catalysts

MDPI

Supplementary Material

GAS-PHASE DEOXYGENATION OF BIOMASS PYROLYSIS TAR CATALYZED BY RARE EARTH METAL LOADED Hβ ZEOLITE

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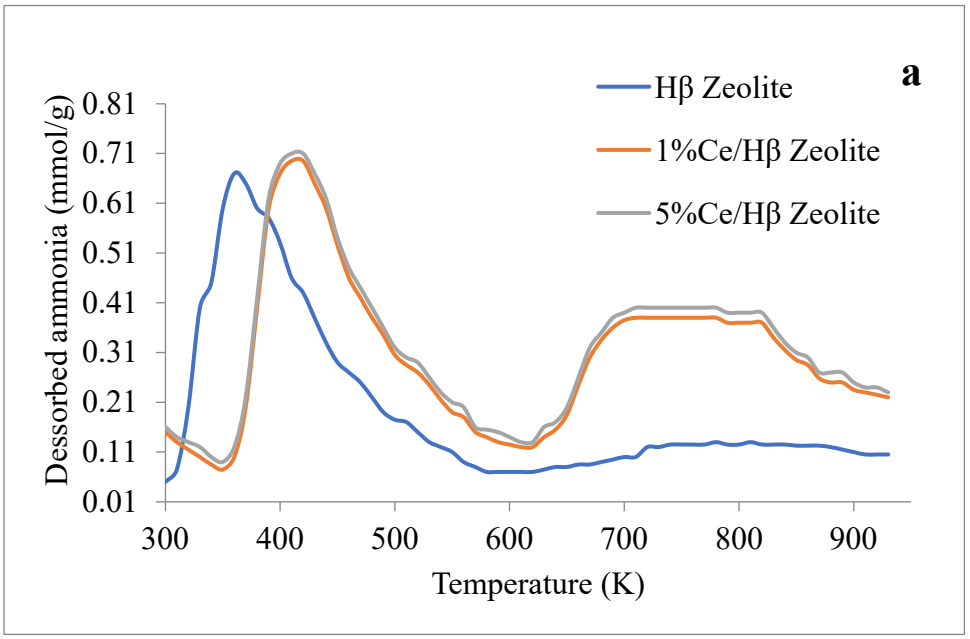
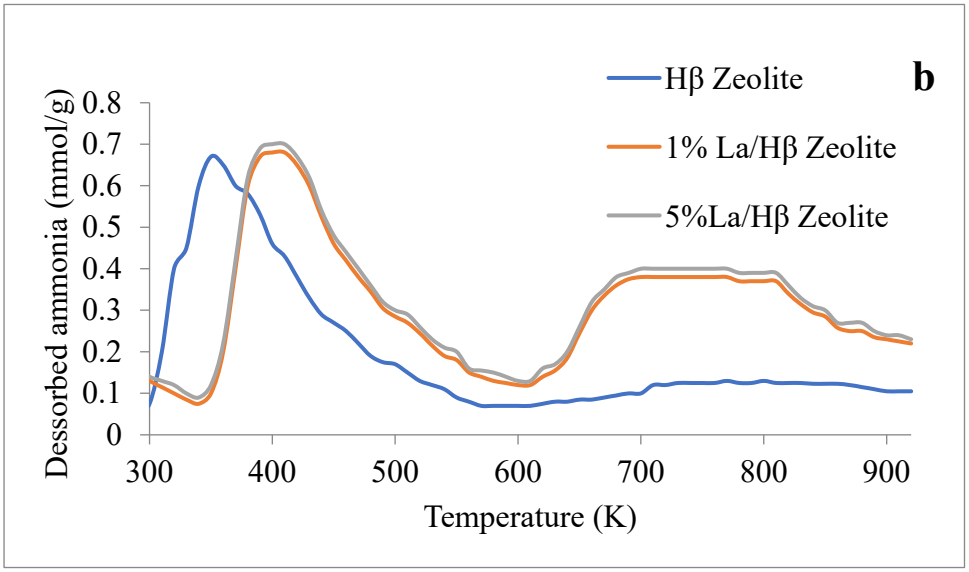




