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Supplementary Information

1-Butyl-3-Methylimidazolium Bromide Functionalized Zeolites: Nature of Interactions and Catalytic Activity for Carbohydrates Conversion to Platform Chemicals

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Table S1: Decomposition temperatures of [BMIM]Br functionalized zeolites under inert and oxidative atmosphere.

Catalyst	T_1 (First decomposition temperature), °C	T_2 (Second decomposition temperature), °C
[BMIM]Br/Nay_5.1	433 (412)	550 (555)
[BMIM]Br/HY_80	450 (454)	586 (566)
[BMIM]Br/HMOR_ 20	475 (495)	588 (681)
The value in the parenthesis indicates the decomposition temperature under oxidative atmosphere.		

Table S2: CHN data for various catalysts studied in this work.

S.No	Sample Name	Carbon (%)	Hydrogen (%)	Nitrogen (%)
1	NaY_5.1	0.22	2.46	0.11
2	[BMIM]Br/NaY_5.1	4.04	2.57	1.11
3	HY_80	0.21	2.02	0.01
4	[BMIM]Br/HY_80	3.04	1.32	0.67
5	HMOR_20	0.37	1.37	1.68
6	[BMIM]Br/HMOR_20	3.85	1.22	2.44

Table S3: N_2 sorption data of bare and [BMIM]Br encapsulated zeolites.

Zeolite Name_ (Si/Al)	S_{BET} ($m^2 \cdot g^{-1}$)	S_μ ($m^2 \cdot g^{-1}$)	V_μ ($cm^3 \cdot g^{-1}$)	V_p ($cm^3 \cdot g^{-1}$)	Average Pore size (nm)	BJH Method		S_μ / S_{BET}	REF
						S_{des} ($m^2 \cdot g^{-1}$)	V_{des} ($cm^3 \cdot g^{-1}$)		
NaY_5.1	712	672	0.351	0.409	2.30	15	0.04	0.94	PW
[BMIM]Br/NaY_5.1	473	439	0.227	0.262	2.41	18	0.05	0.93	PW
HY_80	773	440	0.231	0.581	1.50	333	0.35	0.57	A
[BMIM]Br/HY_80	671	343	0.180	0.530	3.16	328	0.35	0.52	A
HMOR_20	365	306	0.160	0.273	3.00	59	0.11	0.83	A
[BMIM]Br/HMOR_20	36	-	-	0.15	16.24	36	0.15	-	A

S_{BET} - BET surface area
S_{des} - BJH desorption surface area
S_μ- t-plot micropore surface area
P_D - Average pore diameter
V_P - total pore volume calculated at P/Po = 0.99
V_μ- t-plot micropore volume
V_{des} - BJH pore volume from the desorption
A – [Chemistry Select 2017 (2), 10379–10386]

Table S4: The fitted values of binding energies of NaY_5.1, [BMIM]Br/NaY_5.1, HMOR_20 and [BMIM]Br/HMOR_20 catalysts for Al2p and O1s.

Sample	Al_{2p}	Area (%)	Si_{2p}	Area (%)	O_{1s}	Area (%)
NaY_5.1	73.57	68.28	101.88	79.69	531.18	59.18
	74.46	31.72	103.43	20.31	532.53	40.82
[BMIM]Br/NaY_5.1	73.41	86.72	101.72	81.15	531.16	57.00
	75.44	13.28	103.22	18.85	532.86	43.00
HMOR_20	73.57	71.58	102.49	83.50	532.06	73.21
	75.18	28.42	104.95	16.50	534.10	26.79
[BMIM]Br/HMOR_20	73.95	67.75	102.83	73.17	532.77	81.47
	75.14	32.25	104.29	26.83	534.58	18.53

Table S5: Comparison of the performance of [BMIM]Br functionalized zeolites with literature data.

