Pore Blocking by Phenolates as Deactivation Path during the Cracking of 4-Propylphenol over ZSM-5

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Supporting Information

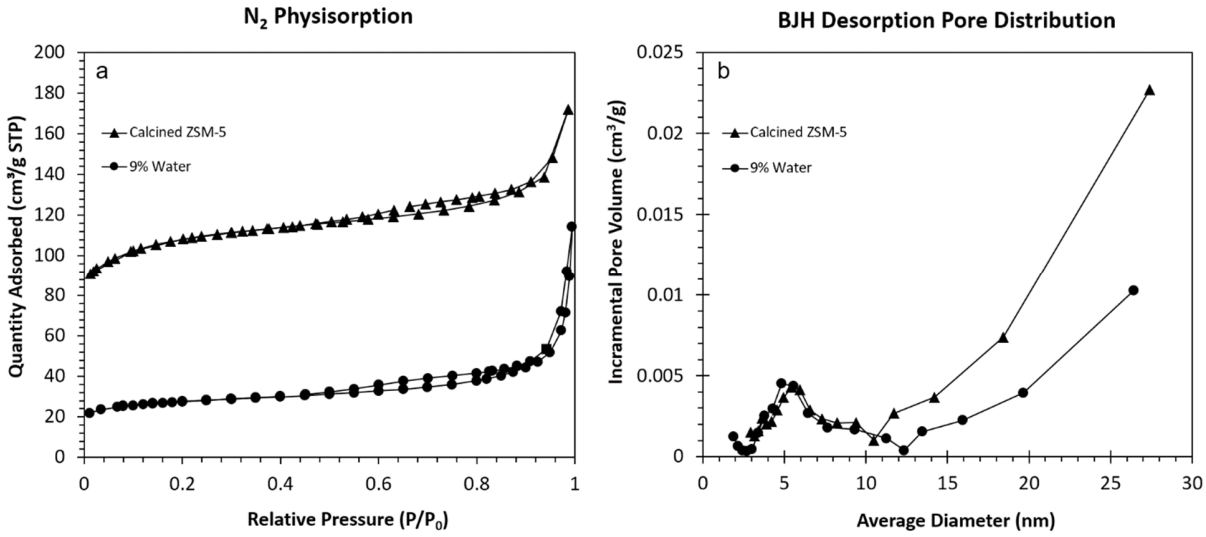

Figure S1 – a) N_2 adsorption/desorption isotherms of the pre and post reaction catalyst. b) Pore volume distribution taken from the desorption isotherm calculated using the BJH method. Samples were pretreated under <10 µm Hg pressure at 250 °C for 300 min prior to analysis.

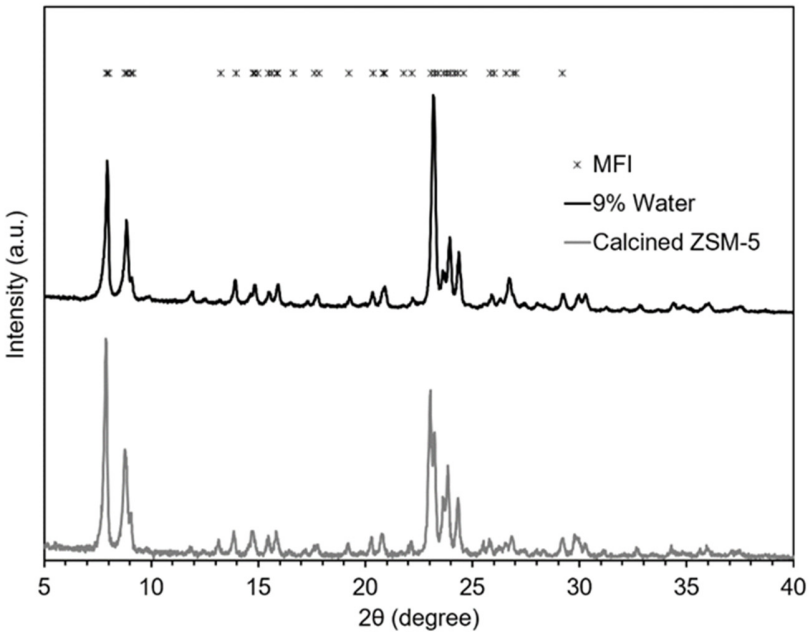

Figure S2 – XRD of calcined ZSM5, 9% water sample post reaction, and reference MFI peak locations.