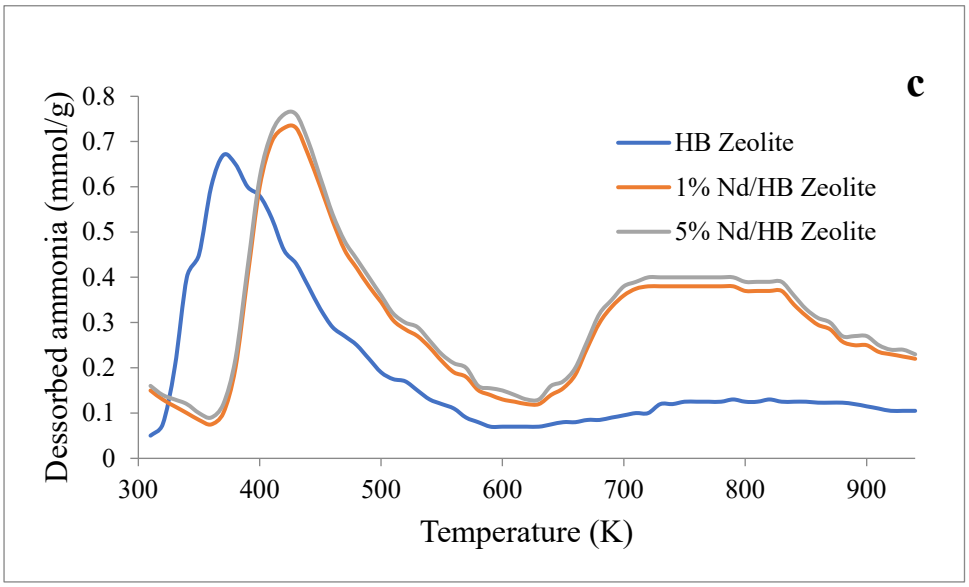


Figure S1. Ammonia-TPD profiles for for pure Hβ zeolite, 1wt% loaded Hβ zeolite, and 5wt% loaded Hβ zeolite before and after their regeneration at 800°C for 2h (a) Ce loaded Hβ zeolite, (b) La loaded Hβ zeolite, and (c) Nd loaded Hβ zeolite (All catalysts were calcined for 6h at 550°C).

