

Supporting information

Metal/acid bifunctional catalysis and intimacy criterion for ethylcyclohexane hydroconversion: when proximity does not matter

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Table S1. List of products of ECH hydroconversion.

Reaction	Product Family	Products
Isomerization	TMCP	1,1,3-trimethylcyclopentane
		1-trans-2-cis-4-trimethylcyclopentane
		1-cis-2-cis-4-trimethylcyclopentane *a
		1,trans-2-cis-3-trimethylcyclopentane
		1,1,2-trimethylcyclopentane
	DMCH	1,trans-4-dimethylcyclohexane
		1,cis-3-dimethylcyclohexane *
		1,trans-2-dimethylcyclohexane
		1,cis-4-dimethylcyclohexane
		1,1-dimethylcyclohexane
		1 ,cis-2-dimethylcyclohexane
	EMCP	1-methyl-trans-3-ethylcyclopentane
		1-methyl-cis-3-ethylcyclopentane
		1-methyl-trans-2-ethylcyclopentane
		1-methyl-cis-2-ethylcyclopentane
		1-ethyl-1-methylcyclopentane
	PCP	isocyclopentane
		n-propyl-cyclopentane *b
	MCHP	methylcycloheptane
Ring opening	P8	2-methylheptane
		4-methylheptane
		2,3-dimethylhexane

		2,4-dimethylhexane
		2,5-dimethylhexane*
		n-Octane
		3,4-dimethylhexane
Cracking	C1	ethane
	C2	methane
	C3	propane
	C4	n-butane
		isobutane
	C5	n-pentane
		isopentane
		cyclopentane
	C6	methylcyclopentane
		2-methylpentane
		3-methylpentane
		cyclohexane
		n-hexane
	C7	1,1-dimethylcyclopentane
		1,cis-3-dimethylcyclopentane
		1,trans-3-dimethylcyclopentane
		2-methylhexane
		3-methylhexane
		3-methylpentane
		ethylcyclohexane
n-heptane		
Dehydrogenation	A8	ethylbenzene

		m-xylene
		p-xylene
		o-xylene

* In coelution with low amounts of paraffin C₈

*a In coelution with low amounts of 3-methylheptane

*b In coelution with the ECH. Compound in negligible amount.