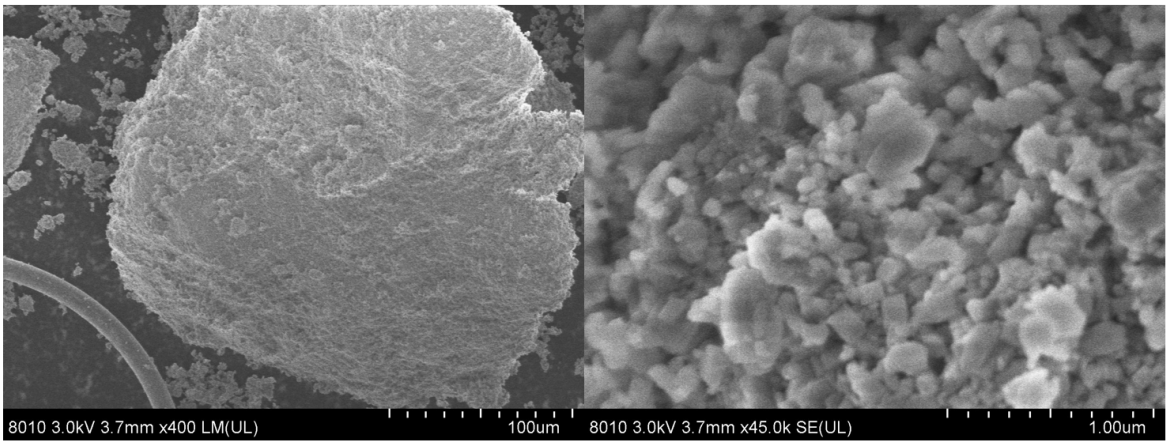

Figure S3 - SEM of ZSM-5 catalyst used in 9% water atmosphere. MFI crystalizes are still clearly visible as part of the catalyst particle agglomerate and there is no visible evidence of large quantities of surface coke.