S. No.	Reactant	Catalyst	Reaction conditions Temp (°C), time (h)	5HMF Yield (%)	Ref
1	Fructose	HBETA + [BMIM]Cl	150, 0.84	86.8	[38]
2		Carbonaceous catalyst + [BMIM]Br	160, 0.25	81.4	[42]
3		$CrCl_3.6H_2O$ + TEAC	130, 0.16	73.8	[43]
4		[BMIM]Br /NaY_5.1	180, 1	80	PW
5	Glucose	HBETA + [BMIM]Cl	150, 0.84	50.3	[38]
6		[BMIM]Br/HMOR_20	170, 3	39	[25]
7		Carbonaceous catalyst + [BMIM]Br	160, 0.25	46.4	[42]
8		Sn-Mont	160, 3	48.2	[44]
9		$CrCl_3.6H_2O$ + TEAC	130, 0.16	71.3	[43]
10		[BMIM]Br /NaY_5.1	180, 2	62	PW
11	Cellulose	HBETA + [BMIM]Cl	150, 0.84	46.5	[38]
12		$CuCl_2/CrCl_2$ + [EMIM]Cl	100, 8	57.5	[9]
13		Carbonaceous catalyst + [BMIM]Br	160, 0.25	40.5	[42]
14		$CrCl_2/RuCl_3$ + [EMIM]Cl	120, 2	60	[45]
15		[BMIM]Br /NaY_5.1	180, 3	59	PW
16		[BMIM]Br /HY_80	180, 3	39	PW
17		[BMIM]Br /HMOR_20	180, 3	40	PW
PW: Present Work					

Table S6: Weight losses in TGA in the temperature range of 200-600°C.

Sample	Weight loss (%)
NaY_5.1	2.8
[BMIM]Br/NaY_5.1	3.66
Recycle [BMIM]Br/NaY_5.1	49.01

