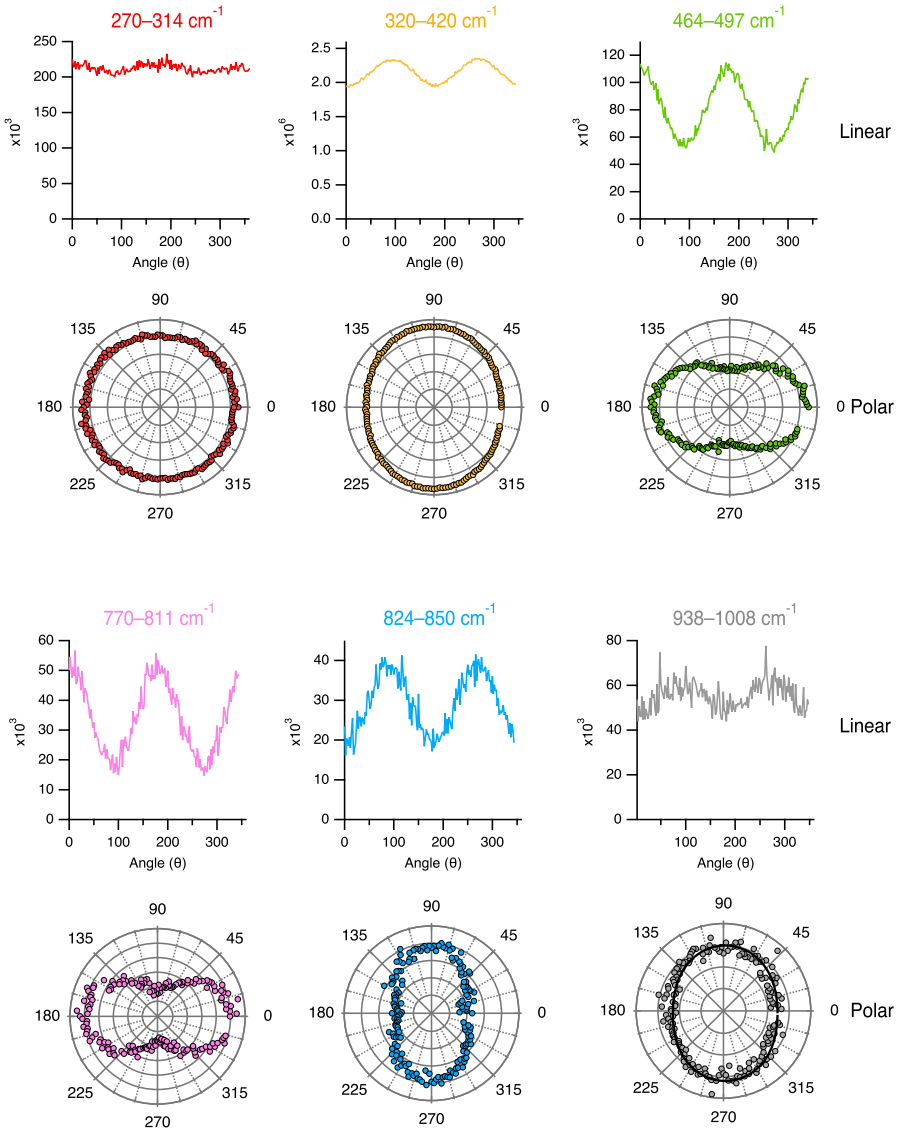

FIGURE 6. Figure S6. Angular dependence of the Raman intensity recorded without an analyser before the detector as a function of θ for a single crystal of ZSM-5 with a MFI crystal structure.

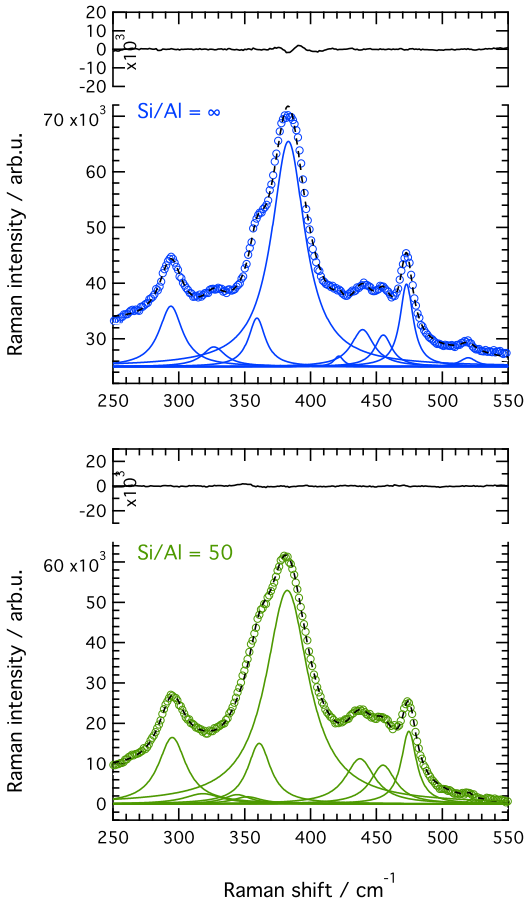

FIGURE 7. Figure S7. The same peak fit model as explained in Figure S2, but applied to a single crystal of Silicalite-1 as compared to the case of a single crystal of ZSM-5. The comparison reveals mainly a broadening of the peaks in ZSM-5, but same vibrational frequencies and number of modes. The feature at ca 520 cm^{-1} arises from the aluminium foil over which the crystals were placed and has nothing to do with the vibrational modes of the framework structure.