

Supporting information

Dehydrogenation of the liquid organic hydrogen carrier perhydrodibenzyltoluene – reaction pathway over Pt/Al₂O₃

Libin Shi ^{1,2,3}, Suitao Qi ^{*1}, Kevin J. Smith ^{*2}, Majed Alamoudi ^{2,4}, Yiming Zhou ¹

1 Shaanxi Key Laboratory of Energy Chemical Process Intensification, School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, P.R. China

2 Department of Chemical & Biological Engineering, University of British Columbia, 2360 East Mall, Vancouver, BC, V6T 1Z3, Canada

3 SINOPEC Research Institute of Petroleum Processing, Beijing 100083, P.R. China

4 Department of Chemical and Materials Engineering, Faculty of Engineering, King Abdulaziz University, Jeddah 21589, Saudi Arabia

*E-mail: suitaoqi@mail.xjtu.edu.cn (Suitao Qi); kjs@mail.ubc.ca (Kevin J. Smith)

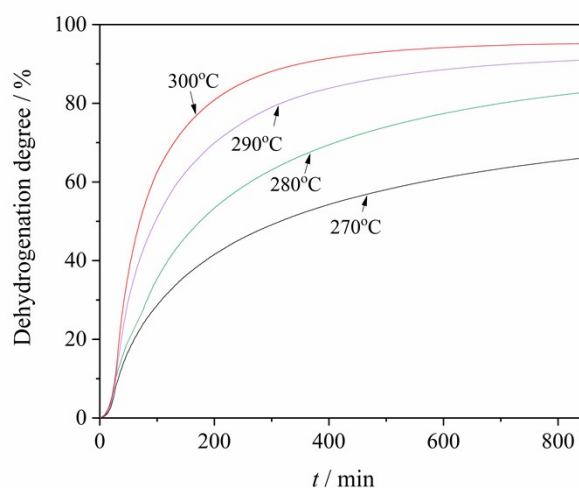


Fig. S1 Dehydrogenation of H18-DBT at different temperature

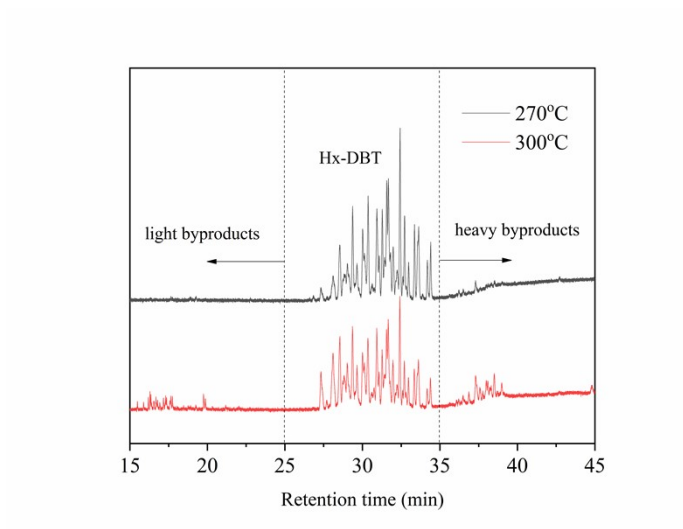


Fig. S2 GC-MS results of dehydrogenation products at 270 °C and 300 °C

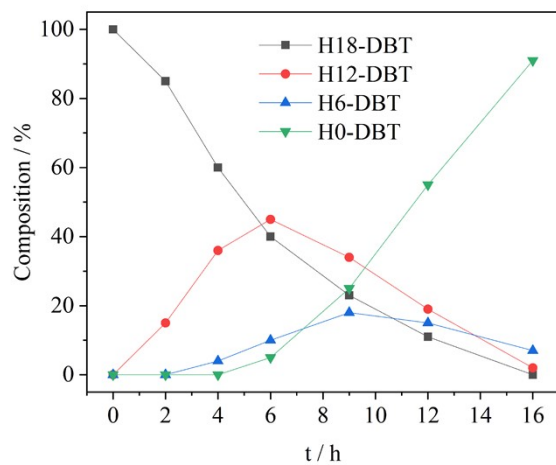


Fig. S3 Hx-DBT species from GC-MS results: composition change during dehydrogenation reaction for H18-DBT species to H12-, H6-, and H0-DBT species versus time.

