An imidazole–based DES Serving as a "Courier" for the Efficient Coupling of HCl Capture and Conversion under Mild Conditions

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Keywords: Deep eutectic solvent (DES); Courier; HCl; Mechanism; Capture and Conversion

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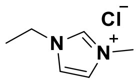
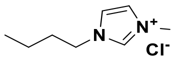
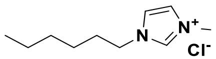
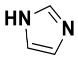
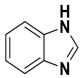
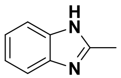
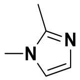
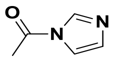
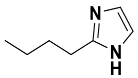
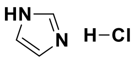
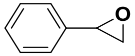
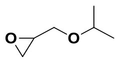
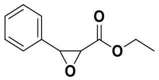
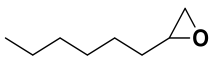
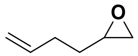
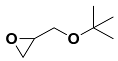
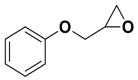
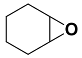
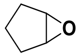
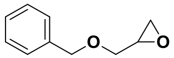
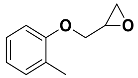
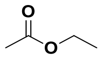
Table S1.

Specifications and sources of chemicals used in this work.

Molecular structure	Chemical name	Abbr. or (number)	CAS number	MW. (g/mol)	Purity (%)	Source
	1–Ethyl–3–methylimidazolium chloride	EmimCl	65039–09–0	146.62	0.98	Macklin
	1–Butyl–3–methylimidazolium chloride	BmimCl	79917–90–1	174.67	0.99	Adamas
	1–Hexyl–3–methylimidazolium chloride	HmimCl	171058–17–6	202.72	0.99	Adamas
	Imidazole	Im	288–32–4	68.08	0.99	Macklin
	1H–benzimidazole	BIm	51–17–2	118.14	0.99	Adamas
	2–Methylbenzimidazole	MeBIm	615–15–6	132.16	0.98	Adamas
	1, 2–Dimethylimidazole	DMIm	1739–84–0	96.13	0.98	Adamas

	1–Acetylimidazole	AceIm	2466–76–4	110.11	0.99	Adamas
	2–Buthylimidazole	BuIm	50790–93–7	124.18	0.98	Adamas
	1H–imidazole hydrochloride	Im–HCl	1467–16–9	104.54	0.99	Macklin
	Styrene oxide	1a	96–09–3	120.15	0.98	Adamas
	Glycidyl isopropyl ether	2a	4016–14–2	116.16	0.96	Aladdin
	Ethyl 3–phenylglycidate	3a	121–39–1	192.21	0.90	Macklin
	2–hexyl–oxirane	4a	2984–50–1	128.21	0.97	Adamas
	1,2–Epoxy–5–hexene	5a	10353–53–4	98.14	0.96	Aladdin
	Tert–butyl glycidyl ether	6a	7665–72–7	130.19	0.96	Aladdin
	Glycidyl phenyl ether	7a	122–60–1	150.17	0.98	Macklin

	Cyclohexene oxide	8a	286–20–4	98.14	0.98	Aladdin
	Cyclopentene oxide	9a	285–67–6	84.12	0.98	Adamas
	Benzyl glycidyl ether	10a	89616–40–0	164.20	0.97	Macklin
	o–Cresyl glycidyl ether	11a	2210–79–9	164.20	0.90	Aladdin
	Ethyl acetate	EA	141–78–6	88.11	99	Adamas
–	Petroleum ether	PE	–	–	Boiling range 60–90 °C	Adamas

Pure HCl and the mixed HCl gas were supplied from Nanjing Special Gas Co., Ltd and Shandong Kanbao Co., Ltd., respectively.

Table S2

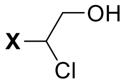
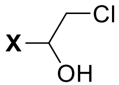
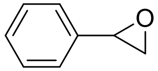
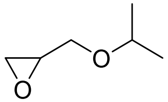
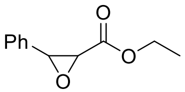
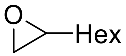
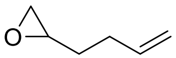
Comparison of absorption solubility of HCl in different absorbents at 30 °C and 1.0 bar.

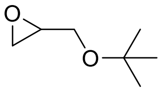
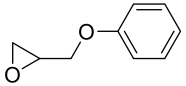
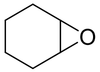
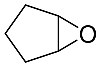
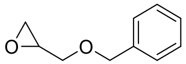
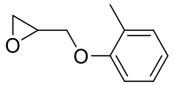
Entry	Absorbent	Molar ratio (mol/mol)	Mass ratio (g/g)	Mole fraction (%)	Reference
1	**EmimCl/Im**	**3.95**	**0.672**	**80**	**This work**
2	[Bmim]Cl [a]	0.68	0.142	40	1
3	[Hmim]Cl [a]	0.69	0.124	41	1
4	[Omim]Cl [a]	0.68	0.108	40	1
5	ImE3 [b]	0.03	0.005	3	2
6	TrizE3 [b]	0.86	0.146	46	2
7	TetzE3 [b]	0.05	0.008	5	2
8	BentrizC4 [b]	1.07	0.220	52	2
9	ChCl–Urea	2.49	0.457	71	3
10	ChCl–Gly	1.61	0.255	62	3
11	ChCl–GA	1.26	0.214	56	3
12	ChCl–EG	1.091	0.395	52	4
13	ChCl–LA	0.90	0.286	47	4
14	ChCl–OA	0.59	0.188	37	4
15	ChCl–MA	0.60	0.179	37	4
16	EmimCl–AA–EG	4.34	0.591	81	5
17	EG	0.72	0.420	42	5
18	EmimCl–EG	2.71	0.476	73	5
19	EmimCl–AA	3.07	0.546	75	5
20	EG–AA	2.71	0.820	73	5
21	Glycerol [c]	0.50	0.199	33	5
22	Tetraglycol [c]	1.40	0.263	58	5
23	PEG–200 [c]	1.42	0.259	59	5

