Supporting Information

for

Standard and Rapid-Scan Infrared Spectroscopic Studies of *o*-Xylene Transformations in Terms of Pore Arrangement of 10-ring zeolites - 2D COS Analysis

Kinga Gołąbek, Karolina A. Tarach*, and Kinga Góra-Marek*

Faculty of Chemistry, Jagiellonian University in Kraków, 3 Ingardena St., 30-060 Kraków, Poland, phone: +48 12 663 2081, fax: +48 12 634 0515

Corresponding Author

*Karolina A. Tarach, Faculty of Chemistry, Jagiellonian University in Kraków, 3 Ingarden St., 30-060 Kraków, Poland, phone +48 (12) 663-20-81, fax. +48 (12) 634-05-15 E-mail address: karolina.tarach@uj.edu.pl

*Kinga Góra-Marek, Faculty of Chemistry, Jagiellonian University in Kraków, 3 Ingarden St., 30-060 Kraków, Poland, phone +48 (12) 663-20-81, fax. +48 (12) 634-05-15 E-mail address: <u>kinga.goramarek@gmail.com</u>



Figure 1_SI. XRD patterns (A) and N₂ adsorption (full symbols) and desorption (empty symbols) isotherms (B), pore size distribution (C) as well as the IR spectra of the zeolites studied in the region of the O-H groups vibrations (D).



Figure 2_SI. A: The coloured curves represent all the bands found for individual reagent upon deconvolution procedure. The shaded curve represents the diagnostic band used in quantitative studies. The black dashed curve is the sum of the spectrum of the already considered product and the spectra of the products presented above. **B:** a – the IR spectrum reconstructed from the spectra of reactants, b - the spectrum recorded upon contact with o-xylene with zeolite ZSM-5 at 250 °C in 15 min.



Figure 3_SI. The 2D synchronous and asynchronous correlation maps of ortho-xylene isomerization reaction at 250 °C for zeolite ZSM-5 in 15 min. of the reaction. The IR spectra subjected the correlation procedure are presented in the upper part. The correlations are listed in the table.



Figure 4_SI. The 2D synchronous and asynchronous correlation maps of ortho-xylene isomerization reaction at 250 °C for zeolite TNU-9 in 15 min. of the reaction. The IR spectra subjected the correlation procedure are presented in the upper part. The synchronous and asynchronous correlations are listed in the table.



Figure 5_SI. The 2D synchronous and asynchronous correlation maps of ortho-xylene isomerization reaction at 250 °C for zeolite IM-5 in 15 min. of the reaction. The IR spectra subjected the correlation procedure are presented in the upper part. The synchronous and asynchronous correlations are listed in the table.



Figure 6_SI. The 2D synchronous and asynchronous correlation maps of ortho-xylene isomerization reaction at 250 °C for zeolite TNU-10 in 15 min. of the reaction. The IR spectra subjected the correlation procedure are presented in the upper part. The synchronous and asynchronous correlations are listed in the table.



Figure 7_SI. The 2D synchronous and asynchronous correlation maps of ortho-xylene isomerization reaction at 250 °C for zeolite ZSM-22 in 15 min. the reaction. The IR spectra subjected the correlation procedure are presented in the upper part. The synchronous and asynchronous correlations are listed in the table.



Figure 8_SI. The IR spectra collected during Rapid Scan measurements of ortho-xylene isomerization at 250 °C all the zeolites studied in 4 min. the reaction. These spectra were subjected the correlation procedure.