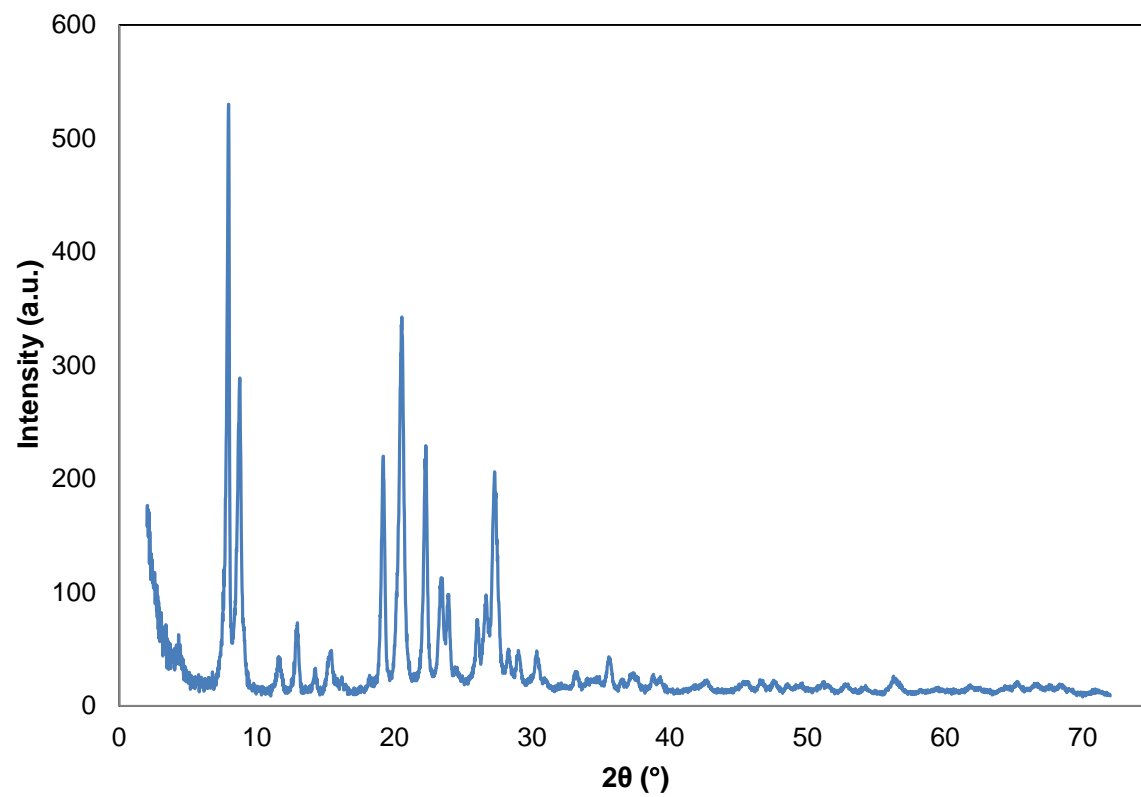


Figure S1. XRD diffractogram for HEU-1

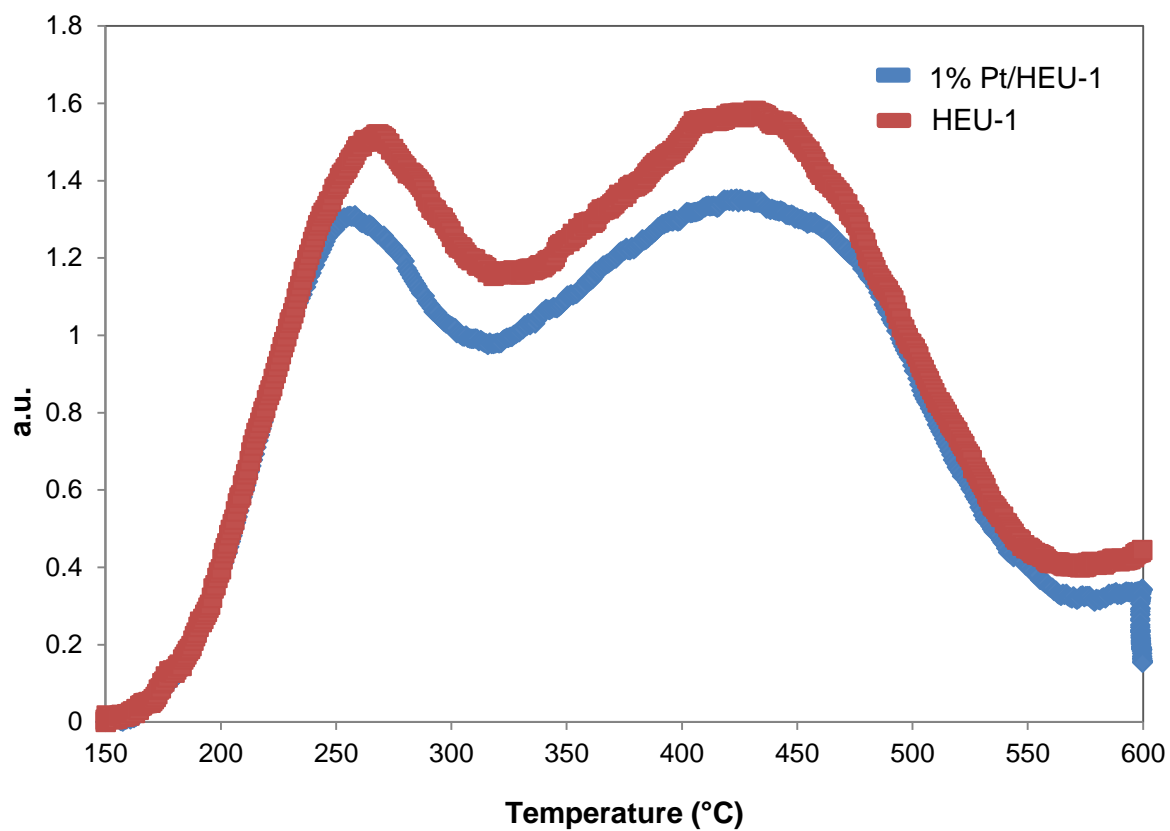


Figure S2. NH₃-TPD profiles for the parent HEU-1 zeolite and the zeolite impregnated with platinum (1% Pt-HEU-1/Al₂O₃)