[a] 0.01 bar, [b] 25 C, [c] 40 C

Table S3

Detailed synthesis parameters of all products in this work (isolated yield is in parentheses)

Entry	Molecular structure	Conversion (%)	Purity (%)	 (%)	 (%)	Solvent usage (g)			Solvent consumption (2%, g)	Water consumption (g)	Mass intensity (g/g)	E·factor (g/g)
						EmimCl/Im	EA	PE				
1		99	99	78 (75)	22 (18)	0.1021	45	100	2.9	6	3.1	2.1
2		99	99	10 (9)	90 (87)	0.1063	45	100	2.9	6	3.0	2.0
3		90	99	83 (80)	17(14)	0.1023	45	100	2.9	6	3.4	2.4
4		99	99	27 (23)	73 (69)	0.1033	45	100	2.9	6	3.2	2.2
5		99	99	22 (20)	78 (74)	0.1095	45	100	2.9	6	2.9	1.9

6		99	99	89 (85)	11 (8)	0.1027	45	100	2.9	6	3.1	2.1
7		99	99	-	100 (94)	0.0977	45	100	2.9	6	3.2	2.2
8		99	99	100 (95)	-	0.1095	45	100	2.9	6	2.9	1.9
9		99	99	100 (95)	-	0.1044	45	100	2.9	6	2.8	1.8
10		99	99	-	100 (94)	0.1041	45	100	2.9	6	3.3	2.3
11		99	99	-	100 (95)	0.0994	45	100	2.9	6	3.3	2.3

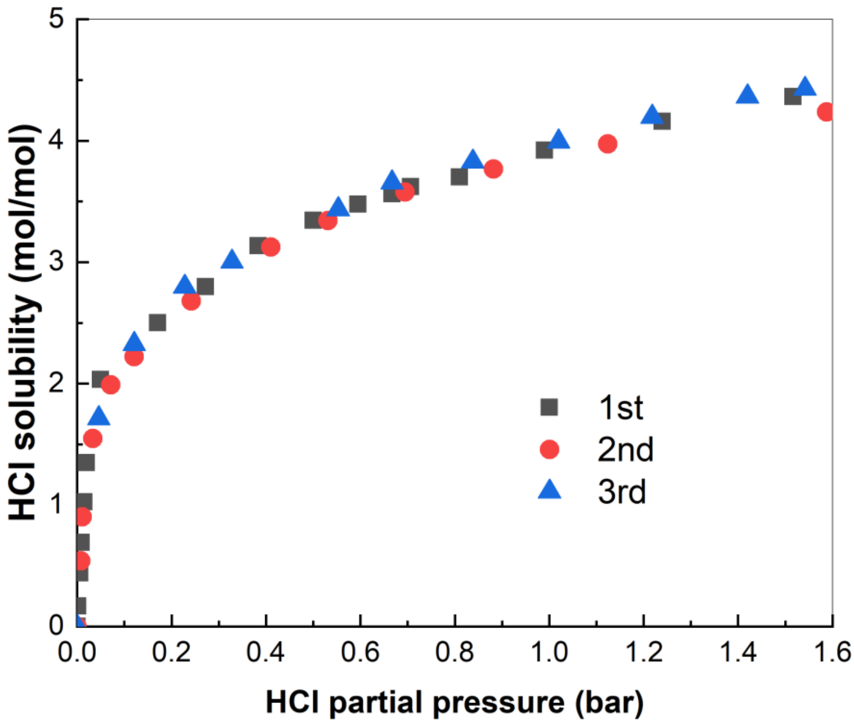


Fig. S1 Three parallel experiments for the independent measurements of HCl solubility.

