Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2018

Supplementary Information

Insights into the reaction mechanism of *n*-hexane dehydroaromatization to benzene over gallium embedded HZSM-5: Effect of H_2 incorporated on active sites

Anawat Thivasasith,[a] Thana Maihom,[b] Sitthiphong Pengpanich,[c] Jumras Limtrakul,[d] and Chularat Wattanakit[*a]*

[a]School of Energy Science and Engineering, Nanocatalysts and Nanomaterials for Sustainable Energy and Environment Research Network of NANOTEC, Vidyasirimedhi Institute of Science and Technology, Rayong 21210, Thailand.

[b]Department of Chemistry, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, Nakhon Pathom 73140, Thailand.

[c]PTT Global Chemical Public Company Limited (PTTGC), Bangkok 10900, Thailand

[d]School of Materials Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong 21210, Thailand.

Corresponding Author's E-mail: chularat.w@vistec.ac.th

Characterization results of catalysts

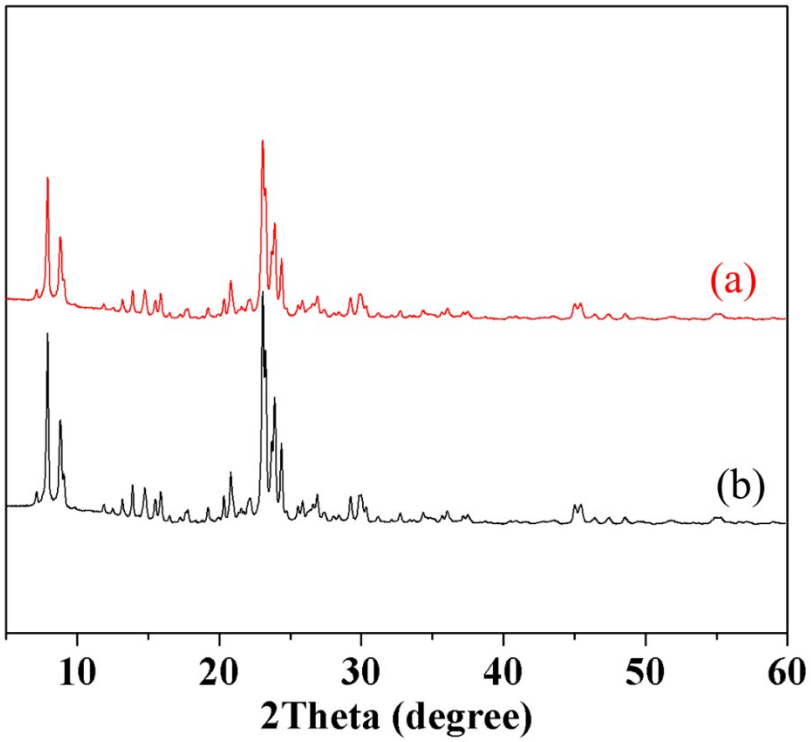

Figure S1 XRD patterns of (a) HZSM-5 and (b) Ga exchange HZSM-5 (Si/Al of 15)

Table S1 Ga contents and Si/Al ratio obtained over the Ga exchange HZSM-5 (Si/Al of 15)

Sample	Ga (wt%)	Si/Al
HZSM-5	-	16.2
1%Ga-Exc-HZSM-5	1.0	16.2

Table S2 Textural properties of Ga exchange HZSM-5 (Si/Al of 15)

Sample	S_{BET}[a] (m^2/g)	S_{micro}[b] (m^2/g)	S_{ext}[c] (m^2/g)	V_{total}[d] (cm^3/g)	V_{micro}[e] (cm^3/g)	V_{meso}[f] (cm^3/g)
HZSM-5	426	391	35	0.32	0.15	0.17

[a] S_{BET}: BET specific surface area ($m^2\ g^{-1}$). [b]S_{micro}: micropore surface area ($m^2\ g^{-1}$). [c] S_{ext}: external surface area ($m^2 g^{-1}$). [d] V_{total}: total pore volume ($cm^3\ g^{-1}$) obtained at $P/P_0 = 0.99$.

[e]V_{micro}: micropore volume ($cm^3\ g^{-1}$). [f] $V_{meso} = V_{total}-V_{micro}$ ($cm^3\ g^{-1}$).

Table S3 Optimized geometrical parameters of hexa-1-ene dehydrogenation to hexa-1,3-diene over the Ga/ZSM-5.