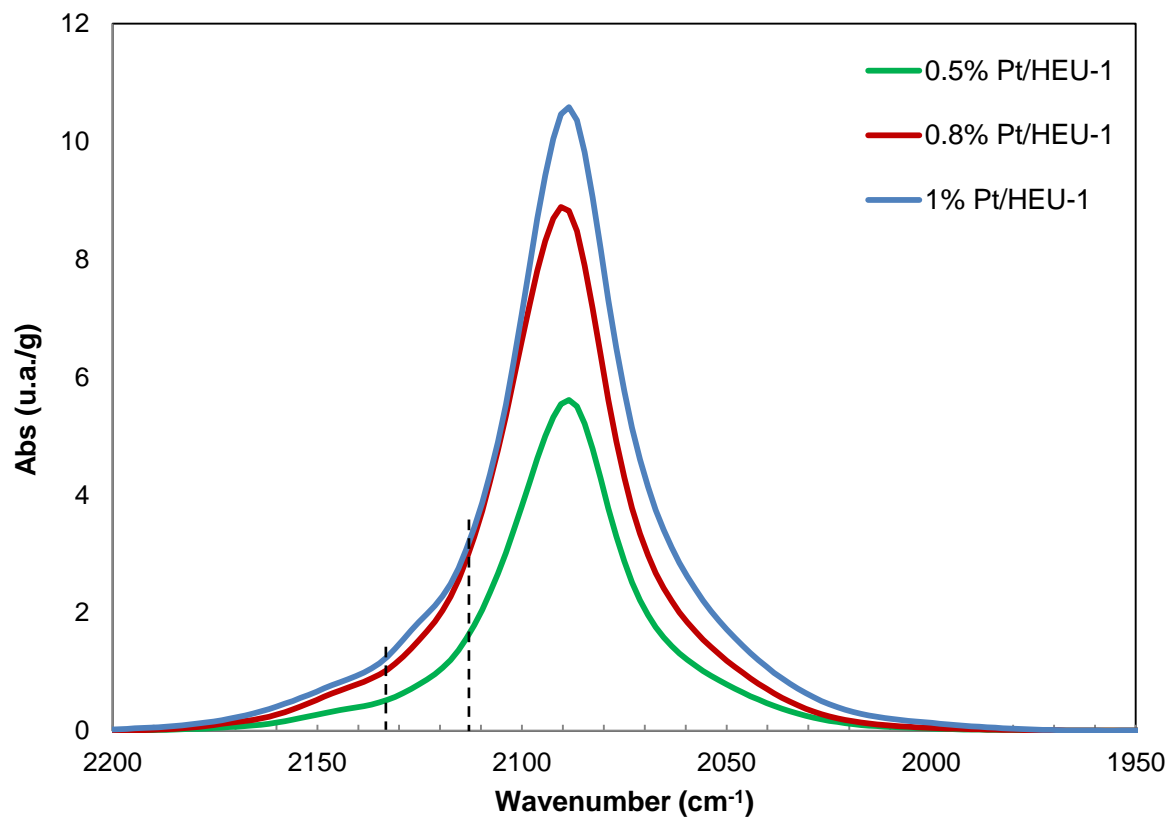


Figure S3. IR spectra at CO saturation plus desorption at 25°C in the CO region (2300-1900)-common scale for the Pt-HEU-1/Al₂O₃ samples.