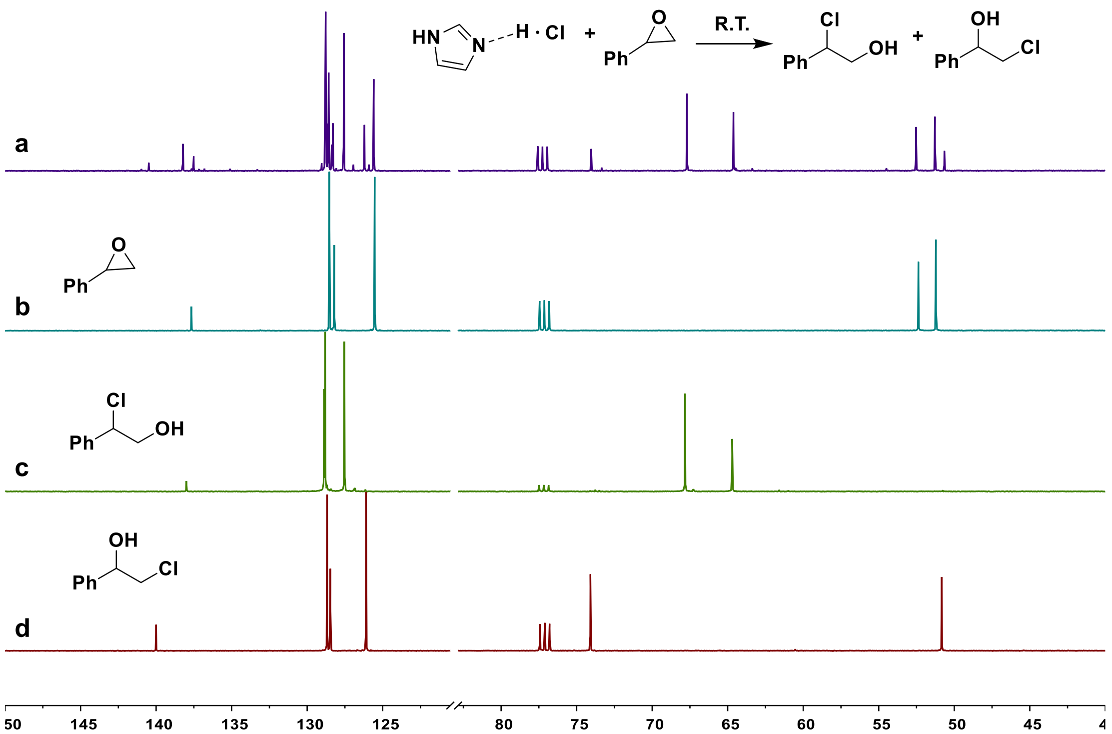


Fig. S2 Comparative experiment of styrene oxide with imidazole hydrochloride as catalyst characterized by ^{13}C NMR

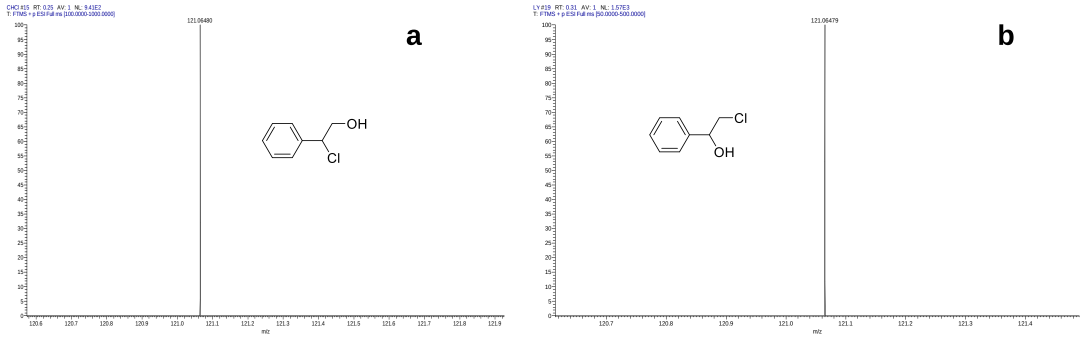


Fig. S3 ESI–MS of 1b (a) and 1c (b) in at *m/z* [M–Cl] $^{+}$.