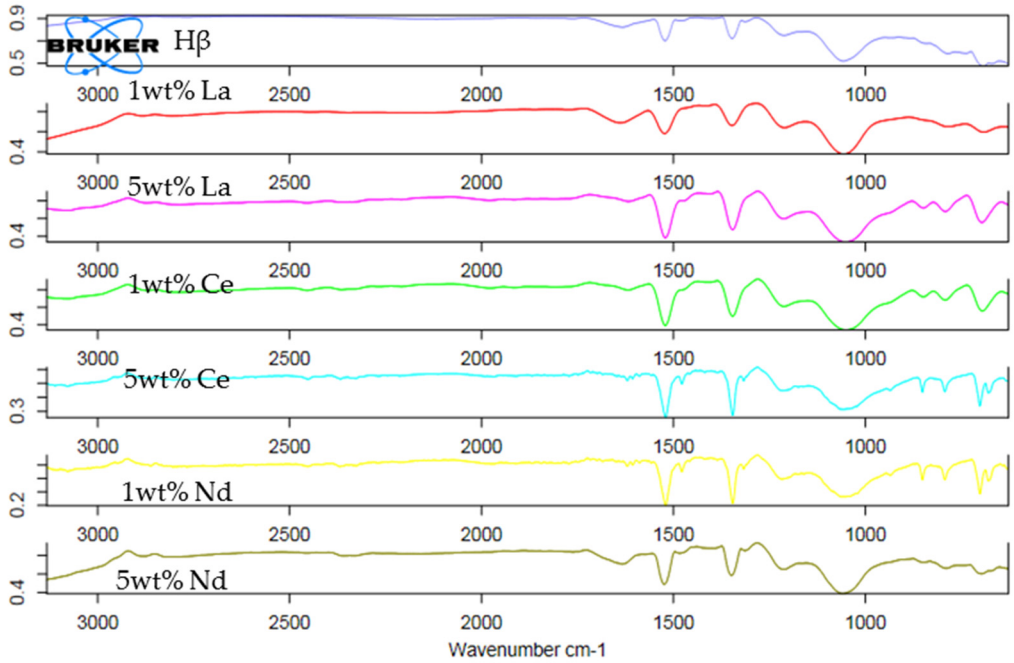
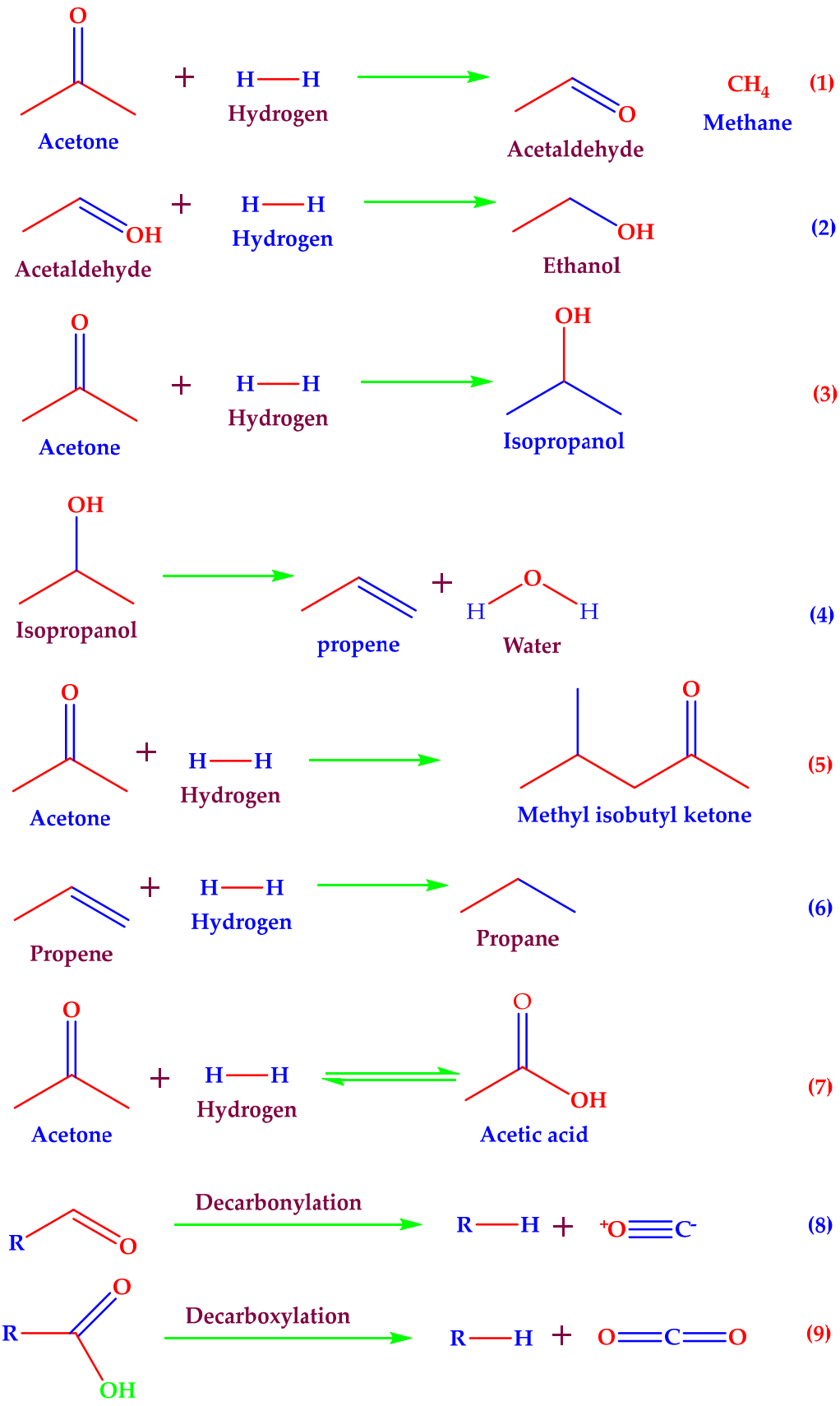