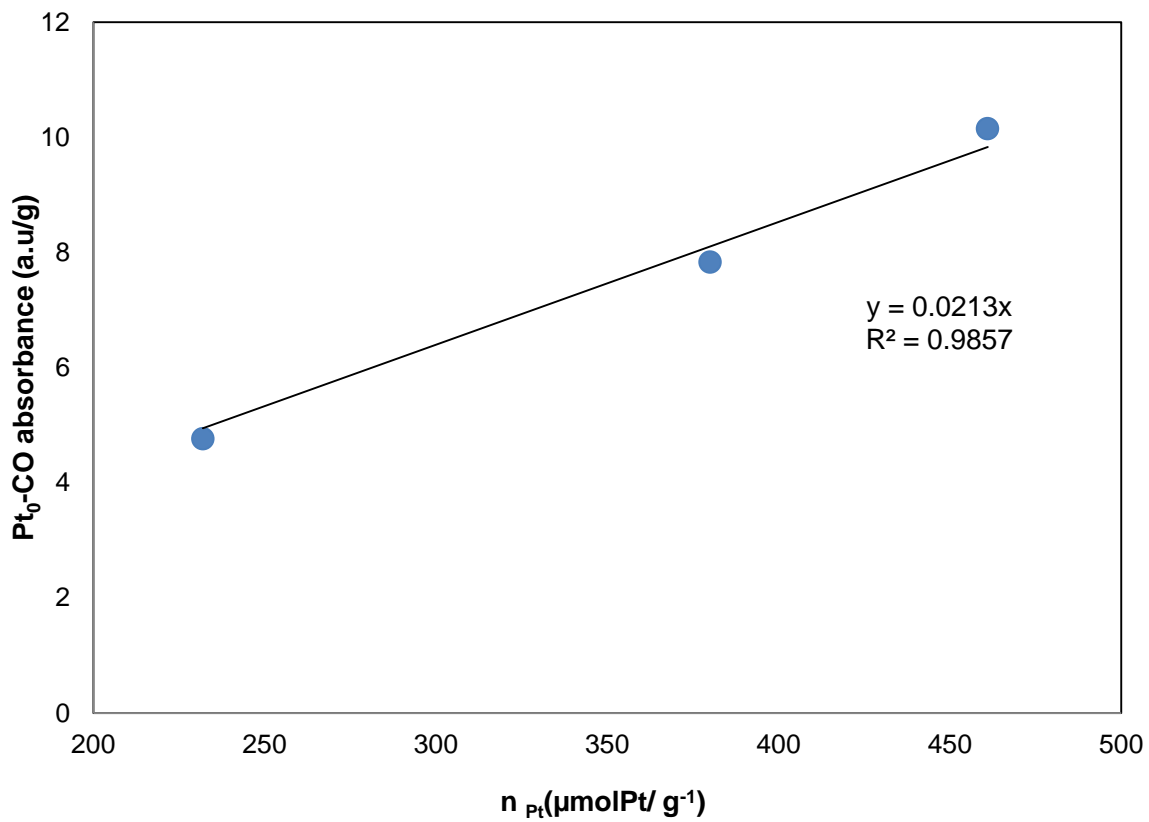


Figure S4. Amount of micromoles of platinum plotted as a function of the peak area of CO at 2090 cm^{-1} from Pt^0 -CO species for HEU-1 impregnated samples