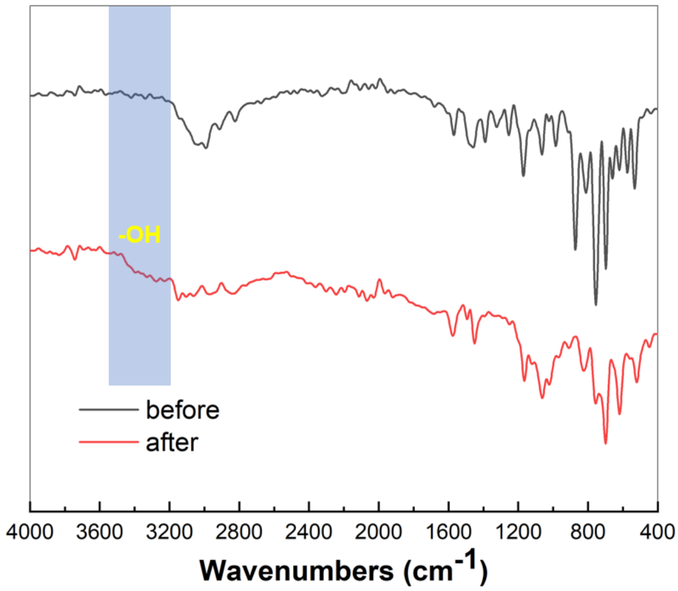


Fig. S4. The infrared spectra before and after the reaction

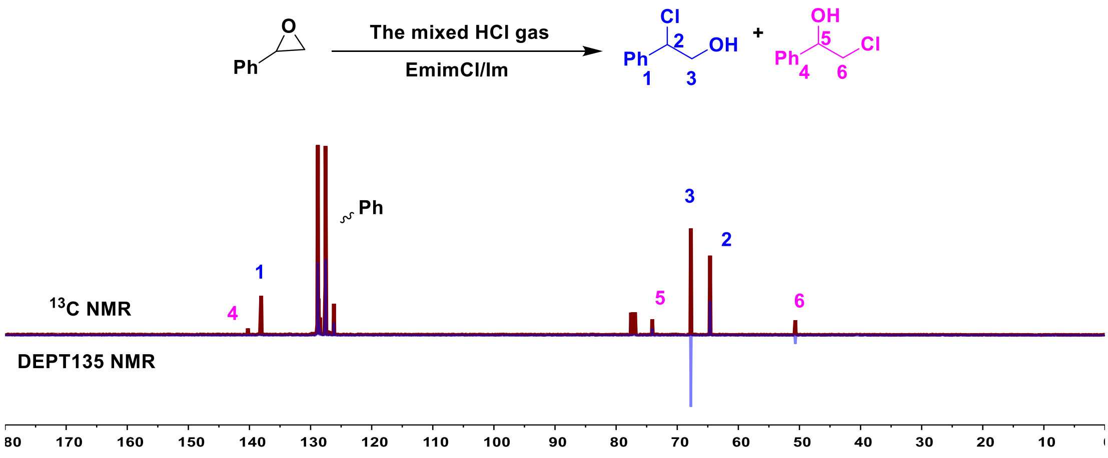


Fig. S5 the ^{13}C NMR detection of mixed HCl–SO_2 gas experiment after the removal of EmimCl/Im by water extraction

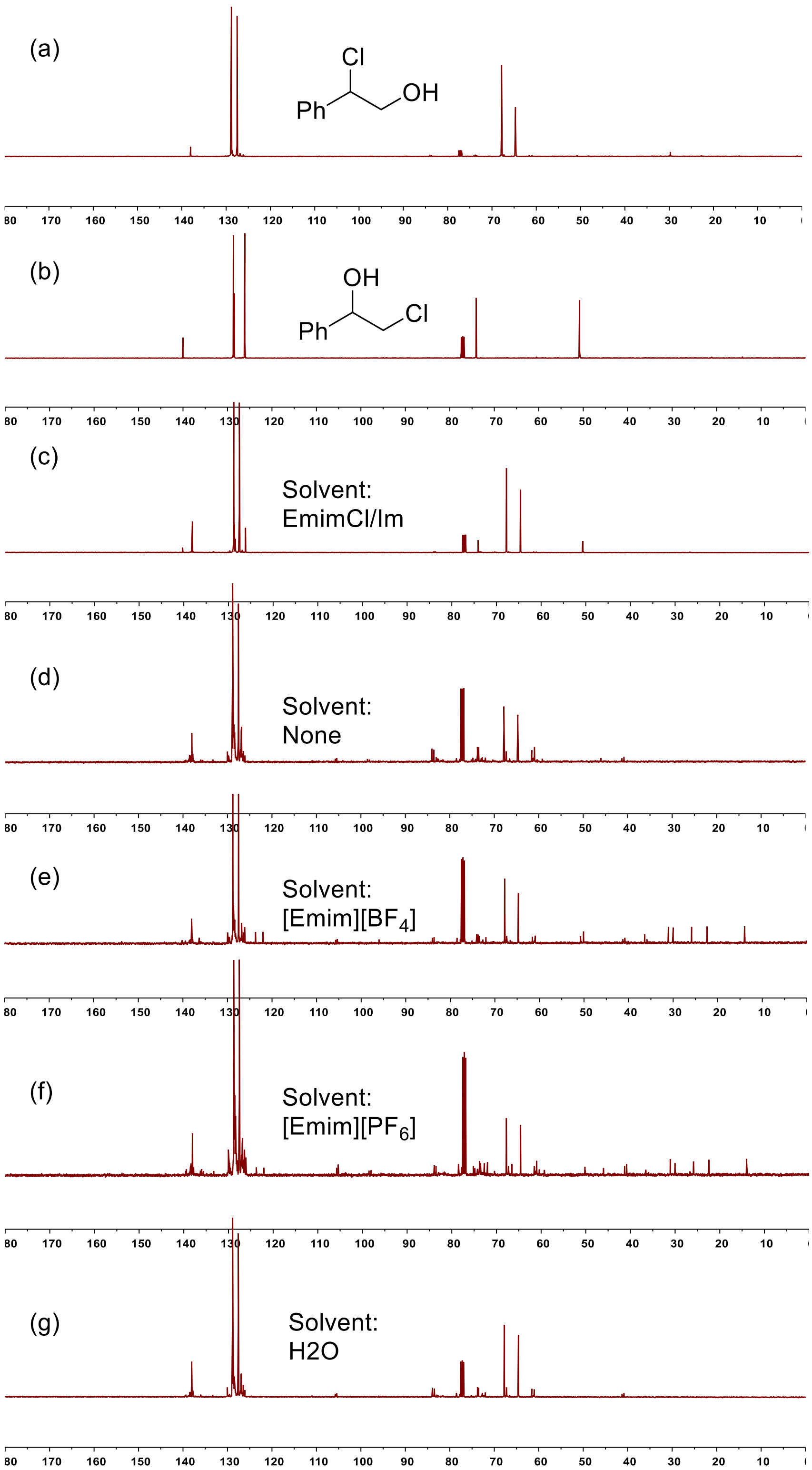


Fig. S6. ^{13}C NMR in different green solvents on HCl conversion.