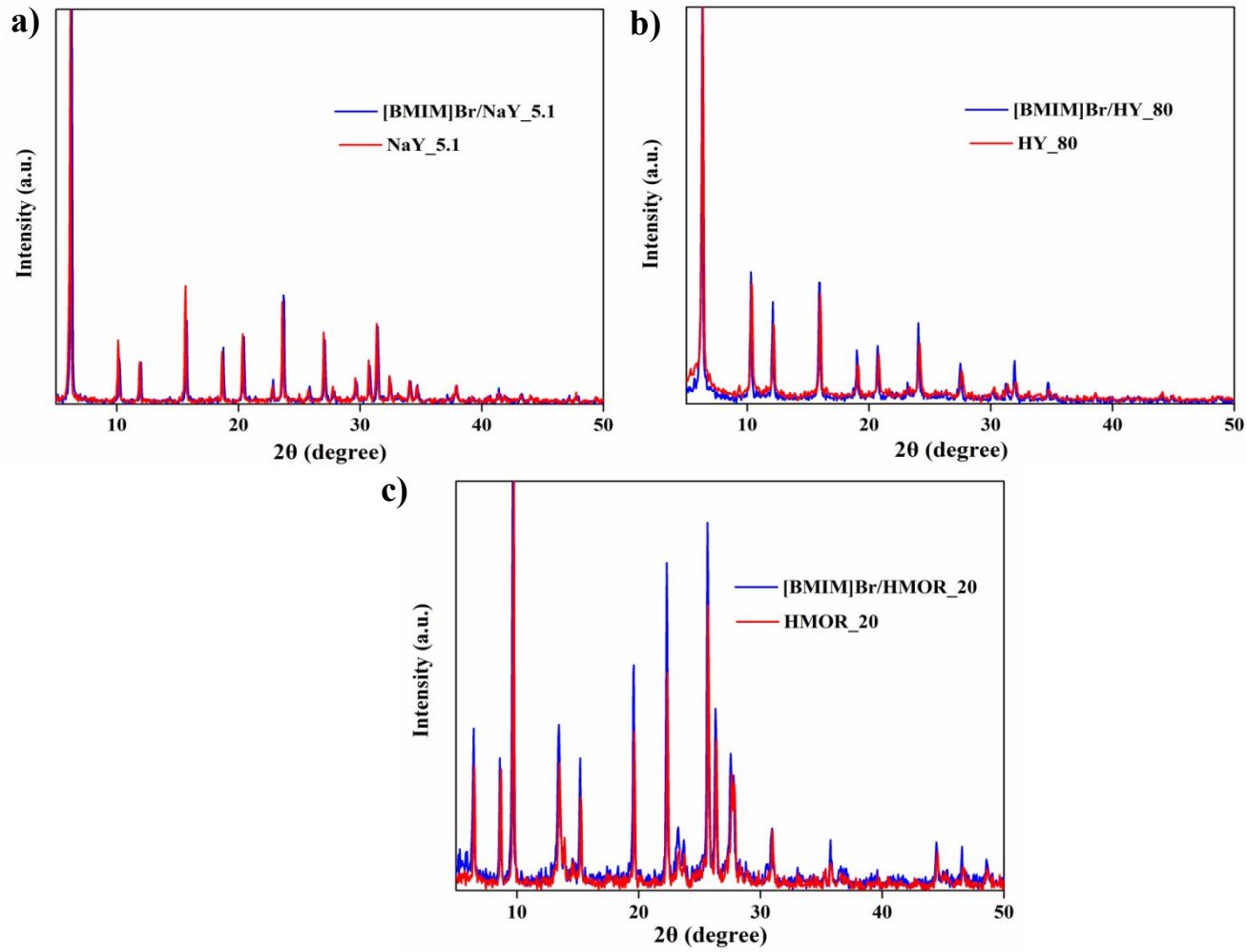

Figure S1: The detailed analysis of XRD pattern after [BMIM]Br encapsulation over zeolites: (a) NaY_5.1 and [BMIM]Br/NaY_5.1, (b) HY_80 and [BMIM]Br/HY_80, and (c) HMOR_20 and [BMIM]Br/HMOR_20.