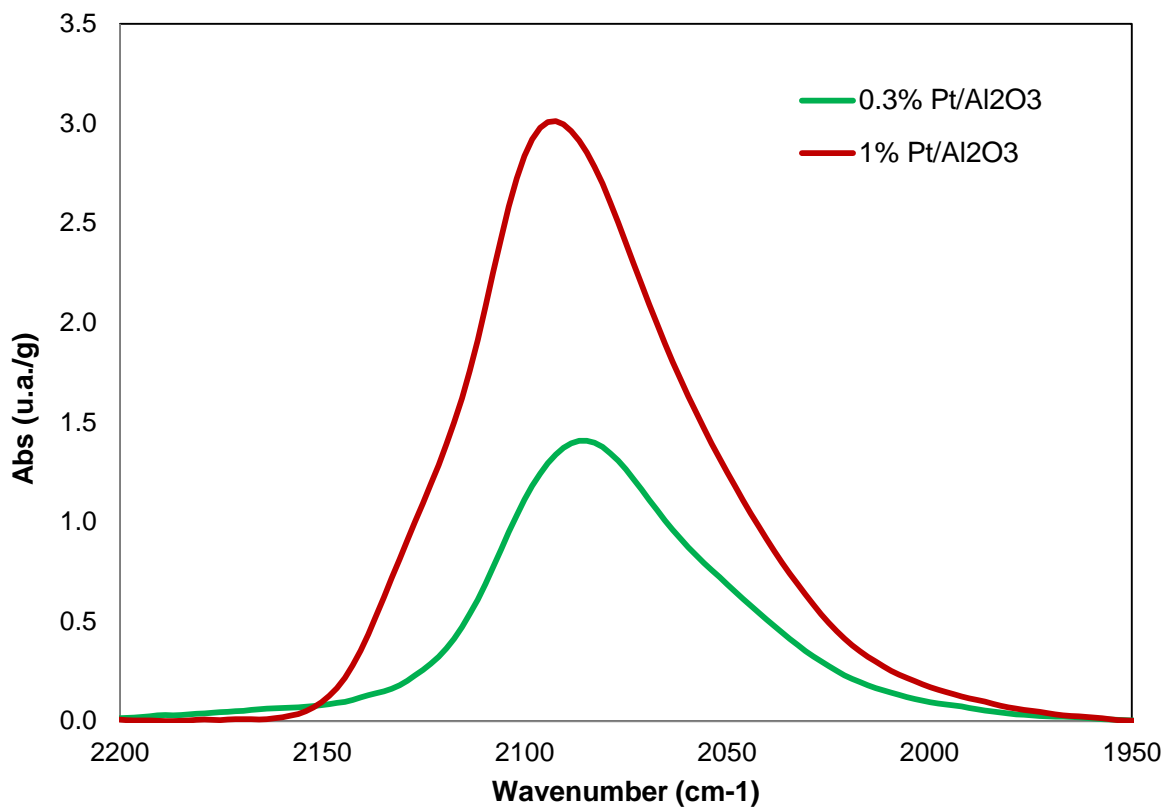


Figure S5. IR spectra at CO saturation plus desorption at 25°C in the CO region (2300-1900)-common scale for the Pt-Al₂O₃/ HEU-1 samples.

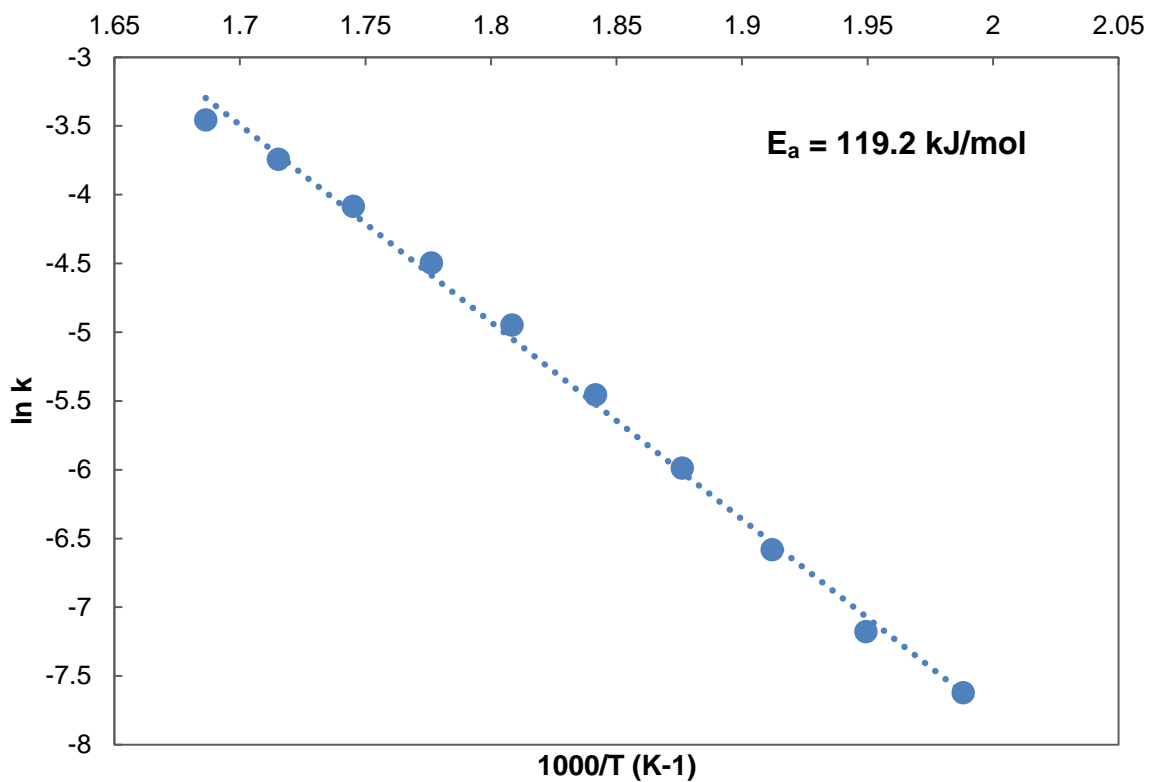


Figure S6. Arrhenius plot for 1 %Pt-HEU-1/Al₂O₃. The rate constant k [m³mol⁻¹s⁻¹] is on a concentration basis and calculated from the integral expression for a first order reaction in a fixed-bed reactor. The corresponding pre-exponential factor, A^0 , is equal to $1.2 \cdot 10^9$ [m³mol⁻¹s⁻¹].

