

Kinetics of Hydrodeoxygenation of Octanol over Supported Nickel Catalysts: A Mechanistic Aspect

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Supplementary Materials

Table S1. HDO of *l*-octanal, *l*-octanol, *l*-heptanol, and *l*-hexanol. ^a

reactant	conversion, %	selectivity, %									
		<i>n</i> -heptane	heptenes	<i>n</i> -octane	octenes	<i>l</i> -octanol	DOE	HEXD	TETD	OC	OA
<i>l</i> -octanal	49.6	33.4	17.5	0.4	0.1	32.2	3.5	4.8	2.3	0	5.8
<i>l</i> -octanol	45.1	<i>n</i> -heptane	heptenes	<i>n</i> -octane	octenes	<i>l</i> -octanal	DOE	HEXD	TETD	OC	OA
		50.9	24.9	0.7	0.4	10.7	10.1	0.4	0.3	1.2	0.4
<i>l</i> -heptanol	38.3	<i>n</i> -hexane	hexenes	<i>n</i> -heptane	heptenes	heptanal	HPE	<i>n</i> -dodecane	TETD	HPH	
		47.3	0.8	2.5	0.9	10.7	34.3	0.7	1.6	1.2	
<i>l</i> -hexanol	13.4	<i>n</i> -pentane	pentene	<i>n</i> -hexane	hexenes	hexanal	HXE	<i>n</i> -decane	<i>n</i> -dodecane	HXH	
		28.8	3.8	1.6	0.7	27.5	33.4	2.0	1.1	1.1	

^a Reaction conditions: temperature = 518 K, pressure = 1 bar, catalyst = 15NiAl, WHSV = 3.99 h⁻¹, TOS = 240 min.

Table S2. Effects of carrier gas on HDO of *l*-octanol. ^a

carrier gas	conversion of <i>l</i> -octanol, %	selectivity, %									
		<i>n</i> -heptane	heptenes	<i>n</i> -octane	octenes	<i>l</i> -octanal	DOE	HEXD	TETD	OC	OA
H ₂	45.1	50.9	24.9	0.7	0.4	10.7	10.1	0.4	0.3	1.2	0.4
N ₂	24.6	28.8	38.4	0.7	1.0	17.1	10.2	0.5	0.9	1.6	0.8

^a Reaction conditions: temperature = 518 K, pressure = 1 bar, catalyst = 15NiAl, WHSV = 3.99 h⁻¹, TOS = 240 min.

Table S3. Effects of H₂ flow rate on HDO of *l*-octanol. ^a

H ₂ flow rate, mL/min	conversion of <i>l</i> -octanol, %	Selectivity, %									
		<i>n</i> - heptane	heptene s	<i>n</i> - octane	octene s	<i>l</i> - octanal	DO E	HEX D	TET D	OC	OA
20	15.6	34.8	18.4	0.3	0.3	23.1	19.2	0.2	1.0	1.8	0.9
40	15.0	35.1	17.6	0.5	0.7	22.9	18.3	0.2	1.3	2.1	1.3

^a Reaction conditions: temperature = 488 K, pressure = 1 bar, catalyst = 15NiAl, WHSV = 3.99 h⁻¹, TOS = 240 min.

Table S4. Vapor pressure of pure components. ^a

temperature, K	vapor pressure, bars										
	<i>l</i> -octanol	<i>n</i> -heptane	<i>l</i> -heptene	<i>n</i> -octane	<i>l</i> -octene	<i>l</i> -octanal	DOE	TETD	HEXD	water	OA
488	1.76	12.64	13.63	7.26	7.72	2.65	0.13	0.39	0.16	20.96	0.5
503	2.78	17.25	18.72	10.18	10.80	3.95	0.25	0.65	0.28	27.85	0.77
518	3.30	19.42	21.18	11.57	12.28	4.59	0.32	0.79	0.35	36.37	1.16
533	3.58	20.58	22.51	12.32	13.08	4.93	0.36	0.87	0.39	46.77	1.69