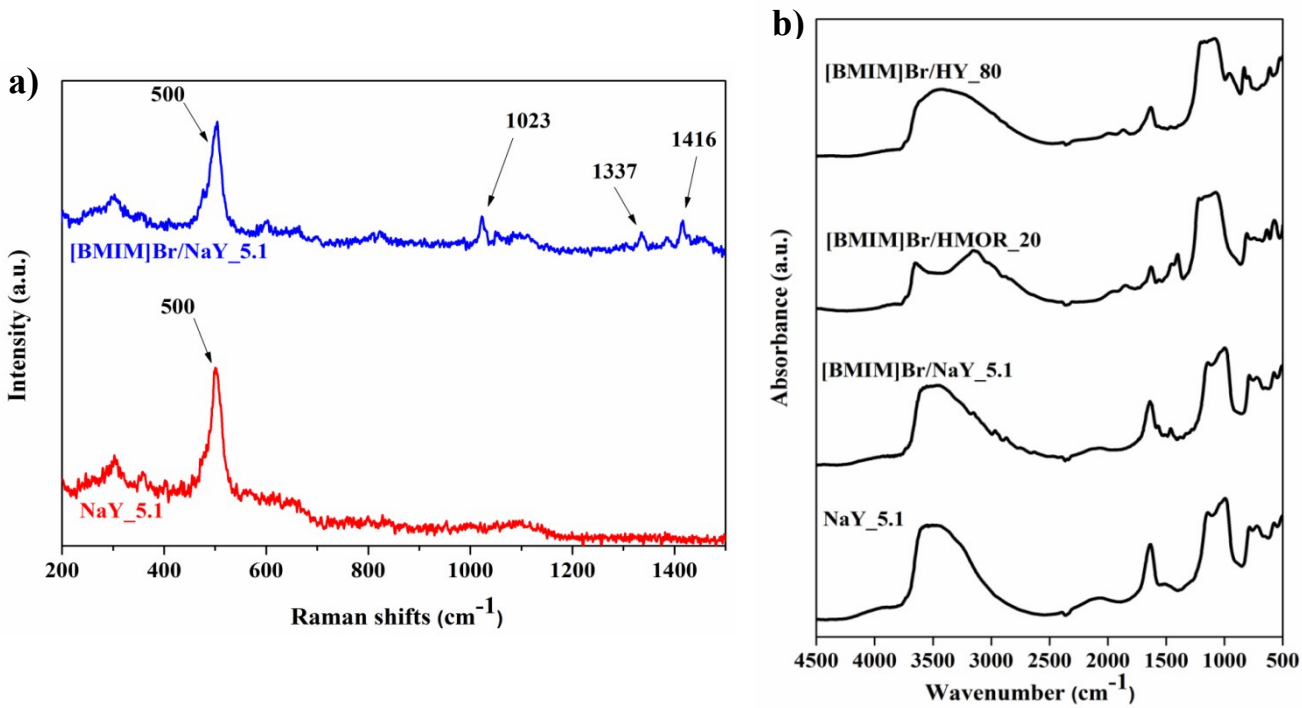

Figure S2: (a) Raman and (b) FTIR spectra of bare and ionic liquid encapsulated zeolites.

