Supporting Information

Catalytic conversion of heavy naphtha to reformate product over phosphorus-ZSM-5 catalyst at lower reforming temperature

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3. Results and Discussion

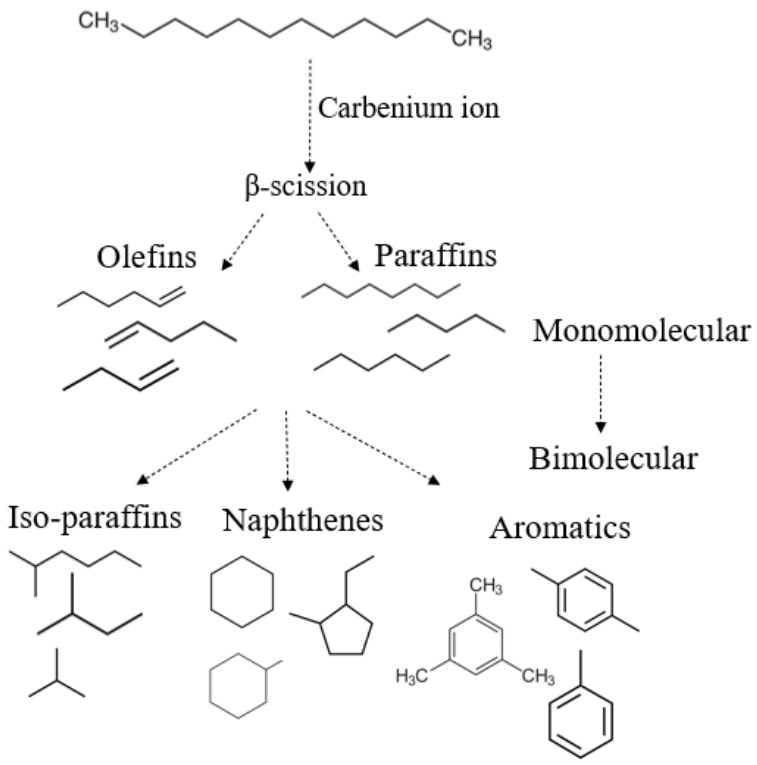

Figure 1S. Schematic diagram of dodecane cracking and reforming via phosphate modified ZSM-5 zeolite catalyst

Figure 1S shows the schematic diagram of dodecane reforming though the carbenium ions via phosphate modified ZSM-5 zeolite catalyst pores and it favored monomolecular reaction through β-scission of dodecane and made high paraffin and olefin (~58%). While bimolecular was also associated with the reaction and promoted the iso-paraffins product via isomerization reaction [1]–[3]. While the parent ZSM-5 (P) showed the pores selectivity favored to the cyclization reaction and produce aromatics and naphthenes products through bimolecular reaction pathway more than the monomolecular reaction pathway [4], [5].

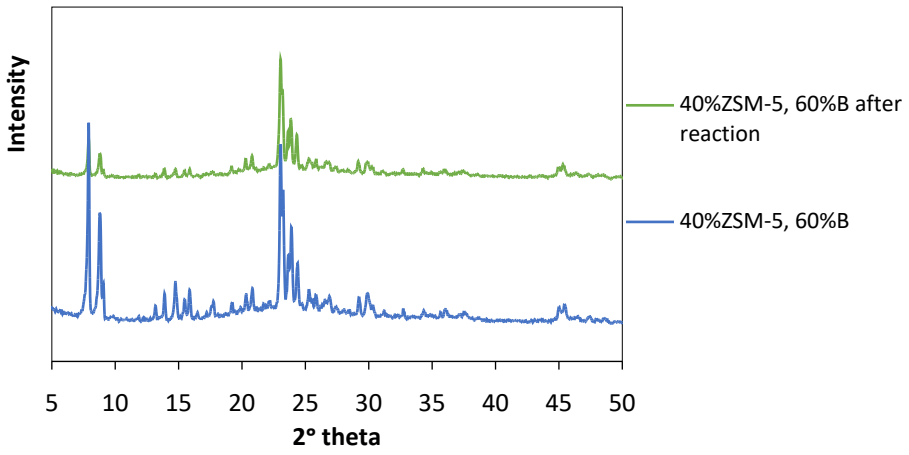

Figure 2S. XRD patterns of hydrothermally treated with steam ZSM-5 zeolite catalysts with binder And after reaction

Table 1S. Nitrogen adsorption analysis and NH_3–TPD profiles of parent and modified ZSM-5