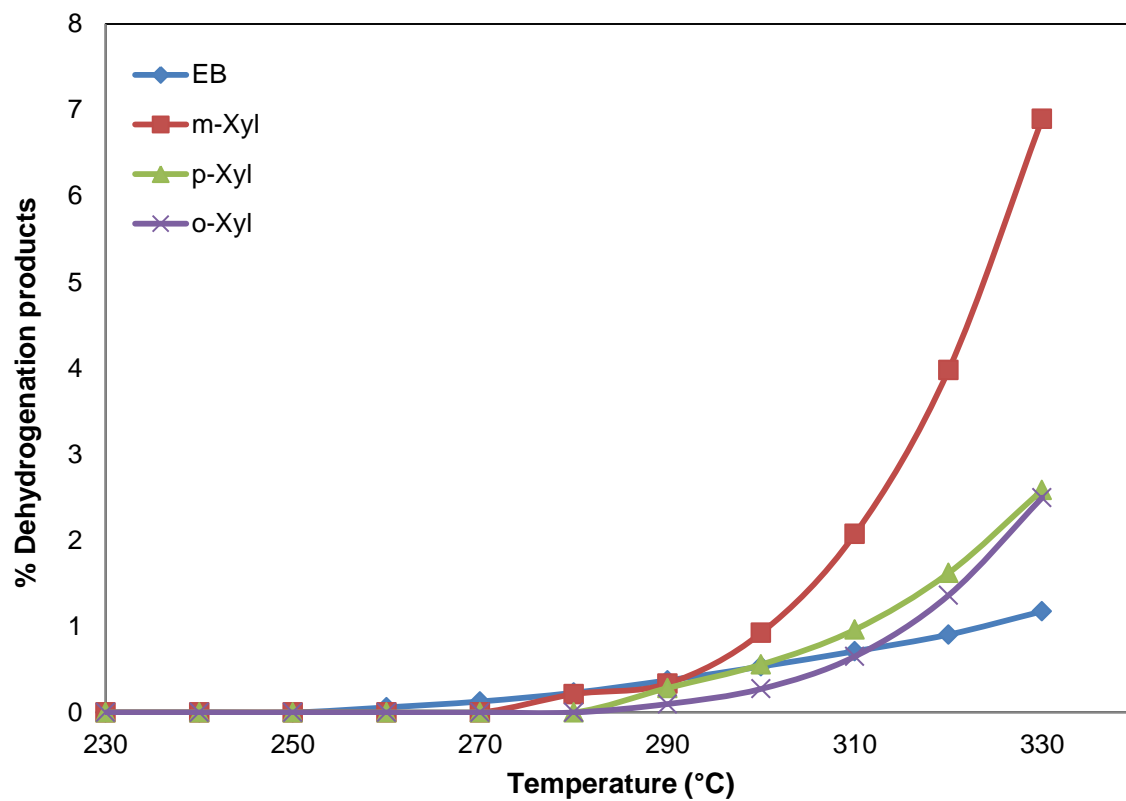


Figure S7. Evolution of different dehydrogenation products for the 1% Pt-HEU-1/Al₂O₃ catalyst.