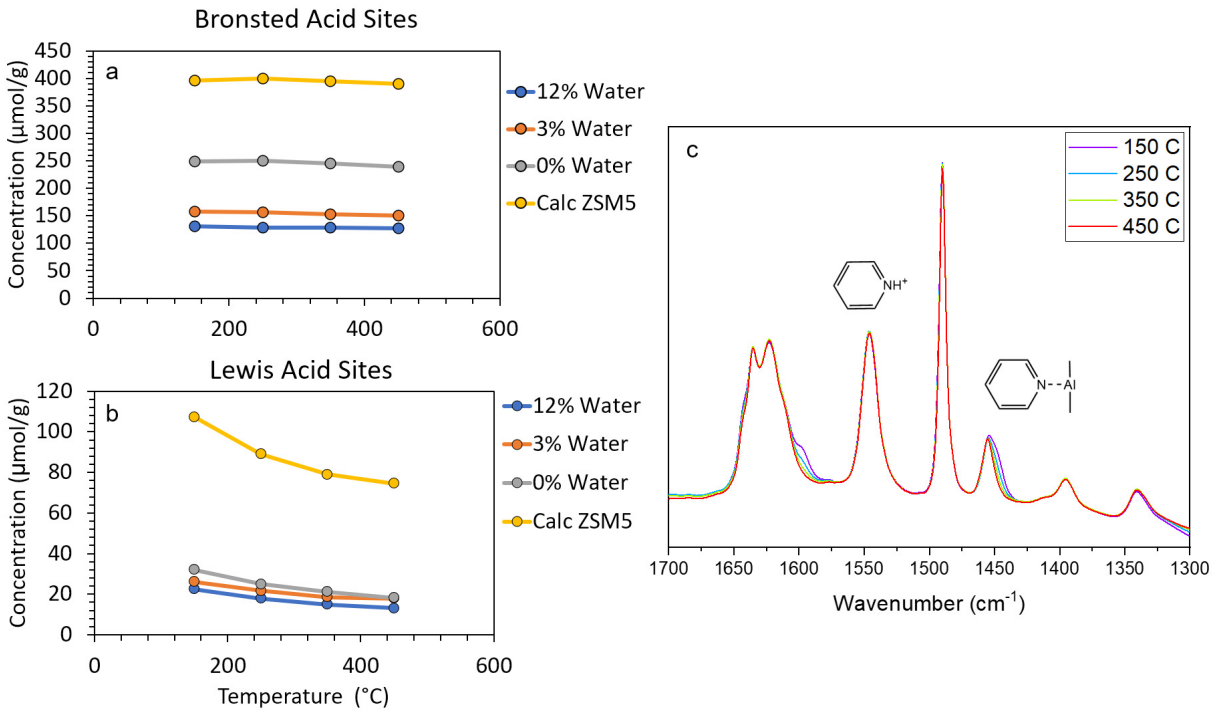

Figure S4 – Brønsted acid site concentration (a) and Lewis acid site concentration (b) as measured by pyridine adsorption followed by FTIR spectroscopy. (c) FTIR spectra collected from pyridine adsorbed on calcined ZSM-5 given as reference.

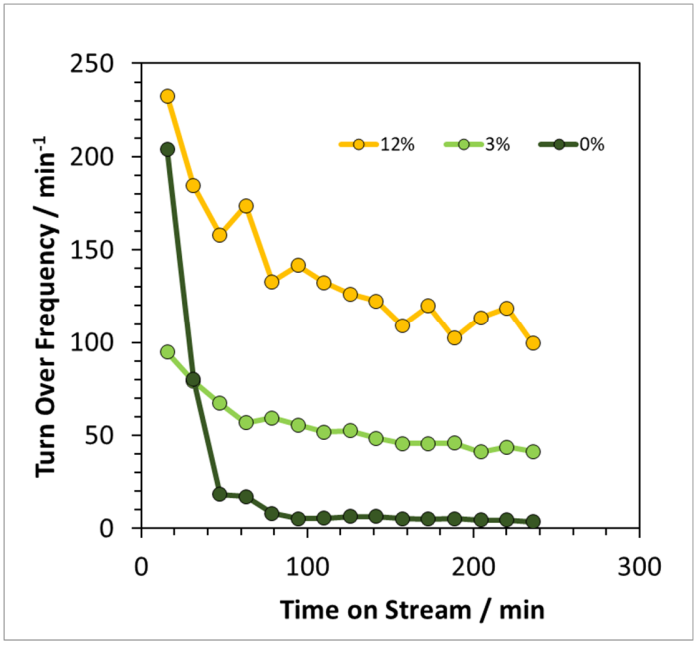

Figure S5 – Turn over frequency of the production of phenol over Brønsted acid sites as a function of water content in the reactant stream.

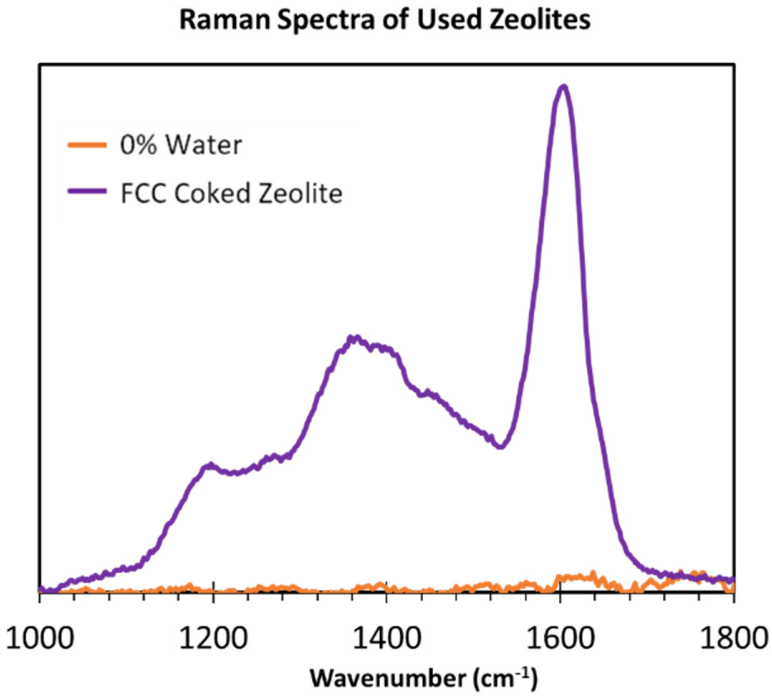

Figure S6 – Raman spectra of fully deactivated ZSM5 compared to fully coked FCC Ecat [38] ($\lambda_0 = 780$ nm).