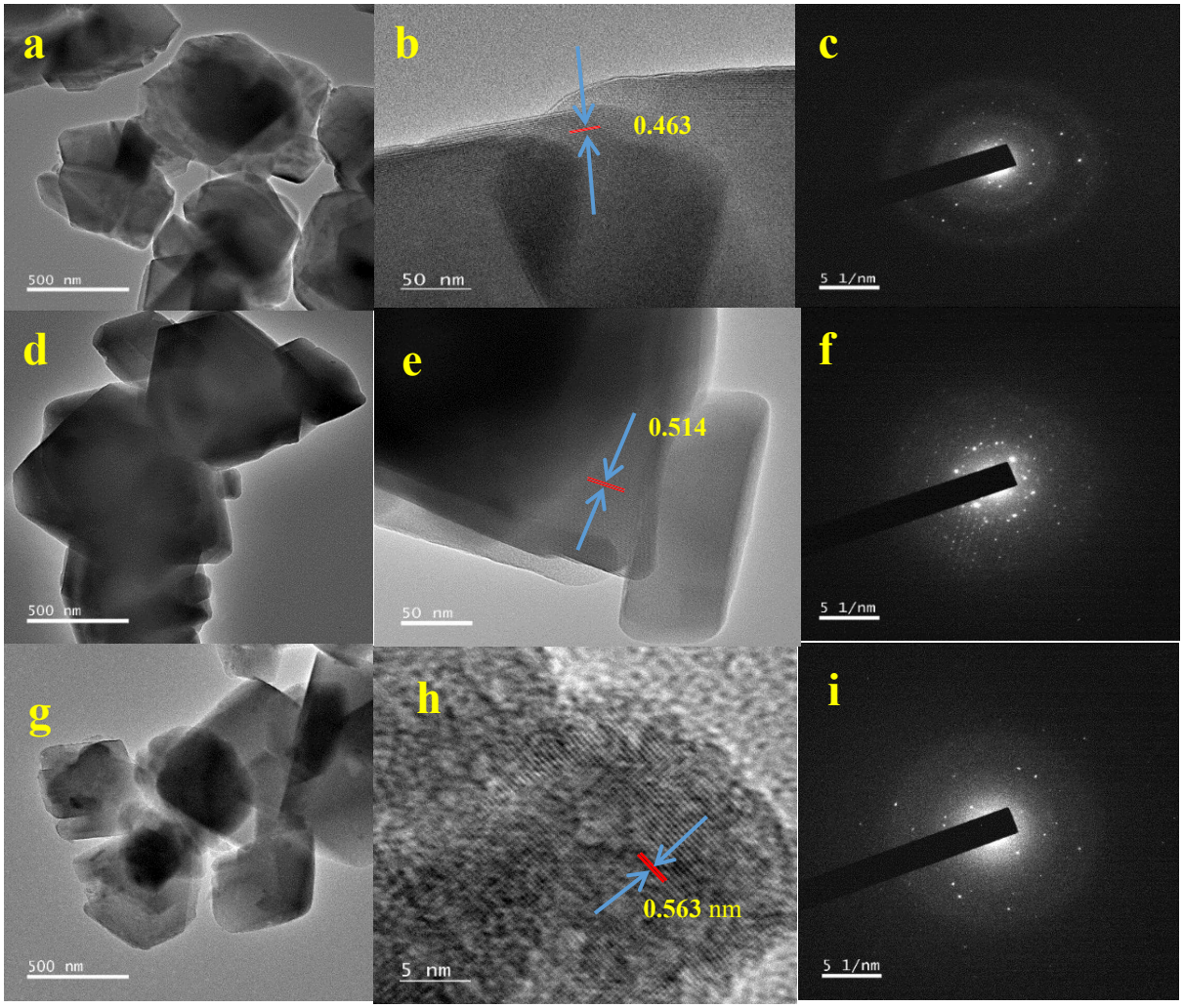

Figure S3: FETEM images and SAED patterns (c, f, and i) of NaY_5.1 (a, b, and c), [BMIM]Br/NaY_5.1 (d, e, and f), and Recycled BMIM]Br/NaY_5.1 (g, h, and i).

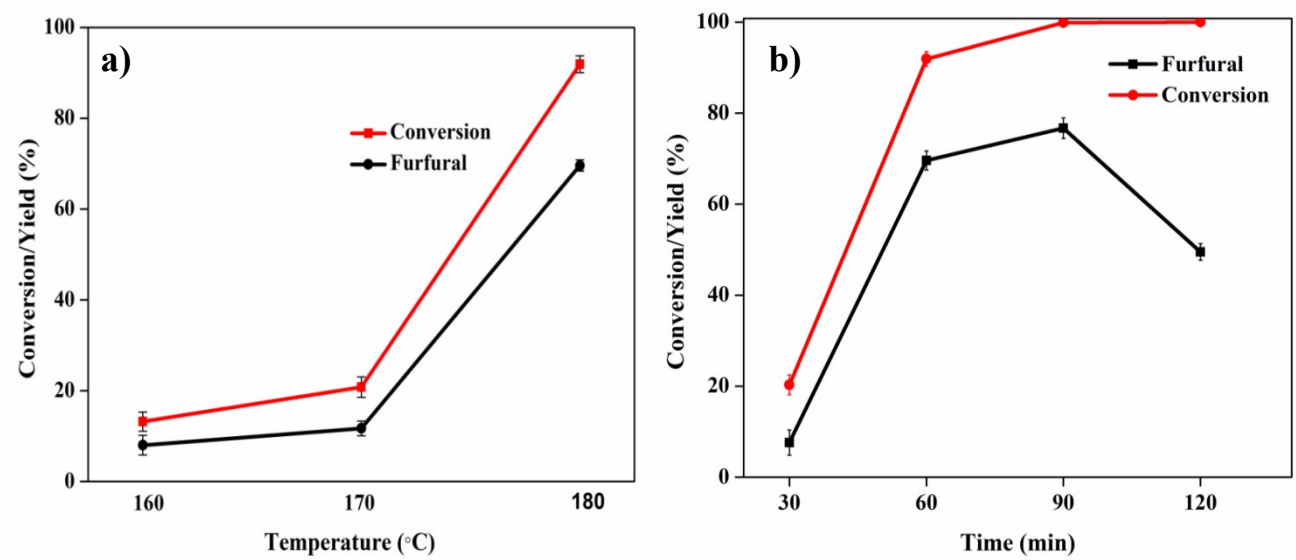

Figure S4: Effect of reaction temperature (at constant time 1h) (a) and time (at constant temperature 180°C) (b) on furfural yield from xylose (Reaction conditions: 2 g DI water, 0.2 g substrate, substrate: catalyst (IL/NaY 5.1) = 3:1 w/w, reaction phase: extractive phase = 1:2 w/w, 0.6 g NaCl).