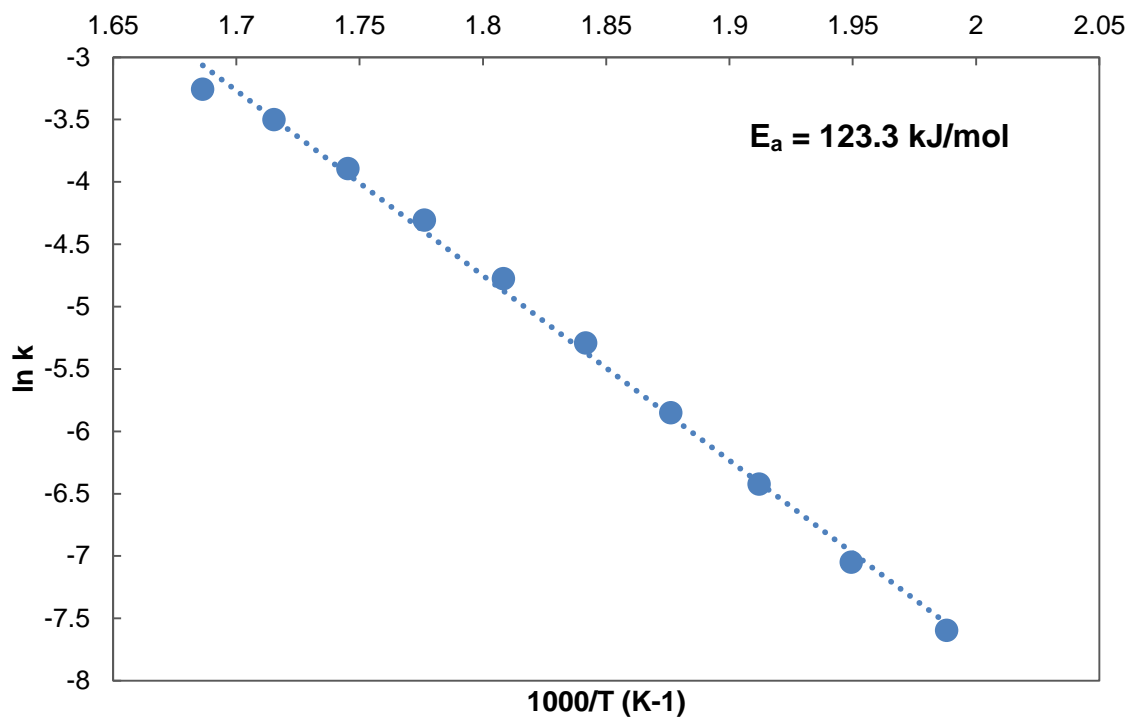


Figure S8. Arrhenius plot for 1% Pt-Al₂O₃/HEU-1. The rate constant k [m³mol⁻¹s⁻¹] is on a concentration basis and calculated from the integral expression for a first order reaction in a fixed-bed reactor. The corresponding pre-exponential factor, A^0 , is equal to $3.4 \cdot 10^9$ [m³mol⁻¹s⁻¹].