Zeolite ID	**BET surface area [m^2g^{-1}]**	**t-Plot* micropore surface area, [m^2/g^{-1}]**	**t-Plot* external surface area, [m^2/g^{-1}]**	**Pore Volume, [cm^3/g^{-1}]**
40% ZSM-5, 60% binder	164	103	61	0.16
40% ZSM-5, 60% binder HT**	170	106	64	0.15
40% ZSM-5, 60% binder after reaction	137	76	61	0.14

* Surface area by t-plot derived from Harkins and Jura equation, **HT: hydrotreatment treatment by steam

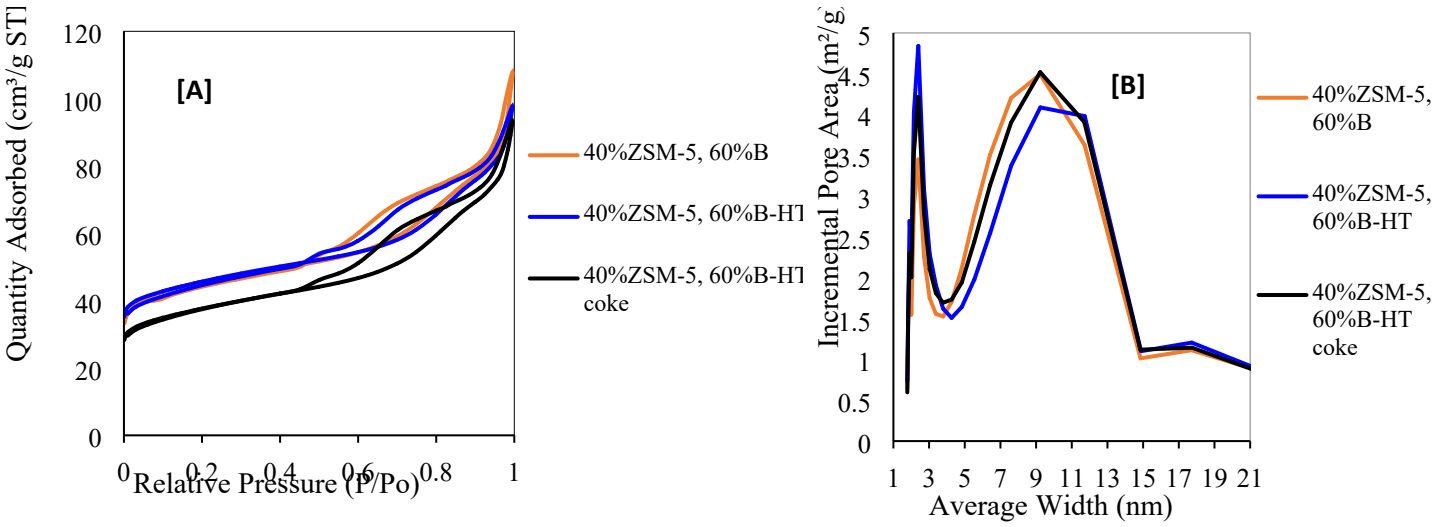

Figure 3S. [A] N_2 adsorption-desorption isotherms [B] pore size distribution curves of parent and modified ZSM-5 zeolite with binder before and after reaction (coke)

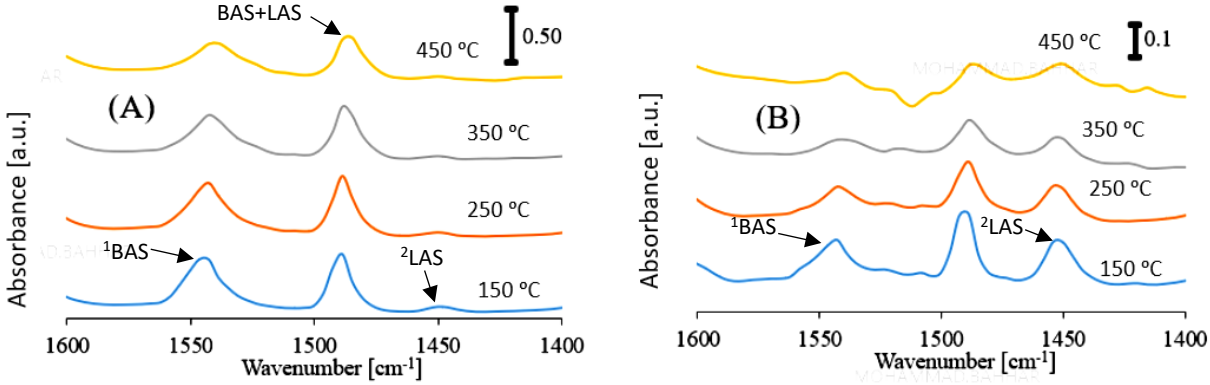

Figure 4S. (A) Py-FTIR of 40% ZSM-5 in 60% binder, (B) Py-FTIR Py-FTIR of 40% ZSM-5 in 60% binder (HT) (^{1}BAS: Brønsted acid sites, ^{2}LAS: Lewis acid sites)

