Supporting Information

Efficient continuous-flow synthesis of long-chain alkylated naphthalene

catalyzed by ionic liquids in a microreaction system

Tian Yang^{1#}, Fajun Wang^{1#}, Jinpei Huang^{2*}, Si Da Ling¹; Suli Liu³, Angui Zhang³, Yundong Wang¹, Jianhong Xu^{1*}

¹ The State Key Laboratory of Chemical Engineering, Department of Chemical Engineering, Tsinghua University, Beijing 100084, P.R. China

² College of life science, China Jiliang University, Hangzhou, Zhejinag 310018, P.R. China

³ Ningxia Coal Industry Group Co. Ltd., CHN ENERGY, Yinchuan 750011, P.R. China

Table of Contents

1. Supplementary Figures
2. Supplementary Tables

1. Supplementary Figures

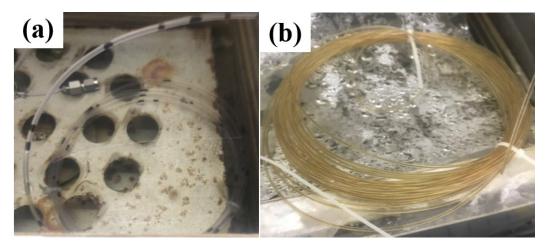


Figure S1. Influence of the delay loop's inner diameter on the dispersion of two phases (a) 2 mm inner diameter; (b) 0.9 mm inner diameter

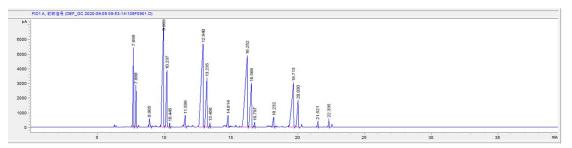


Figure S2. GC profiles for the 1-dodecene alkylation products

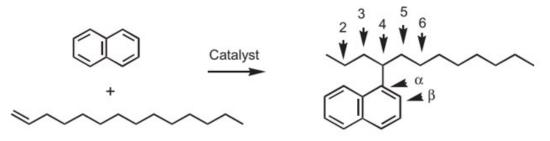


Figure S3. Alkylation reaction between 1-dodecene and naphthalene

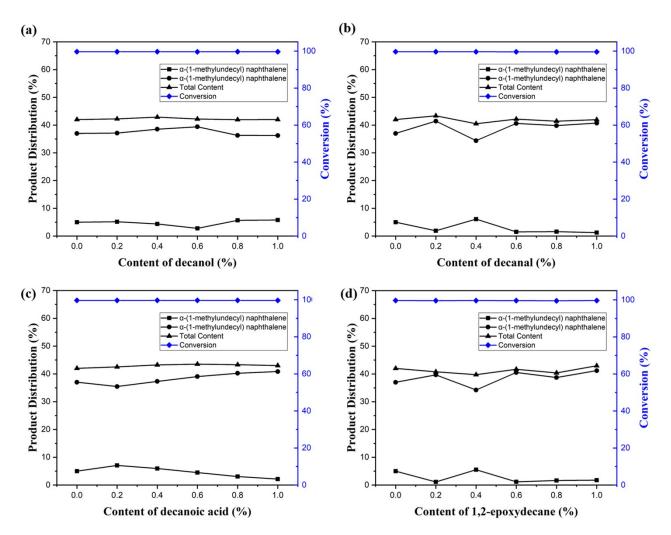


Figure S4. Effects of the content of each kind of oxides on the on the alkylation of 1-dodecene

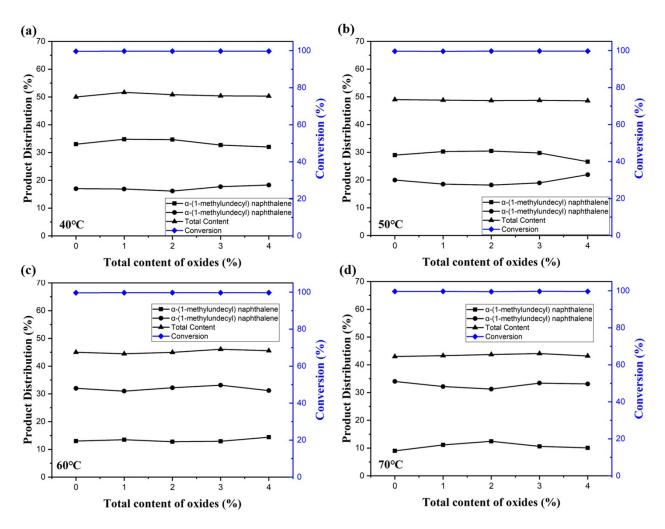
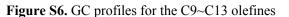


Figure S5. Effects of the total content of oxides on the alkylation of 1-dodecene