Figure S2. Pyridine-Fourier-Transform Infra-Red Spectroscopy for pure Hβ zeolite, 1wt% Ce/ Hβ zeolite, 5wt% Ce/ Hβ zeolite, 1wt% La/ Hβ zeolite, 5wt% La/ Hβ zeolite, 1wt% Nd/ Hβ zeolite, and 5wt% Nd/ Hβ zeolite (All catalysts were calcined for 6h at 550°C).

Table S1. GC-FID analysis of liquid phase products of the GDO reaction of acetone.

Retention time, min	Compound Class	Compound	Formula
1.53	Aromatics	Benzene	C_6H_6
1.696		Toluene	C_7H_8
2.08		O-xylene	C_8H_{10}
2.11		P-xylene	C_8H_{10}
2.30		Ethylbenzene	C_8H_{10}
2.46		Mesitylene	C_9H_{12}
2.49		1-Ethyl-4-methylbenzene	C_9H_{12}
2.51		1-Ethyl-3-methylbenzene	C_9H_{12}
2.53		1-Ethyl-2-methylbenze	C_9H_{12}

2.71		2,3-Dihydro-methyl-1H-indene	$C_{10}H_{12}$
2.83		P-Cymene	$C_{10}H_{14}$
2.97		2,2-Dimethylindene, 2,3-dihydro-	$C_{11}H_{14}$
1.313	Aldehydes	Acetaldehyde	C_2H_4O
1.466	Ketones	Acetone	C_2H_6O
2.19		Methyl isobutyl ketone	C_4H_8O
1.637	Alcohols	Methanol	CH_3OH
1.843		Ethanol	C_2H_6O
1.76		Isopropanol	C_2H_8O
1.52	Alkanes	Butane	C_4H_{10}
1.58		N-Pentane	C_5H_{12}
1.62	Alkenes	4-Methyl-1-pentene	C_6H_{12}
2.12	Esters	5-Hexenyl acetate	$C_8H_{14}O_2$
1.193	Furans	2-Methylfuran	C_5H_6O