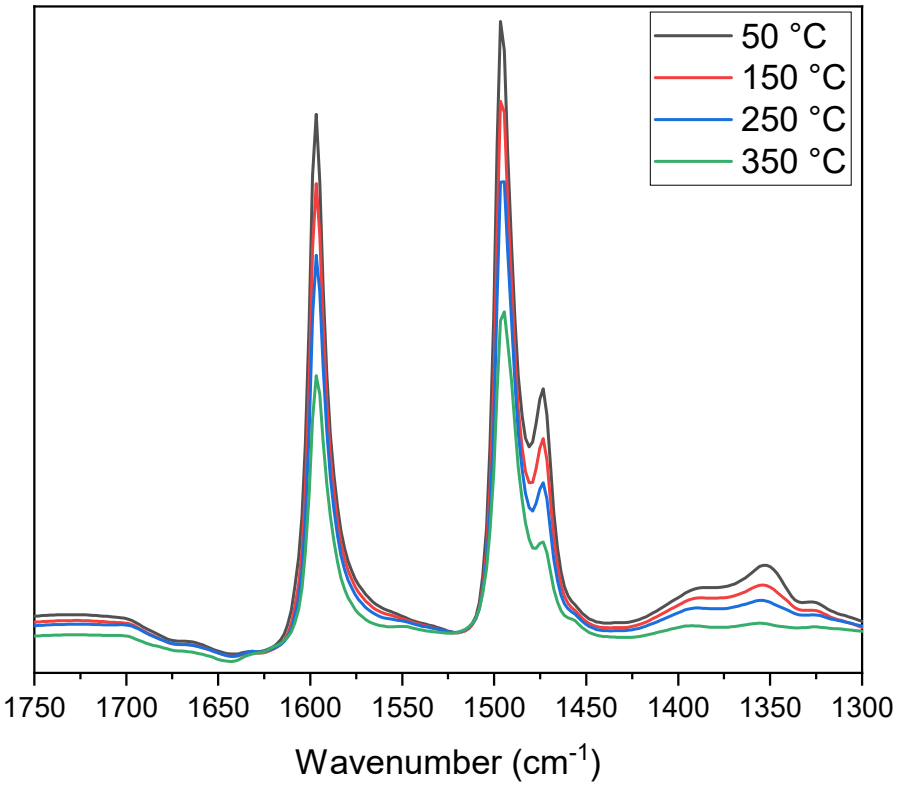

Figure S7 – Common scale infrared spectra in the aromatic region of adsorbed phenol with ZSM-5 support subtracted. All peaks decrease with increasing temperature as expected from thermal desorption.

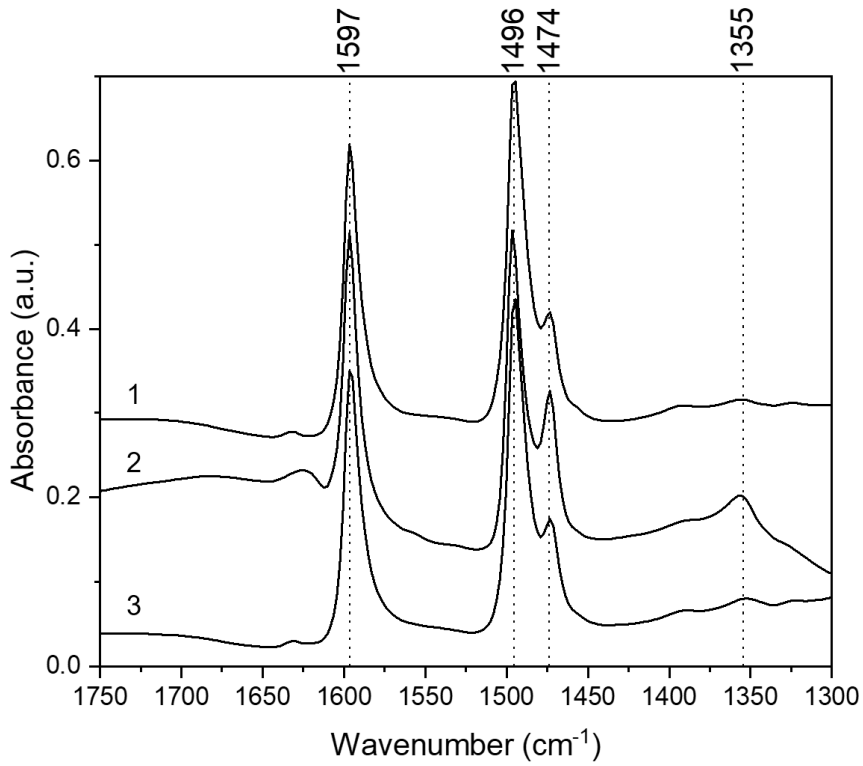

Figure S8 - Transmission infrared spectra of phenol on ZSM-5 after 1) heating to 350 °C, 2) dosing with water vapor at 50 °C, and 3) reheating to 300 °C.