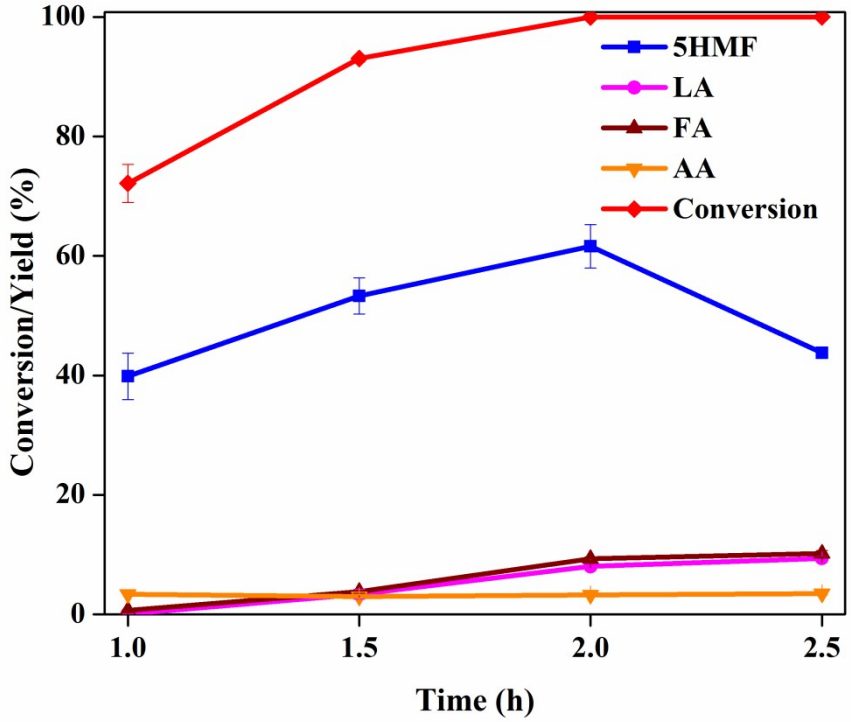

Figure S5: Effect of reaction time on glucose (Reaction conditions: 2 g DI water, 0.2 g substrate, substrate: catalyst ([BMIM]Br/NaY 5.1) = 3:1 w/w, reaction phase: extractive phase = 1:2 w/w, 0.6 g NaCl, and 180°C reaction temperature).

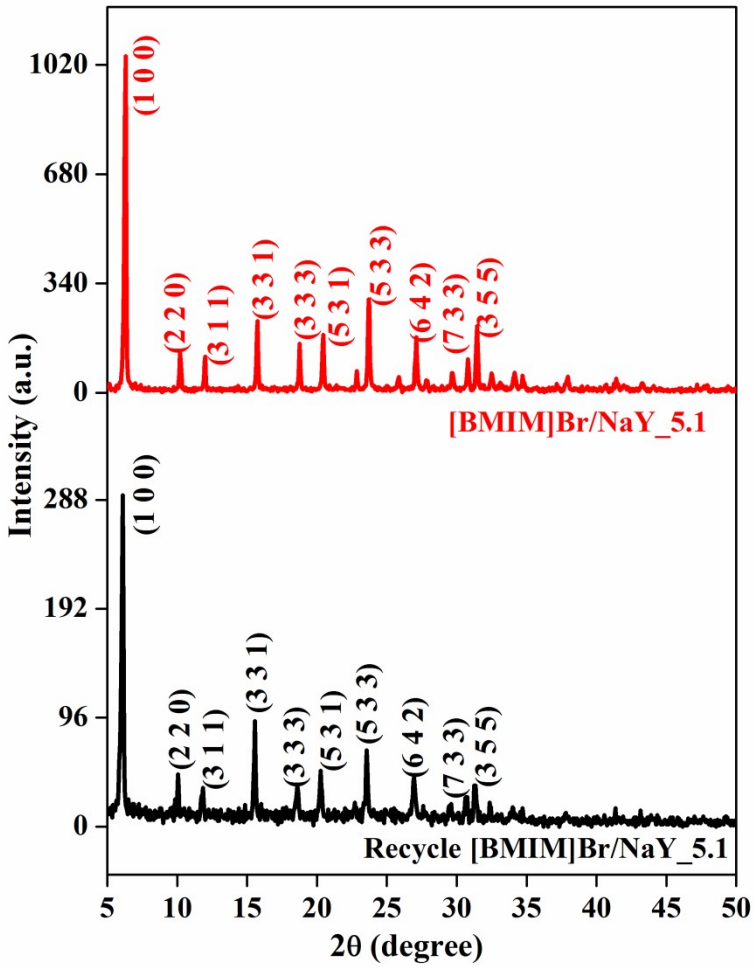

Figure S6: The powder XRD patterns of fresh and recycled [BMIM]Br/NaY_5.1.