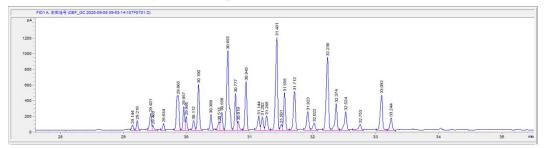


Figure S7. GC profiles for the C9~C13 olefines alkylation products

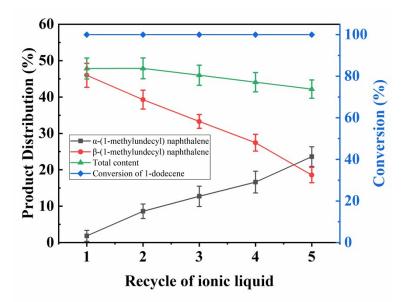


Figure S8. Influence of ionic liquid recycling on the distribution of products

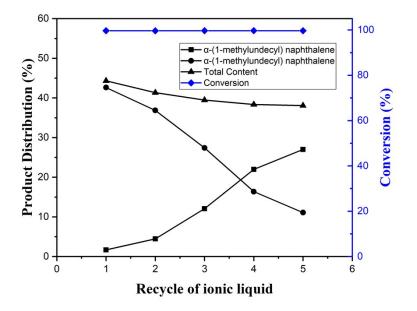


Figure S9. Reuse of ionic liquids at 4% oxides content in 1-dodecene

The flow rates of naphthalene and 1-dodecene were 9 mL/min and 1 mL/min, respectively; the temperature was 70°C; the molar ratio of naphthalene to 1-dodecene was 6:1; the flow rate of ionic liquid was 0.3 mL/min

2.	Suppl	lementary	Tables
----	-------	-----------	--------

Peak	Retention time /min	Products	Molecular formula
1	31.186	α- (1-pentylheptyl) naphthalene	$C_{22}H_{32}$
2	31.251	α- (1-butyloctyl) naphthalene	$C_{22}H_{32}$
3	31.417	α - (1-propylnonyl) naphthalene	$C_{22}H_{32}$
4	31.485	β -(1-pentylheptyl) naphthalene	$C_{22}H_{32}$
5	31.540	β -(1-butyl-octyl) naphthalene	$C_{22}H_{32}$
6	31.704	α- (1-ethyldecyl) naphthalene β- (1-propylnonyl) naphthalene	$C_{22}H_{32}$
7	31.917	β - (1-ethyldecyl) naphthalene	$C_{22}H_{32}$
8	32.237	α - (1-methylundecyl) naphthalene	$C_{22}H_{32}$
9	32.382	β - (1-methylundecyl) naphthalene	$C_{22}H_{32}$

Table S1. Composition	n of products for the all	kylation of 1-dodecene and	l naphthalene
-----------------------	---------------------------	----------------------------	---------------

Table S2. Retention time of GC-MS for C9~C13 olefines

Peaks	Retention time /min	Components	Molecular formula
1	7.699	1-nonene	C ₉ H ₁₈
2	7.888	nonane	$C_{9}H_{20}$
3	9.986	1-decene	$C_{10}H_{20}$
4	10.237	decane	$C_{10}H_{22}$
5	12.937	1- undecene	$C_{11}H_{22}$
6	13.235	undecane	$C_{11}H_{24}$
7	16.264	1-dodecene	$C_{12}H_{24}$
8	16.579	dodecane	$C_{12}H_{26}$
9	19.716	1-tridecene	$C_{13}H_{26}$
10	20.032	tridecane	$C_{13}H_{28}$

Table S3. Composition of C9~C13 olefines after normalization

Commonanta		Olefine				Alkane					
Components	С9	C10	C11	C12	C13		С9	C10	C11	C12	C13
Concentration X_i (wt%)	6.02	17.80	19.73	19.14	10.55		2.70	6.11	6.99	7.27	3.68
$\sum X_i$			73.24						26.76		

Table S4. Productivity of alkylated naphthalene for the alkylation of C9~C13 olefines

Item	Value	Unit
Density of naphthalene (20 wt.% with cyclohexane)	0.80	g/mL
Density of C9~C13 α-olefines	0.75	g/mL
Mass fraction of α -olefines in C9~C13 α -olefines	0.73	1
The average molecular weight of α -olefin in C9~C13 α -olefines	153	g/mol
The average molecular weight of alkylated naphthalene	281	g/mol
Volume flow rate of C9 \sim C13 α -olefines	0.7	ml/min
Conversion rate of α -olefines	0.99	1
Mole flow rate of α -olefines in C9~C13 α -olefines	0.7*0.75*0.73/153=0.002505	mol/min
Mass flow rate of alkylated naphthalene	0.002505*0.99*281=0.697	g/min

Table S5. The proportion of catalytic substance taken away by organic phase

Item	1-dodecene	C9~C13 olefines
Sample mass	20.92 g	22.56 g
Mass of wash water	101.45 g	98.68 g
The concentration of Al ³⁺ in wash water	42.823 mg/L	169.266 mg/L
Al taken away by organic phase	4.344 mg	16.703 mg
The initial mass of ionic liquid	1.0137 g	1.0217 g
Al contained in ionic liquid	151.101 mg	152.286 mg
The proportion of Al taken away by organic phase	2.875%	10.968%