^a The data was generated using Aspen Plus®, Aspen Tech™

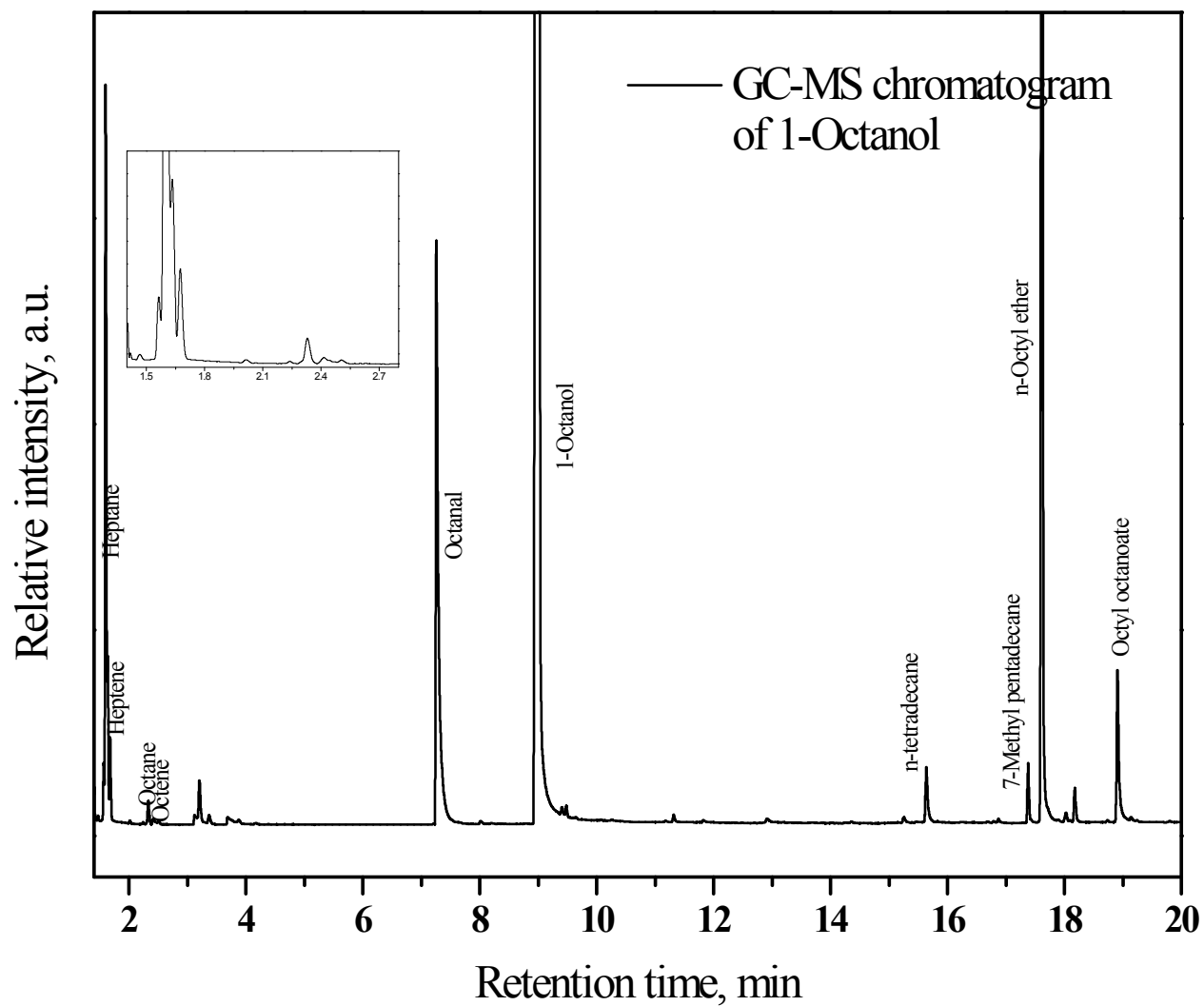


Fig. S1. A typical GC-MS chromatogram of liquid sample for HDO of 1-octanol. Reaction conditions: temperature = 518 K, pressure = 1 bar, catalyst = 15NiAl, WHSV = 3.99 h⁻¹, TOS = 240 min.