(a) product 1b, (b) product 1c, (c) solvent EmimCl/Im, (d) solvent-free, (e) solvent [Emim][BF$_4$], (f) solvent [Emim][PF$_4$], and (g) solvent H_2O.

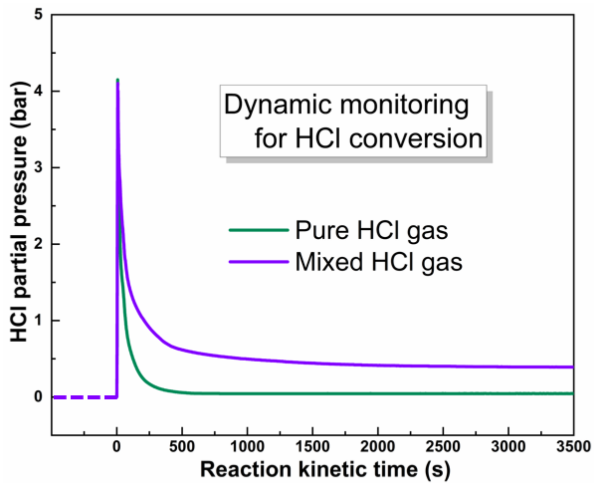


Fig. S7 Pressure–time kinetic curve for dynamic monitoring with different HCl containing gases.

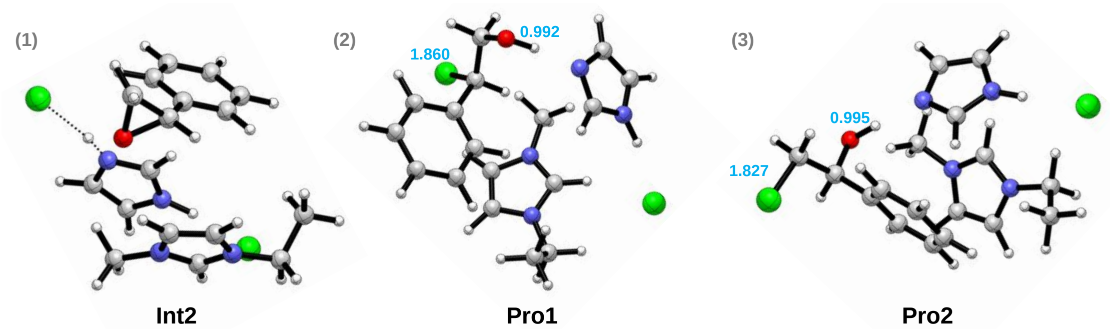


Fig. S8 The optimized structures obtained by the method of B3LYP/6−311G++(d,p) (blue numbers in Å).

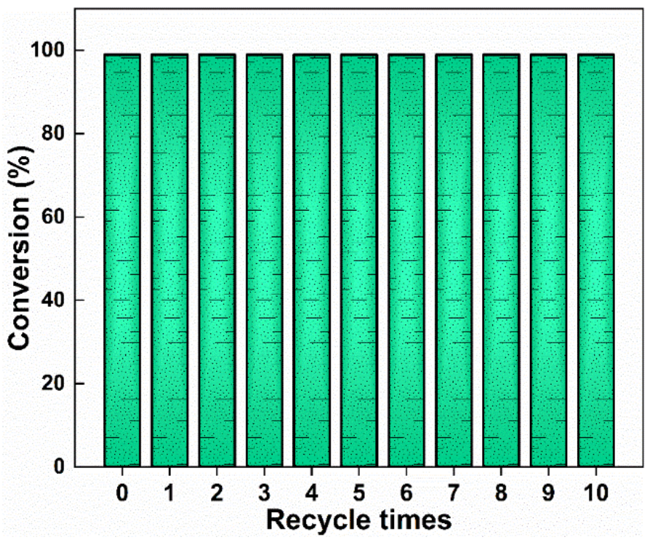


Fig. S9 Cyclic performance with styrene oxide as substrate under equivalent catalyst.

