Supporting information

Propylene Synthesis via Isomerization Metathesis of 1-Hexene and FCC olefins

Gyula Novodárszki,[a] Blanka Szabó,[a] Róbert Auer,[b] Katalin Tóth,[b] László Leveles,[b] Róbert Barthos,[a] Gábor Turczel,[a] Zoltán Pászti,[a] József Valyon,[a] Magdolna R. Mihályi,*[a] and Róbert Tuba*[a]

[a]Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences
Magyar tudósok körútja 2., 1519 Budapest, P.O. Box 286. Hungary
E-mail: tuba.robert@ttk.hu

[b]MOL, Hungarian Oil and Gas Public Limited Company, Október huszonharmadika u. 18., 1117 Budapest, Hungary

Table S1 Propylene yield in ISOMET of 1-hexene (1-H) with ethylene over activated and reactivated $6MoO_3$/HBEA catalyst at different temperatures and 0.5 h and 3 h of TOS, at 3 g_{cat} $g_{1\text{-}H}^{-1}$ h space time under 3 bar ethylene pressure. The ethylene/1-hexene molar ratio was 10.

Temperature (°C)	TOS (h)	Propylene Yield (%)	
		Activated[a]	Reactivated[b]
75	0.5	12	17
	3	4	5
100	0.5	11	18
	3	7	8
125	0.5	14	21
	3	9	11
150	0.5	15	19
	3	4	7

[a]*Activation*: The *ex-situ* calcined catalyst was *in-situ* pre-treated in a flow of Ar (50 ml min^{-1}) at 550 °C for 2 h. The activated catalyst was cooled to the target temperature in a flow of Ar and the ISOMET reaction was performed.
[b]*Reactivation*: After 3 h of TOS, the reactant feed was stopped, the total pressure was reduced to atmospheric pressure. The catalyst was purged with a flow of Ar (50 ml min^{-1}) for 30 min at the reaction temperature to remove olefins, then heated to 550 °C at a ramp rate of 10 °C min^{-1}, and maintained at this temperature for 2 h. The reactivated catalyst thus obtained was cooled to the target temperature in a flow of Ar and the ISOMET reaction was performed again.

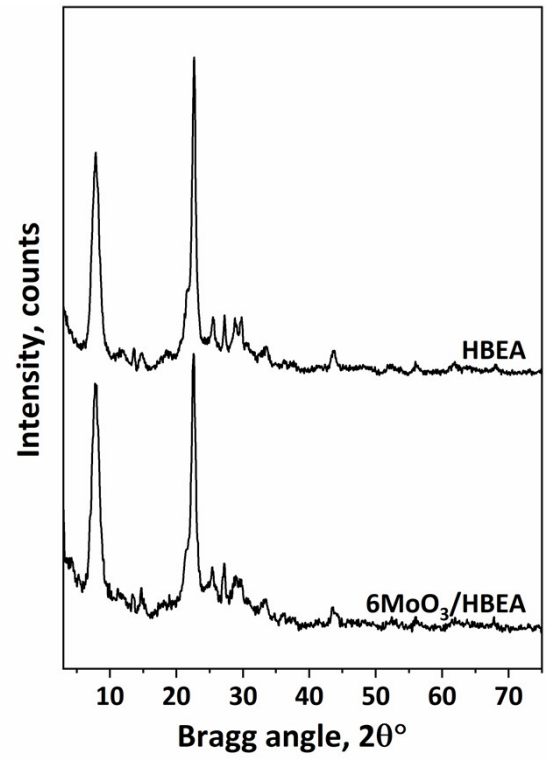

Fig. S1 XRD patterns of HBEA support and $6MoO_3$/HBEA catalyst calcined at 500 °C. The diffractograms were recorded at room temperature.