Parameters	INT2_De	TS3	INT3	TS4	INT4	INT4_De
Distances (Å)						
Ga-O3	2.23	2.34	2.04	2.14	2.26	2.24
Ga-O4	2.16	2.13	2.06	2.17	2.17	2.21
Ga-H3	-	1.64	1.56	1.90	3.56	-
H3-H4	-	-	-	0.88	0.74	-
C4-H3	-	1.68	3.30	-	-	-
Ga-H4	-	4.05	3.42	2.29	3.78	-
C3-H4	-	1.09	1.10	1.62	6.10	-
C3-C4	1.53	1.59	1.56	1.44	1.34	1.35
C4-C5	1.53	1.51	1.54	1.52	1.50	1.50
C3-Ga	3.74	3.62	2.89	2.65	3.51	2.90
C4-Ga	-	2.97	1.98	2.19	3.52	2.87
∠Angle(°)						
O3-Ga-O4	68.2	68.0	74.3	69.9	68.5	68.1

Table S4 Optimized geometrical parameters of hexa-1,3-diene dehydrogenation to hexa-1,3,5-triene over the Ga/HZSM-5.

Parameters	INT4_De	TS5	INT5	TS6	INT6	INT6_De
Distances (Å)						
Ga-O3	2.24	2.13	2.02	2.14	2.18	2.17
Ga-O4	2.21	2.11	2.04	2.11	2.17	2.17
Ga-H5	-	1.71	1.56	1.90	3.30	-
H5-H6	-	-	2.89	0.89	0.74	-
C5-H5	-	1.58	3.06	-	-	-
Ga-H6	-	4.25	2.94	2.37	3.26	-
C6-H6	-	1.09	1.09	1.52	3.86	-
C4-C5	1.50	1.39	1.48	1.46	1.45	1.45
C5-C6	1.53	1.50	1.55	1.39	1.34	1.34
C5-Ga	3.50	2.87	2.00	2.51	3.41	3.45
C6-Ga	4.97	4.03	2.80	3.02	3.21	3.22
∠Angle(°)						
O3-Ga-O4	68.1	69.8	72.7	69.4	69.4	69.7

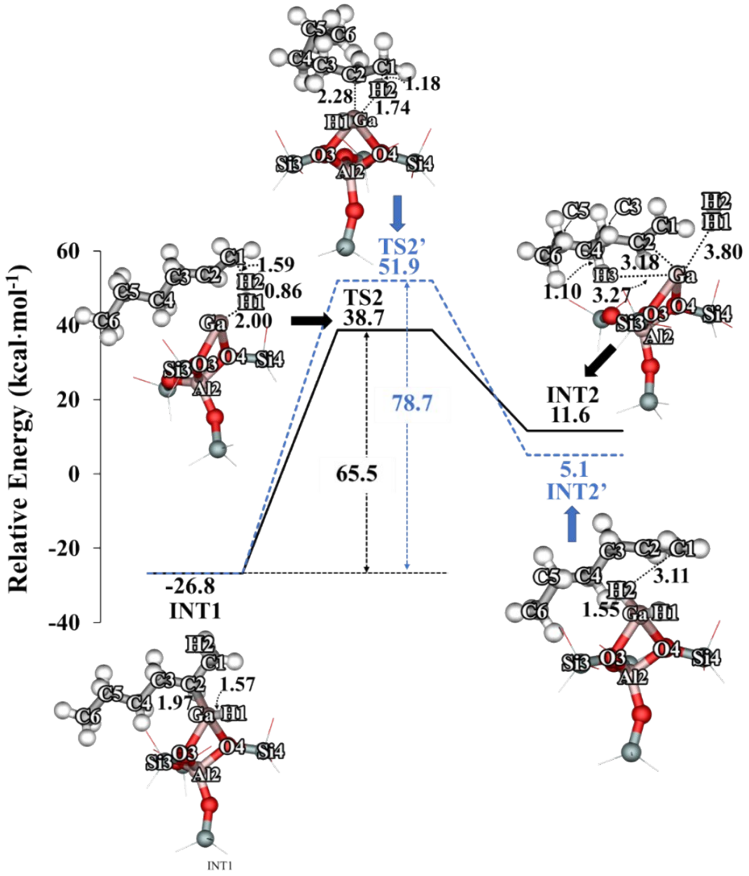

Figure S2 Energy profile of the reaction mechanism of the dehydrogenation of second hydrogen (H2) of C_6H_{13} towards hexa-1-ene over the INT1 (GaH1/HZSM-5) via the production of H_2 molecule and the regeneration of Ga site (black line) and the incorporation of H on the GaH active site to be the GaH_2 site (blue dash line).