Table S2. Metal analysis of zeolite catalysts

Sample ID	O	Al	Si	P
40% ZSM-5, 60% binder	48	16.3	33.6	2.1
40% ZSM-5, 60% binder – HT*	61.6	12.4	24.6	1.4

*HT: hydrothermal treatment by steam, ND: not detected

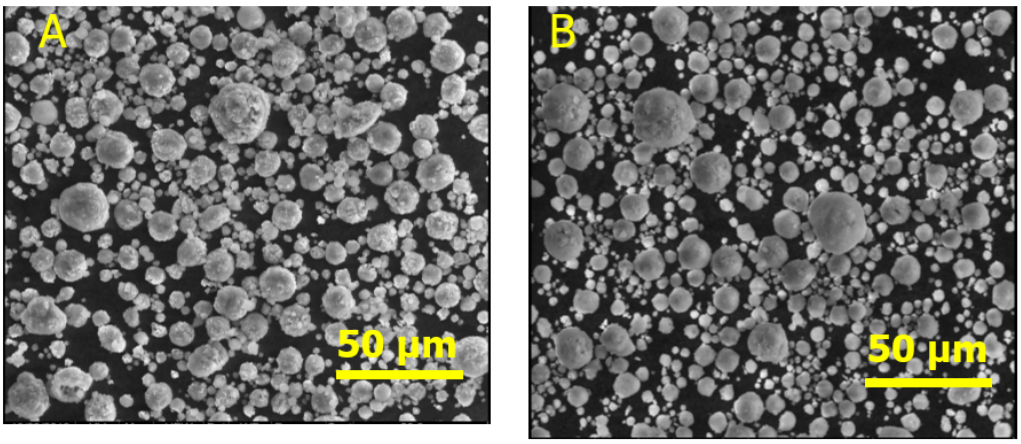

Figure 5S. SEM images [A] 40% ZSM-5 in 60% binder, [B] 40% ZSM-5 in 60% binder after steam treatment

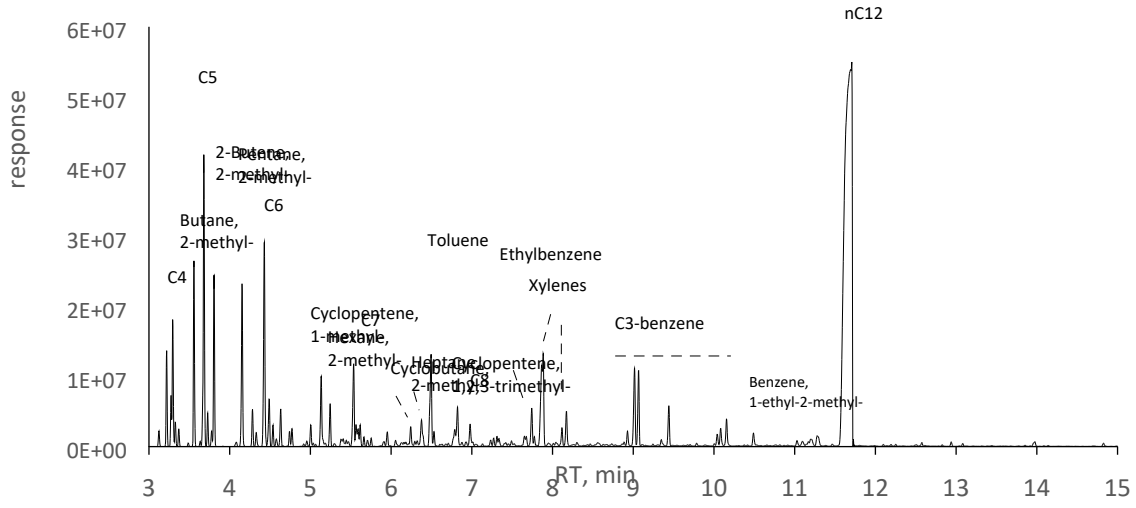

Figure 6S. Gas-chromatograph of n-dodecane conversion over 40% ZSM-5 in 60% binder after steam treatment

References

[1] M. Alabdullah *et al.*, "One-step conversion of crude oil to light olefins using a multi-zone reactor," *Nature Catalysis*, vol. 4, no. 3, pp. 233–241, 2021.

[2] M. Alabdullah *et al.*, "Composition-performance Relationships in Catalysts Formulation for the Direct Conversion of Crude Oil to Chemicals," *ChemCatChem*, vol. 13, no. 7, pp. 1806–1813, 2021.

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