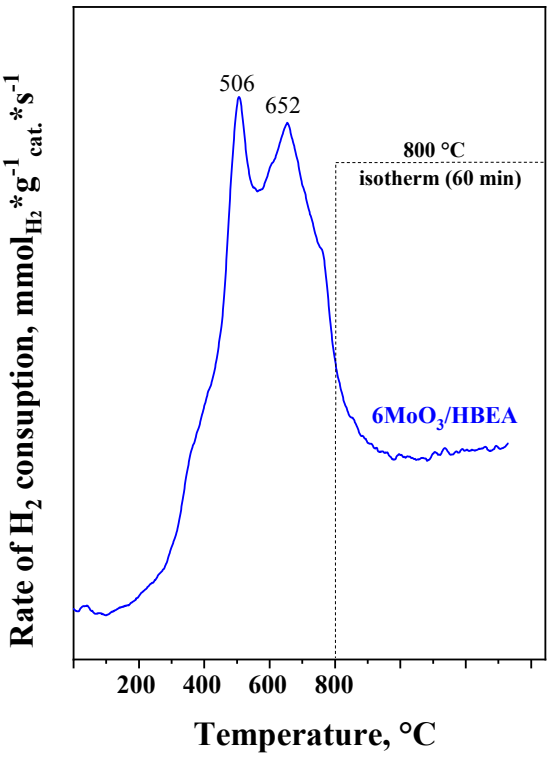

Fig. S2 H_2-TPR curve of the $6MoO_3$/HBEA catalyst. The catalyst was treated in O_2 in a flow rate of 30 ml/min for 1 h at 500 °C, cooled to 25 °C and then heated at a rate of 10 °C min^{-1} up to 800 °C for 1 h in a flow of 9 % H_2/N_2 mixture.

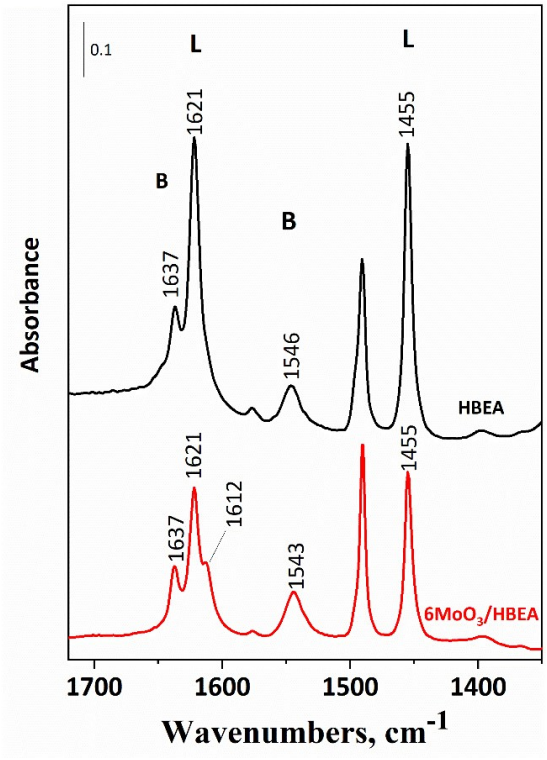

Fig. S3 FT-IR spectra of pyridine adsorbed on the HBEA support and $6MoO_3$/HBEA catalyst. The samples were activated in high vacuum at 550 °C. Pre-treated samples were contacted with Py vapour at 5 mbar, 200 °C for 30 min, and evacuated for 30 min. After evacuation, the spectra were recorded at room temperature. Labels L and B indicate the characteristic bands for Py bonded to Lewis and Brønsted acid sites, respectively.