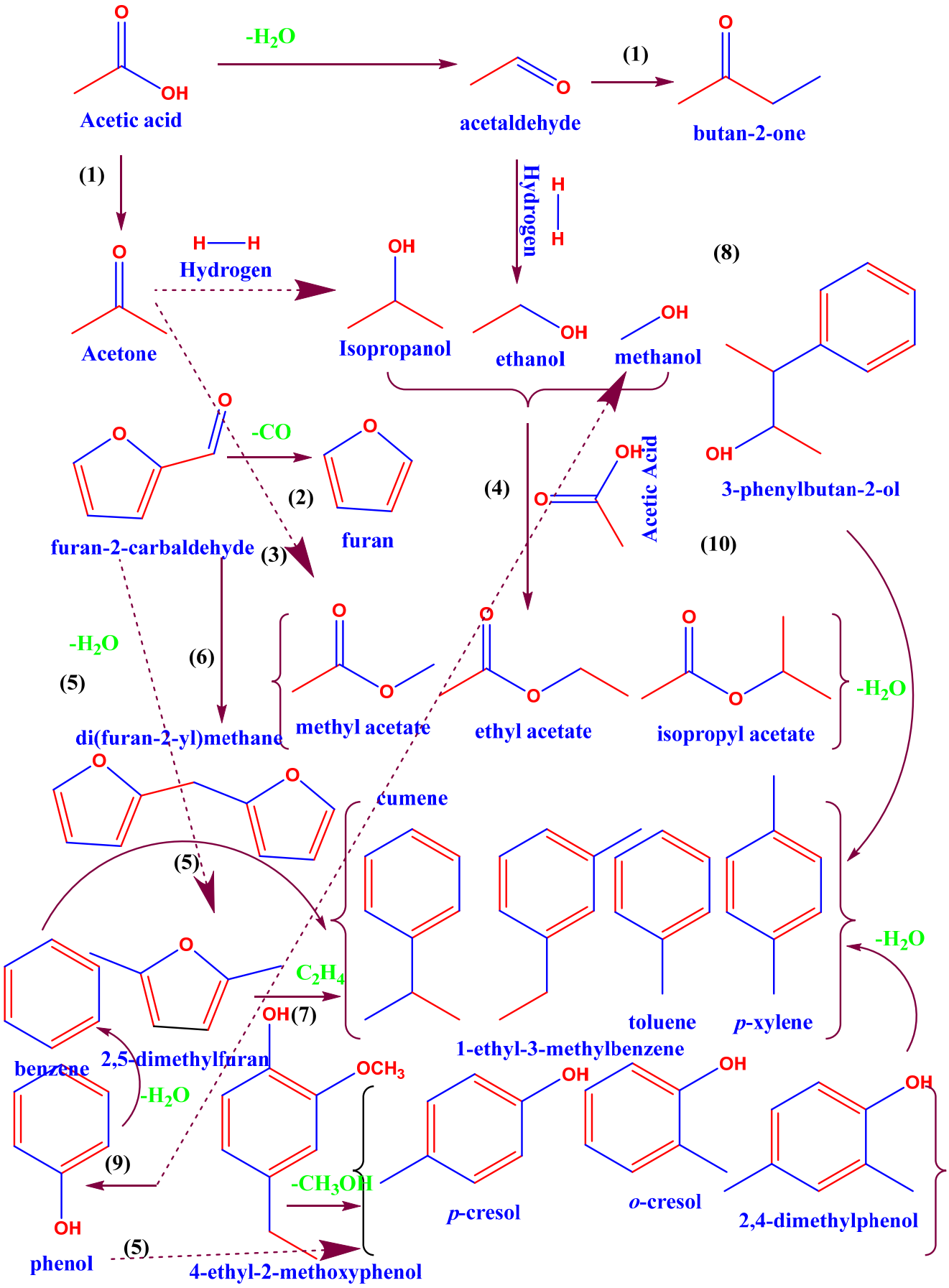

Acetone
Hydrogen
Acetaldehyde
CH_4
Methane
(1)
Acetaldehyde
Hydrogen
Ethanol
(2)
Acetone
Hydrogen
Isopropanol
(3)
Isopropanol
propene
Water
(4)
Acetone
Hydrogen
Methyl isobutyl ketone
(5)
Propene
Hydrogen
Propane
(6)
Acetone
Hydrogen
Acetic acid
(7)
Decarbonylation
(8)
Decarboxylation
(9)

35

36

37

Figure S3. Reaction network for GDO of acetone model compound at 400°C using 1wt% Ce/ Hβ zeolite as the catalyst.


Acetic acid
-H2O
acetaldehyde
(1)
butan-2-one
(1)
Hydrogen
Hydrogen
Acetone
Isopropanol
ethanol
methanol
(8)
3-phenylbutan-2-ol
-CO
(2)
furan
furan-2-carbaldehyde
(3)
(4)
Acetic Acid
(10)
-H2O
(5)
(6)
di(furan-2-yl)methane
methyl acetate
ethyl acetate
isopropyl acetate
-H2O
cumene
(5)
C2H4
(7)
toluene
p-xylene
-H2O
benzene
2,5-dimethylfuran
1-ethyl-3-methylbenzene
-H2O
(9)
-CH3OH
p-cresol
o-cresol
2,4-dimethylphenol
phenol
(5)
4-ethyl-2-methoxyphenol

40
41

Figure S4. Main interaction pathways for biomass pyrolysis of tar GDO using 1wt% Ce/ Hβ zeolite as the catalyst at 400°C and process time of 3h (Decarbonylation and decarboxylation steps are not shown).