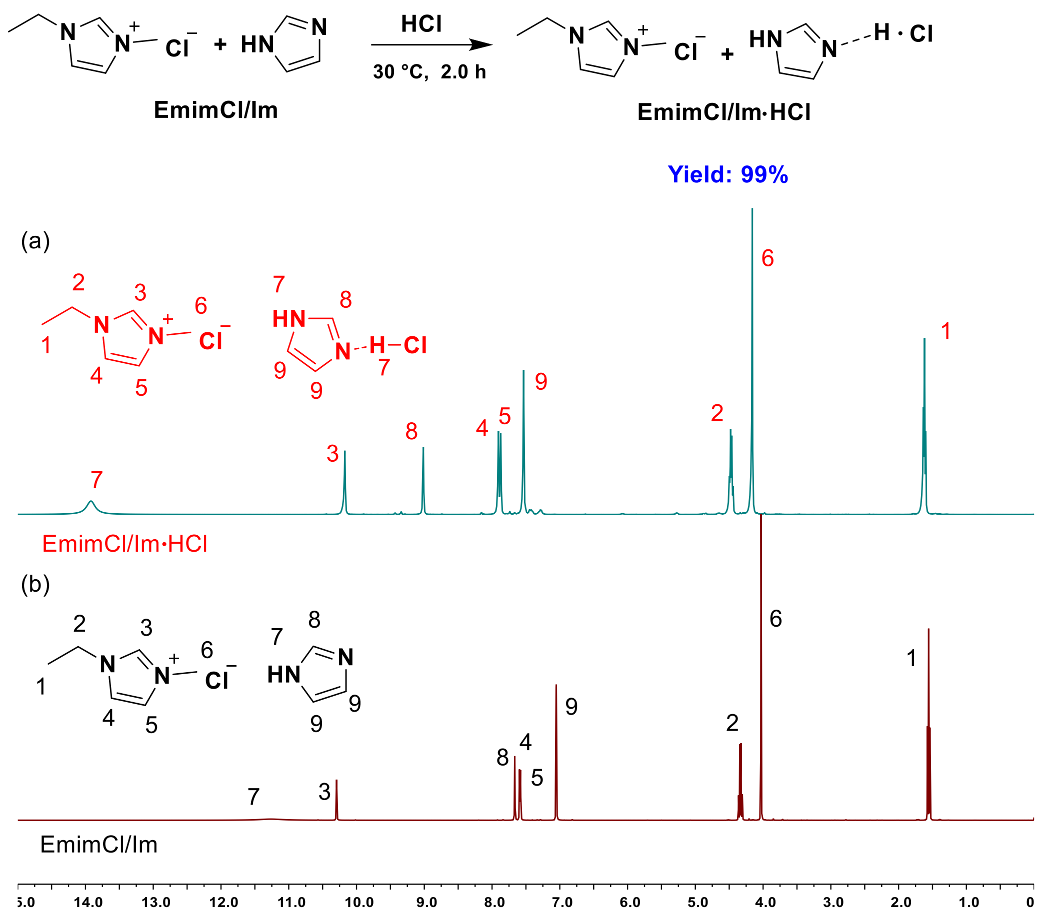


Fig. S10 [1]H NMR of (a) recycled DES and (b) fresh DES.