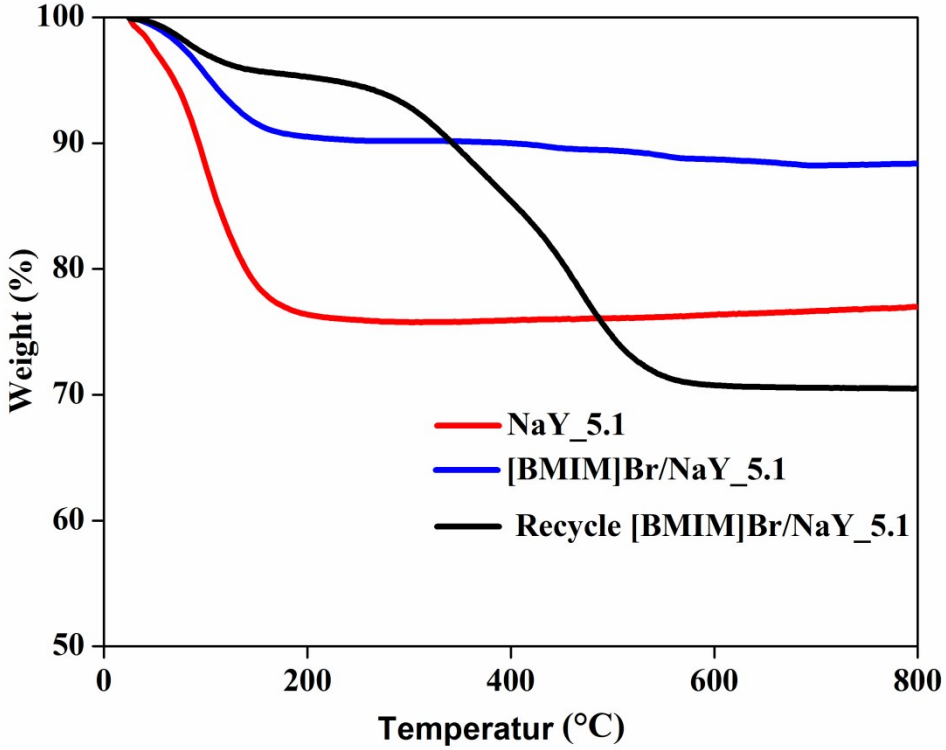

Figure S7: The TGA profiles of NaY_5.1, [BMIM]Br/NaY_5.1 and recycled [BMIM]Br/NaY_5.1.