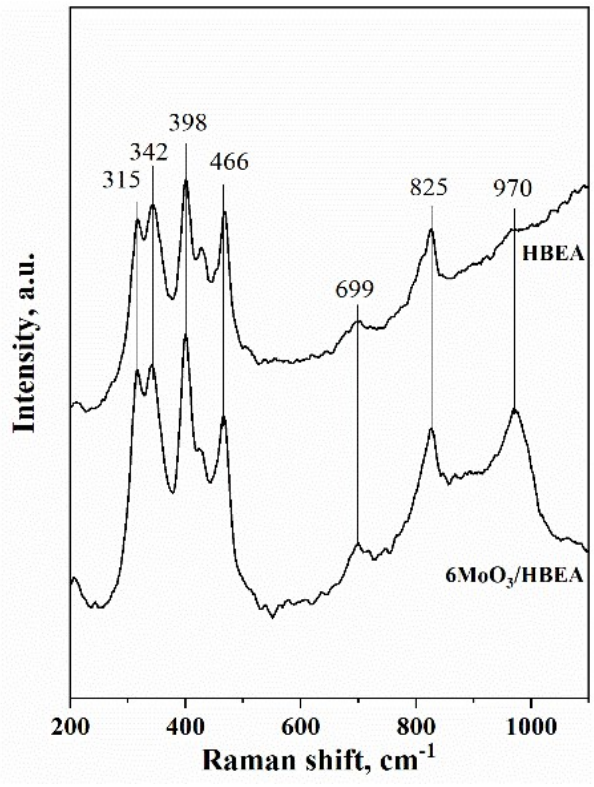

Fig. S4 Raman spectra of HBEA support and $6MoO_3$/HBEA at ambient conditions.

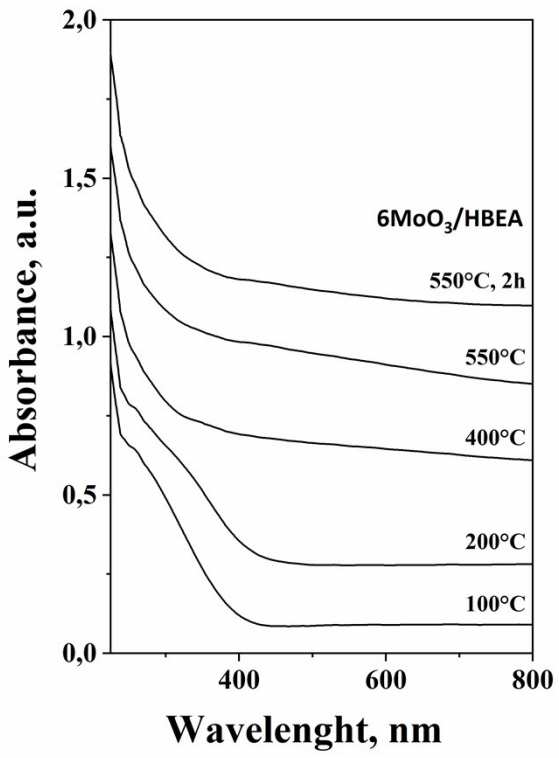

Fig. S5 In-situ UV-VIS spectra of the $6MoO_3$/HBEA catalysts. The catalyst was heated at a rate of 10 °C/min up to 550 °C for 2 h in Ar flow.

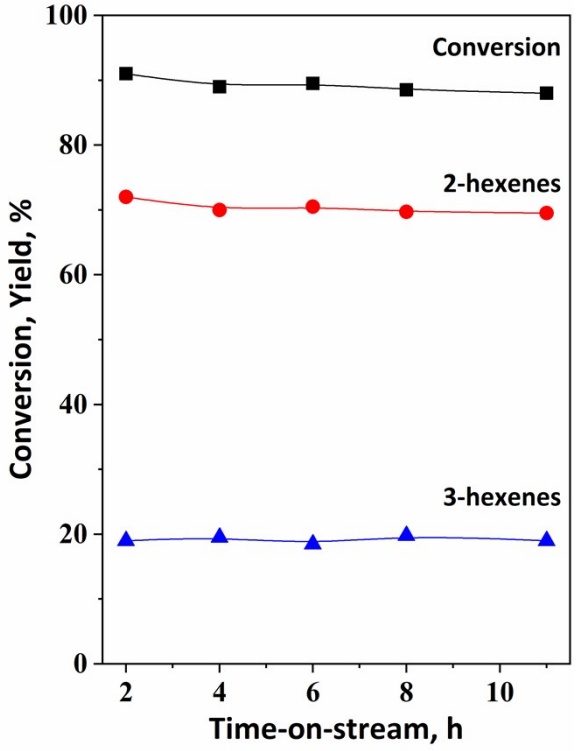

Fig. S6 Isomerization of 1-hexene using H-BEA catalyst at 150 °C and 3 g_{cat} $g_{1\text{-hexene}}^{-1}$ h space time using Ar as carrier gas in atmospheric pressure.