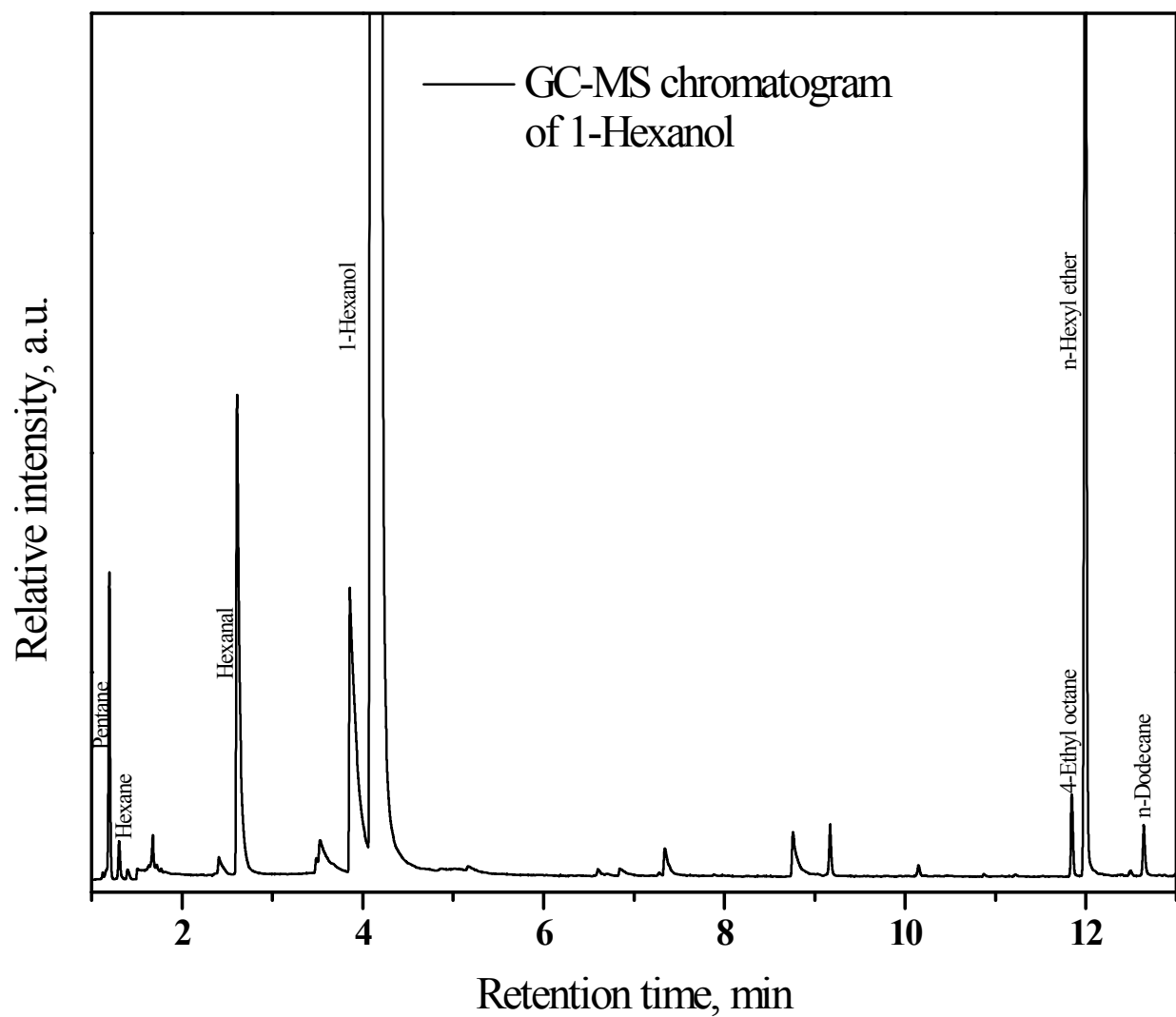


Fig. S2. A typical GC-MS chromatogram of liquid sample for HDO of *l*-hexanol.
Reaction conditions: temperature = 513 K, pressure = 1 bar, catalyst = 15NiAl,
WHSV = 3.99 h⁻¹, TOS = 240 min.