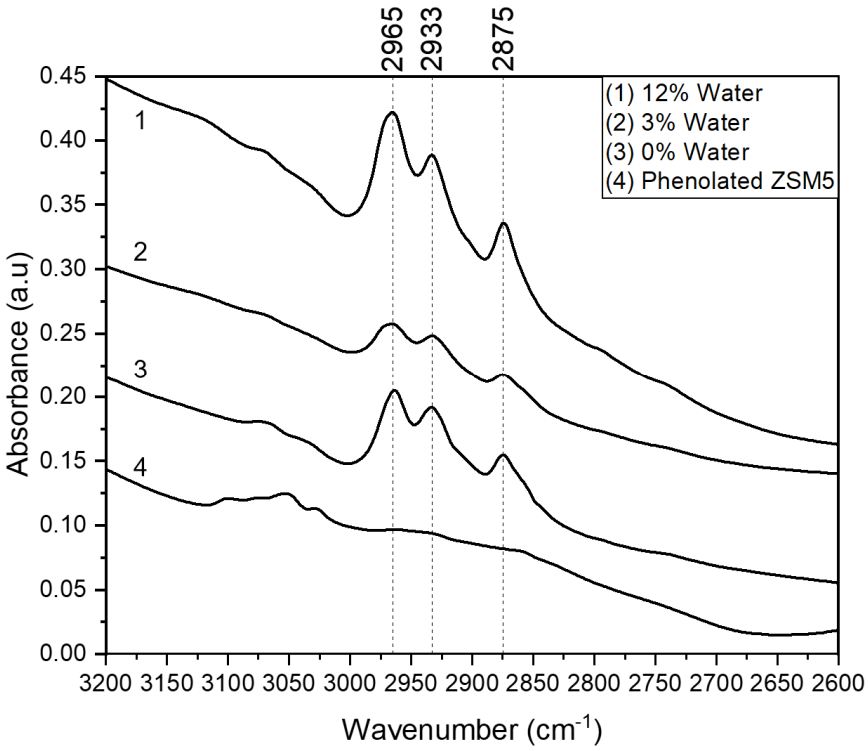

Figure S9 - Infrared spectra in the aliphatic region of post reaction ZSM-5 (1-3) with phenolated ZSM-5 (4) included for reference.

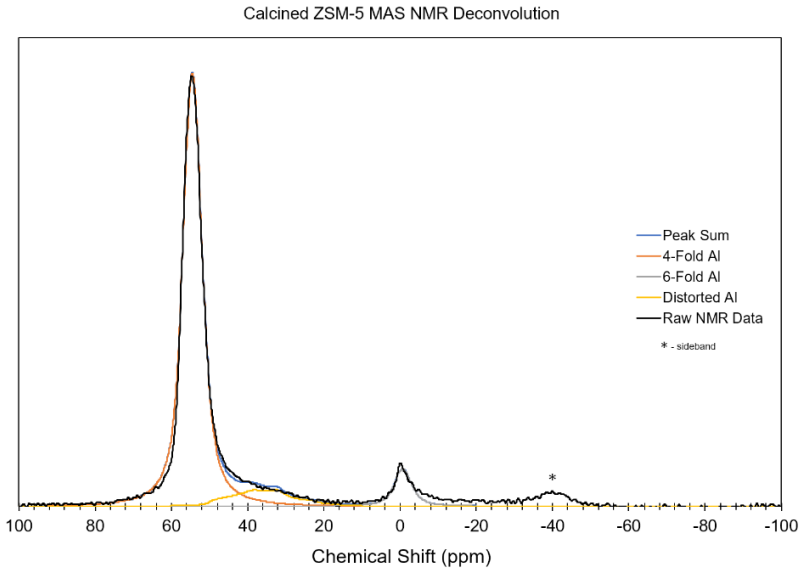

Figure S10 – Representative deconvolution of Calcined ZSM-5 using DMfit2015 software. Peaks fit using ^{27}Al quadrupolar assignment and peak model Q 1/2 mas.