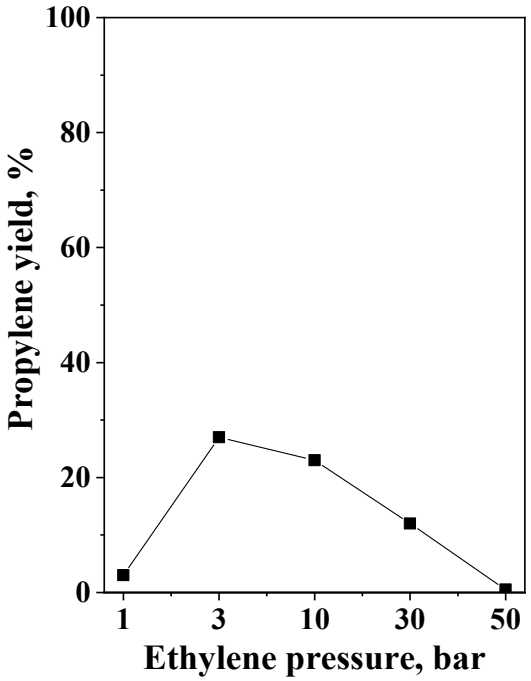

Fig. S7 Propylene yield in ethenolysis of hexene mixture (Fig. S6) at different ethylene pressures using $12MoO_3/Al_2O_3$ at 25 °C and 6 g_{cat} $g_{reactant}^{-1}$ h space time.

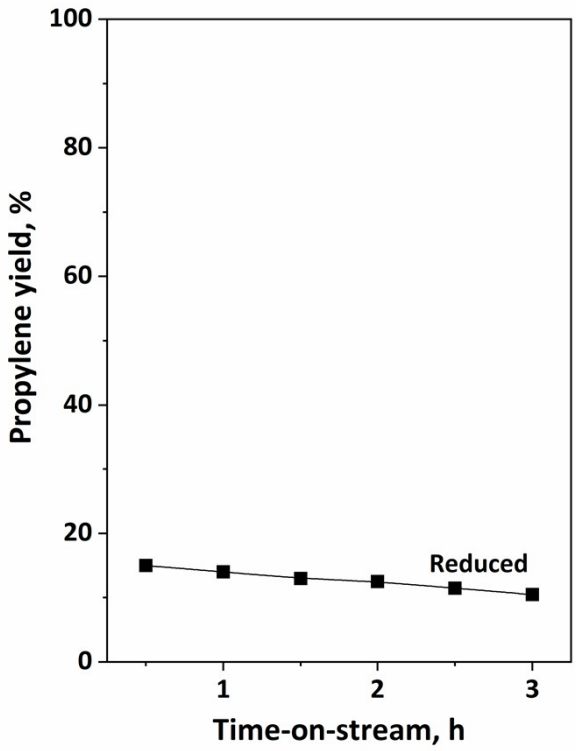

Fig. S8 Propylene yield as a function of time on stream in ISOMET of 1-hexene using HBEA and $12MoO_3/Al_2O_3$ catalyst mixture at 75 °C and 6 $g_{cat.}$ $g_{1\text{-hexene}}^{-1}$ h space time under 3 bar ethylene pressure. The catalyst mixture was reduced at 550 °C for 2 hours under atmospheric pressure using 5 % H_2/Ar.