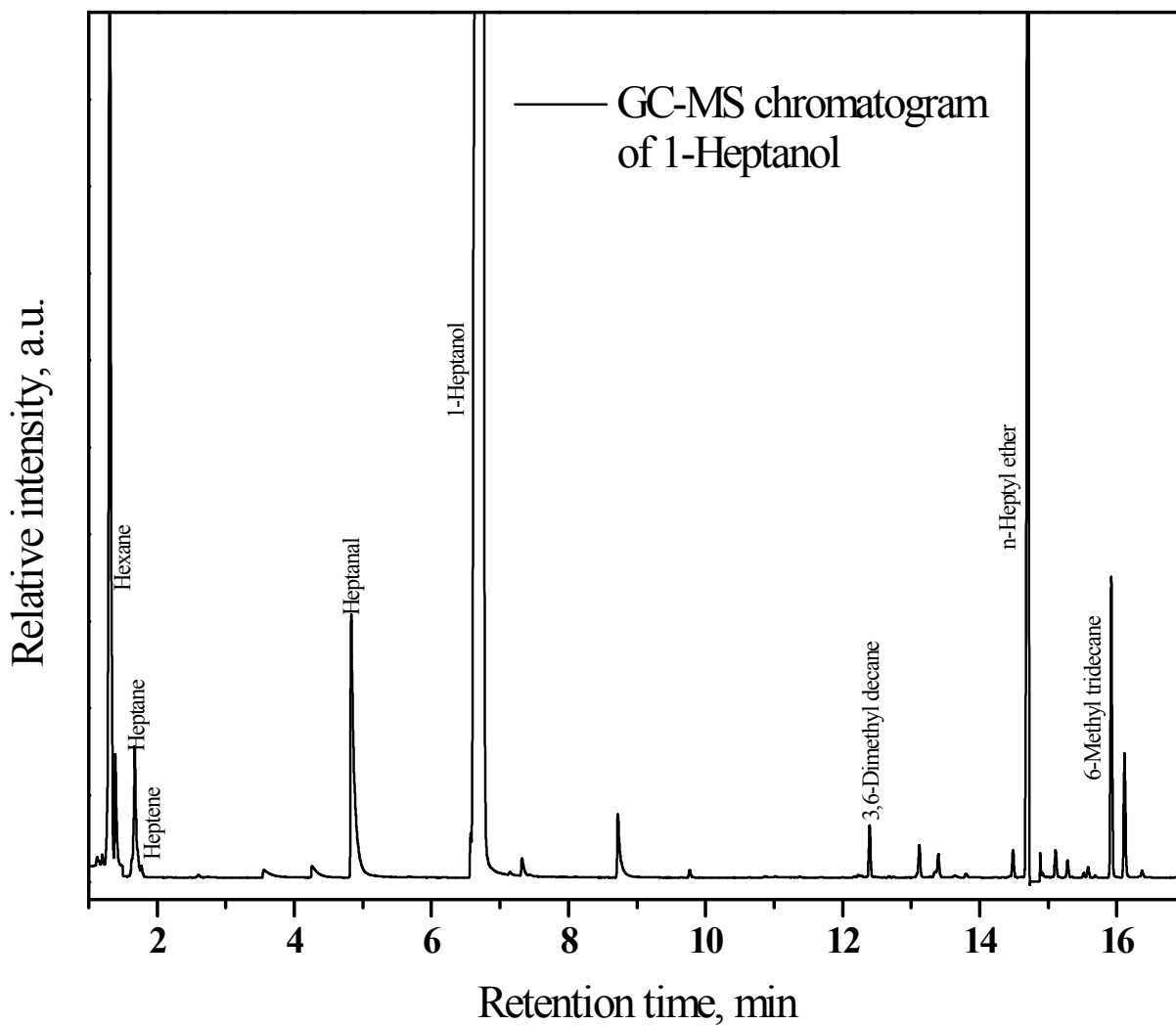


Fig. S3. A typical GC-MS chromatogram of liquid sample for HDO of *l*-heptanol.
Reaction conditions: temperature = 513 K, pressure = 1 bar, catalyst = 15NiAl,
WHSV = 3.99 h⁻¹, TOS = 240 min.