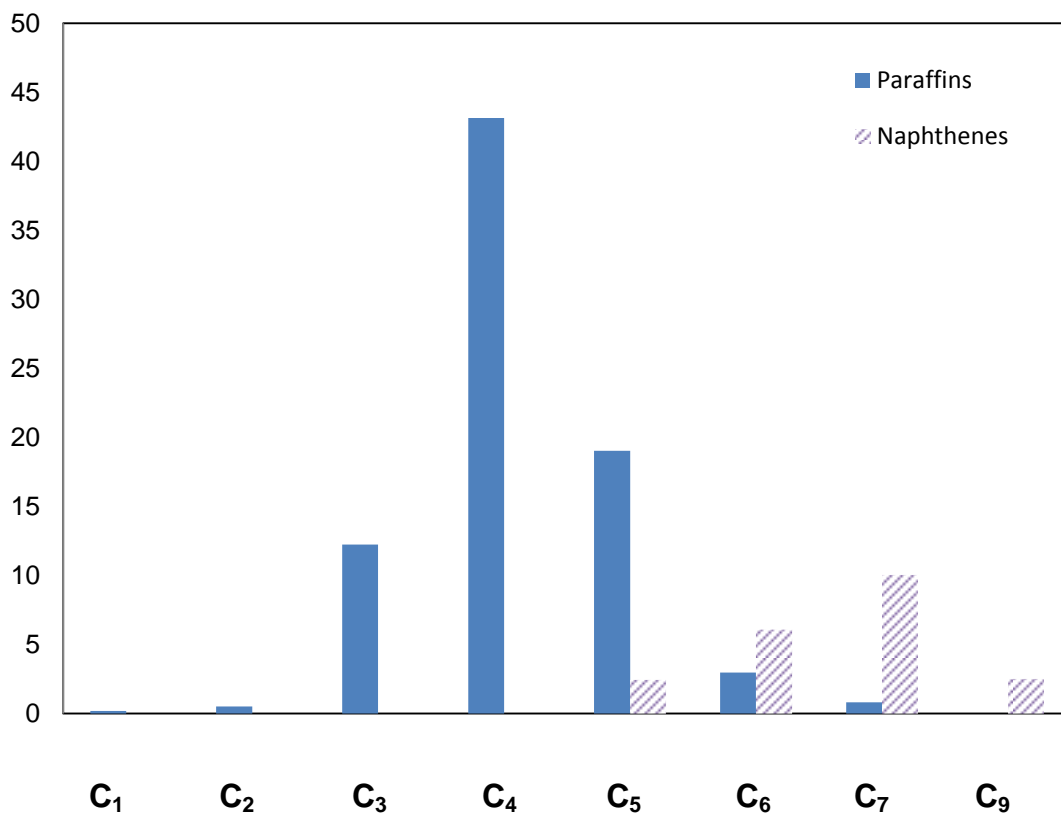


Figure S9. Cracking product distribution at 300°C for the reference catalyst 1% Pt-Al₂O₃/HEU-

1.

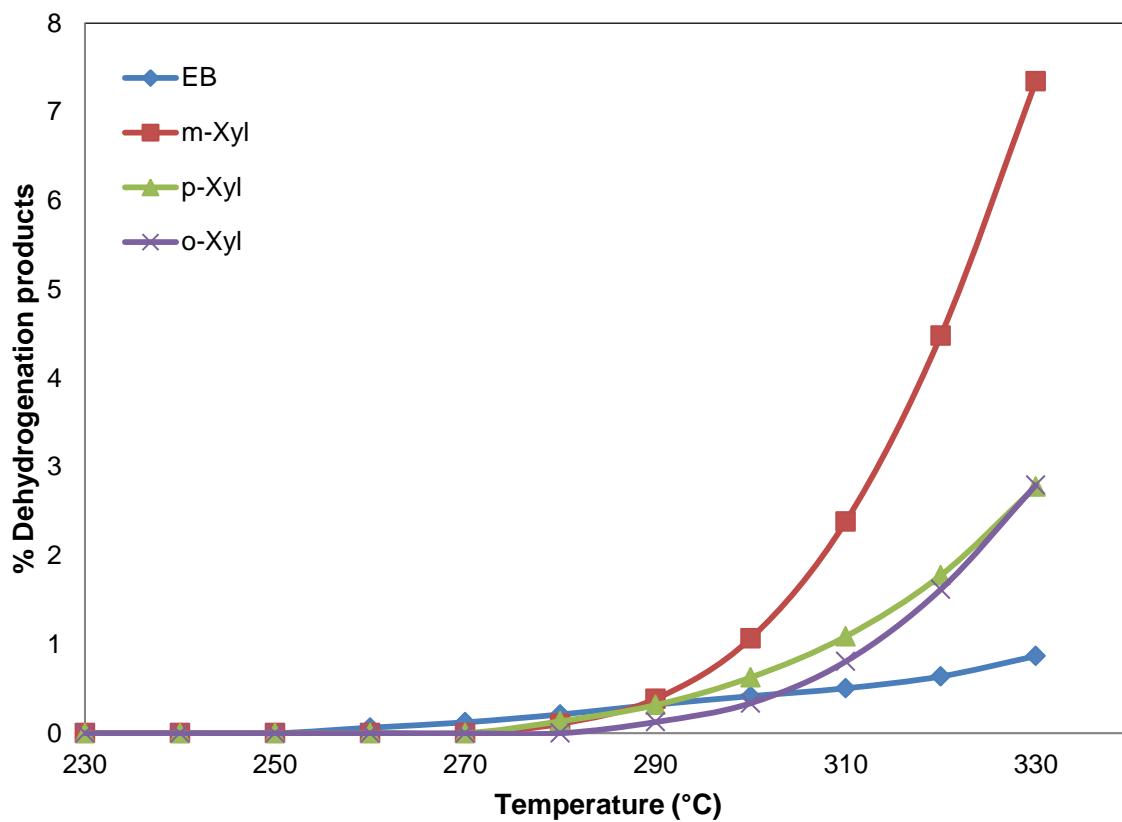


Figure S10. Evolution of different dehydrogenation products for the reference catalyst 1% Pt- $\text{Al}_2\text{O}_3/\text{HEU-1}$.