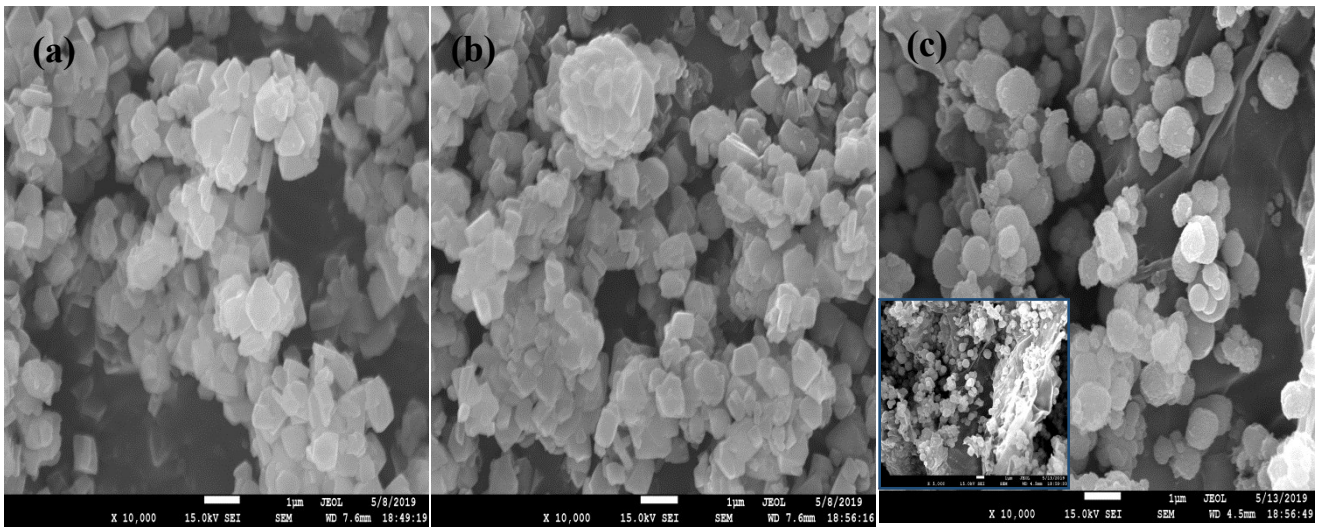

Figure S8: The FESEM images of (a) NaY_5.1, (b) [BMIM]Br/NaY_5.1 and (c) recycled [BMIM]Br/NaY_5.1.

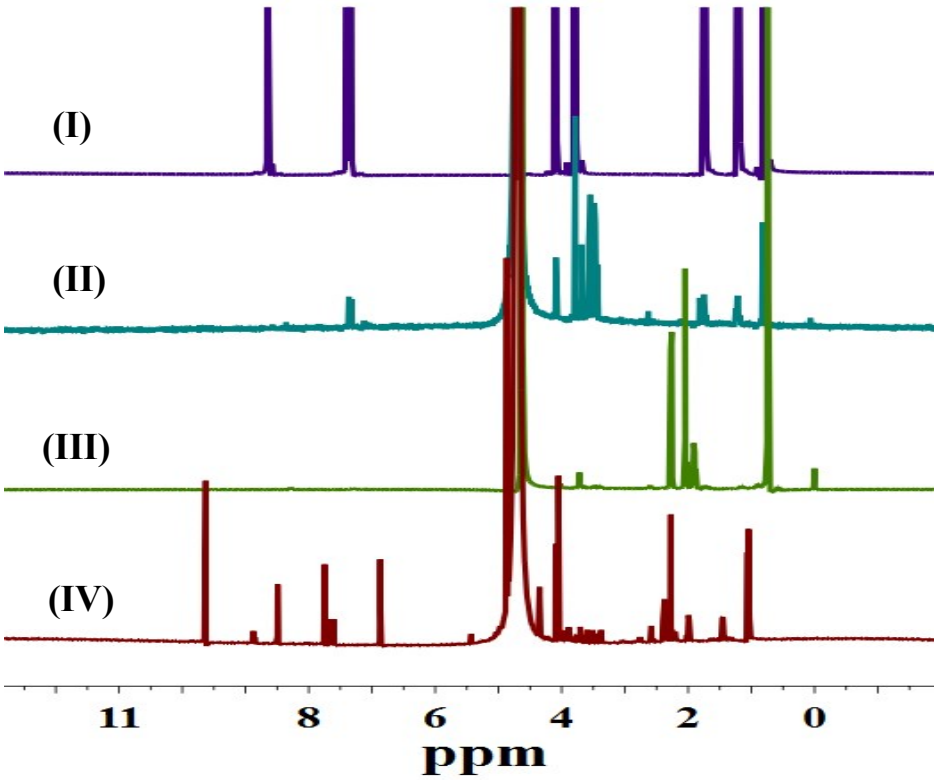

Figure S9: ^{1}H NMR spectra for (I) pure [BMIM]Br, (II) [BMIM]Br/NaY_5.1+D_2O suspension before exposing to reaction conditions (room temperature) and filtration (leaching test) (III) [BMIM]Br/NaY_5.1+D_2O suspension after exposing to reaction conditions (180 °C and 3 h) and filtration (leaching test) and (IV) [BMIM]Br/NaY_5.1+cellulose+NaCl+D_2O suspension after exposing to reaction conditions (180 °C and 3 h) and filtration.