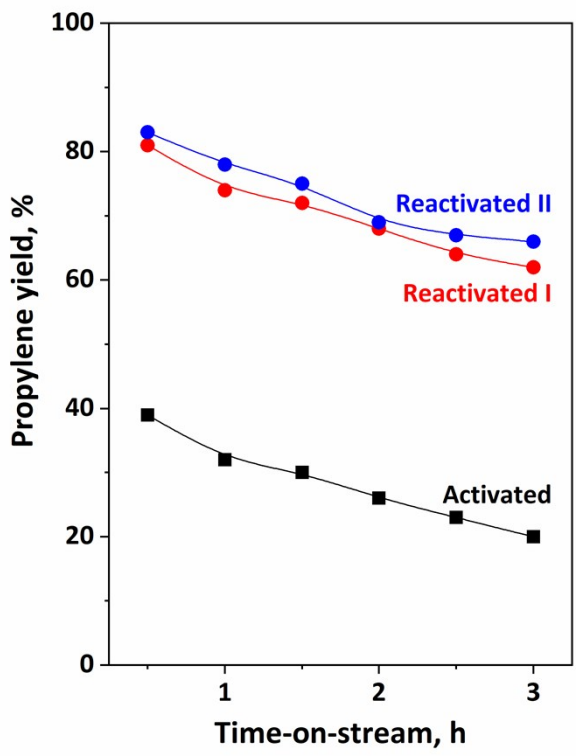

Fig. S9 Propylene yield as a function of time on stream over HBEA and $12MoO_3/Al_2O_3$ catalyst mixture after activation and two consecutive reactivation in Ar in ISOMET of 1-hexene at 75 °C and 6 $g_{cat.}$ $g_{1\text{-hexene}}^{-1}$ h space time under 3 bar ethylene pressure.

Activation: the *ex-situ* calcined catalyst was *in-situ* pre-treated in 5 % H_2/Ar or Ar flow (50 ml min^{-1}) at 550 °C for 2 h. *Reactivation*: after 3 h of TOS in 1-hexene ISOMET the catalyst was purged in a flow of Ar (50 ml min^{-1}) for 0.5 h at 75 °C to desorb olefins, then heated to 550 °C at a ramp rate of 10 °C min^{-1}, and maintained at this temperature for 2 h.

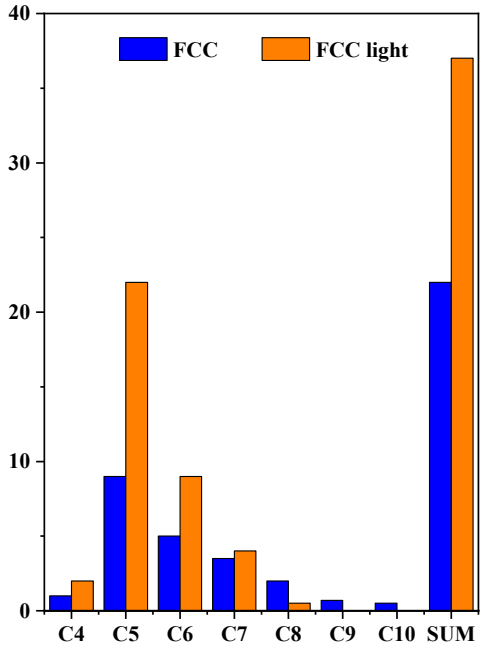

Fig. S10 Olefin content of FCC and FCC light fractions.

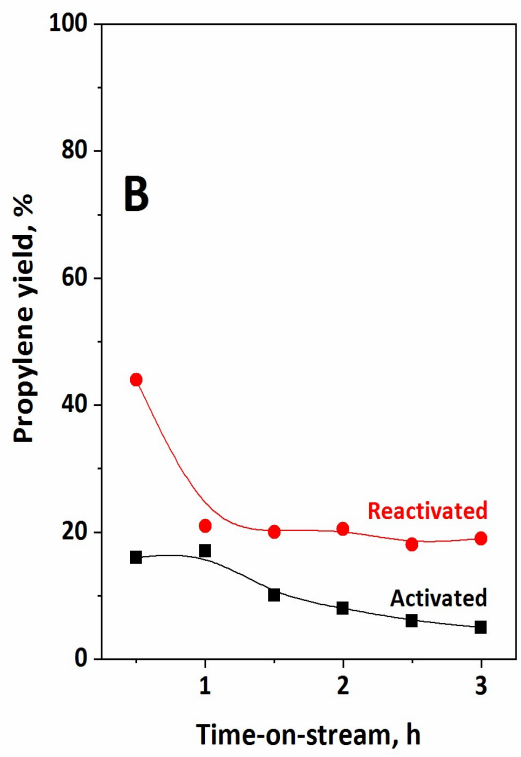

Fig. S11 ISOMET of FCC light using 13MoO_3/HBEA catalyst at 75 °C and under 3 bar ethylene pressure.