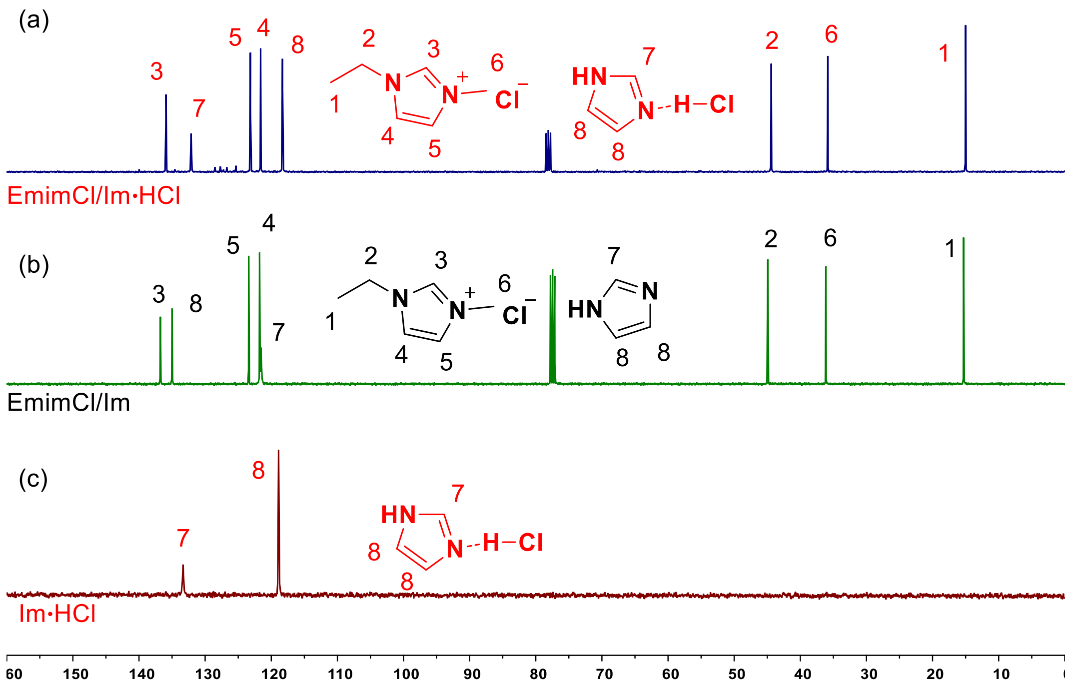


Fig. S11 [13]C NMR of (a) recycled DES, (b) fresh DES, and (c) pure Im·HCl

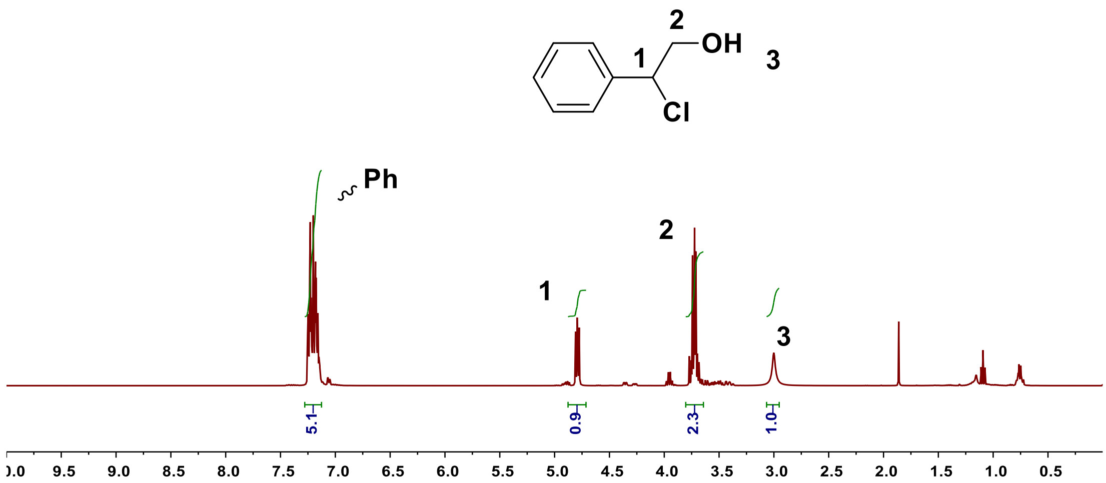


Fig. S12 ^{1}H NMR of 1b.

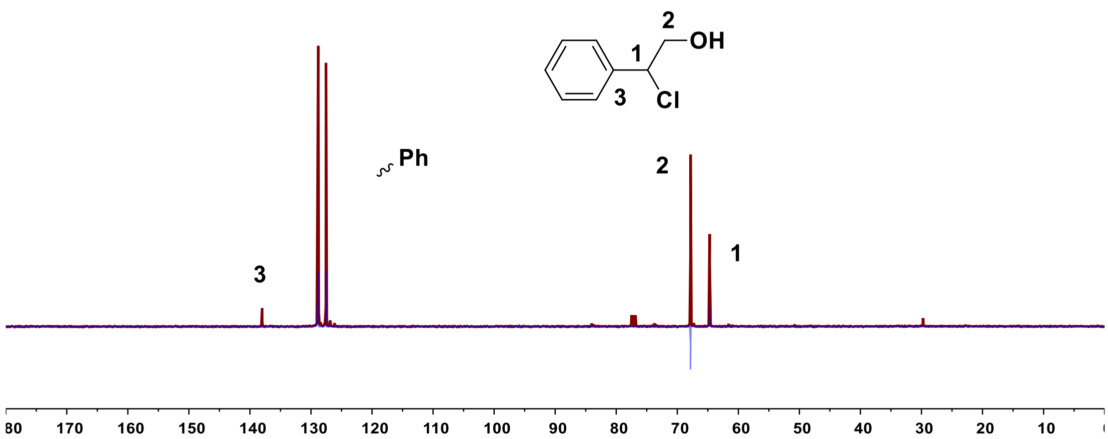


Fig. S13 ^{13}C NMR of 1b.

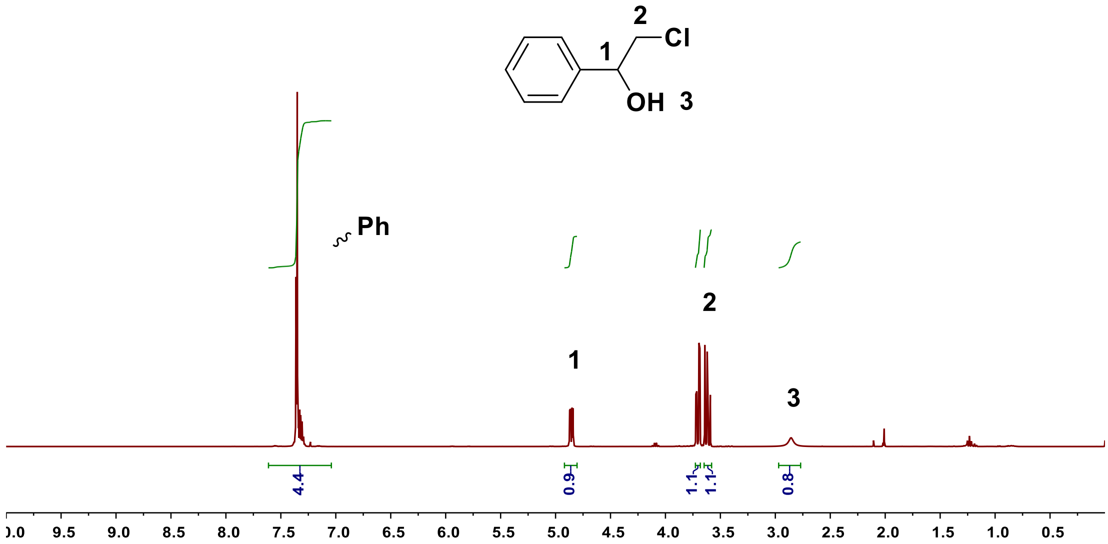


Fig. S14 ^{1}H NMR of 1c.