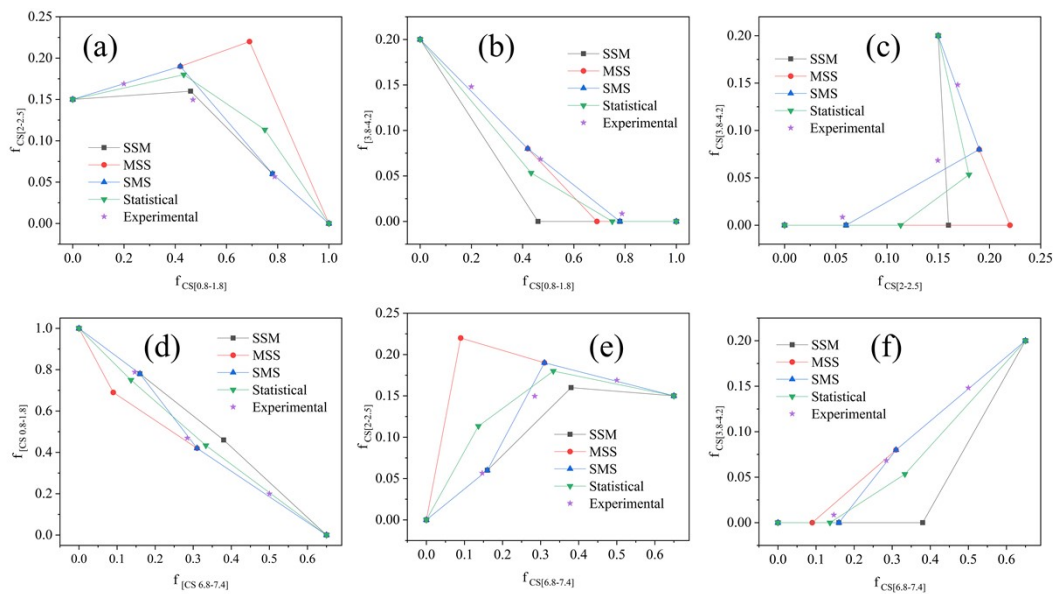


Fig. S4. The experimental ^1H NMR results of dehydrogenation products of $\text{Pt}/\text{Mo}-\text{Al}_2\text{O}_3$ catalysts (five-pointed stars) and the different dehydrogenation pathways (solid lines)

Table S1 The average residual between each experimental point and each dehydrogenation pathway over $\text{Pt}/\text{Mo}-\text{Al}_2\text{O}_3$

Plots	Average residual			
	SSM	MSS	SMS	Statistical
$f_{\text{CS}[0.8-1.8]} \sim f_{\text{CS}[2-2.5]}$	0.016	0.089	0.021	0.043
$f_{\text{CS}[0.8-1.8]} \sim f_{\text{CS}[3.8-4.2]}$	0.074	0.010	0.010	0.031
$f_{\text{CS}[2-2.5]} \sim f_{\text{CS}[3.8-4.2]}$	0.020	0.043	0.014	0.029
$f_{\text{CS}[6.8-7.4]} \sim f_{\text{CS}[0.8-1.8]}$	0.079	0.083	0.012	0.035
$f_{\text{CS}[6.8-7.4]} \sim f_{\text{CS}[2-2.5]}$	0.033	0.122	0.014	0.052
$f_{\text{CS}[6.8-7.4]} \sim f_{\text{CS}[3.8-4.2]}$	0.122	0.012	0.009	0.032