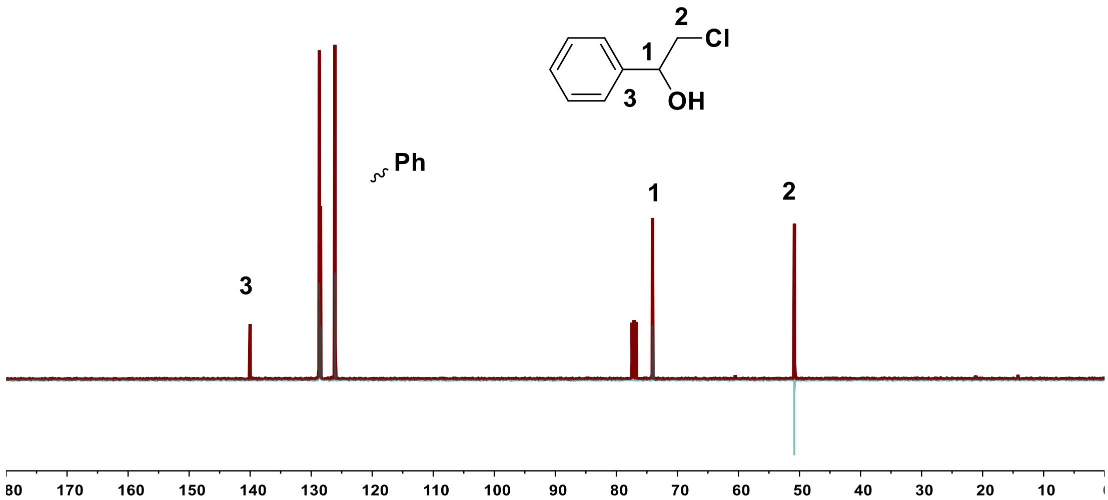


Fig. S15 ^{13}C NMR of 1c.

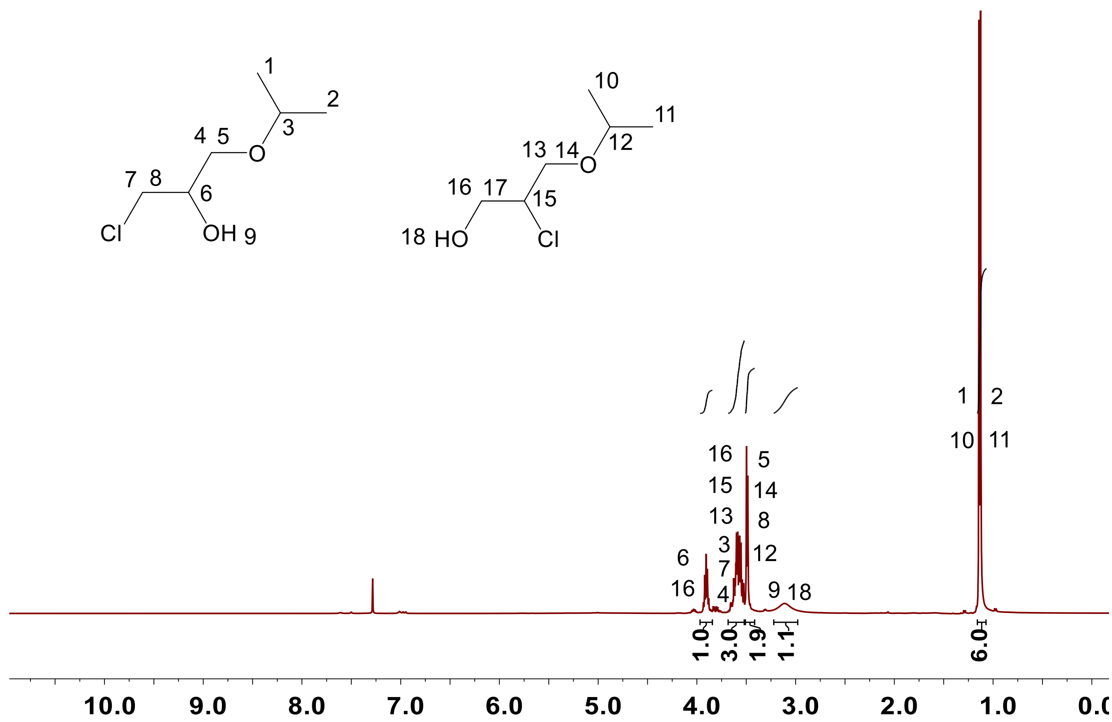


Fig. S16 [1]H NMR of 2b+2c.

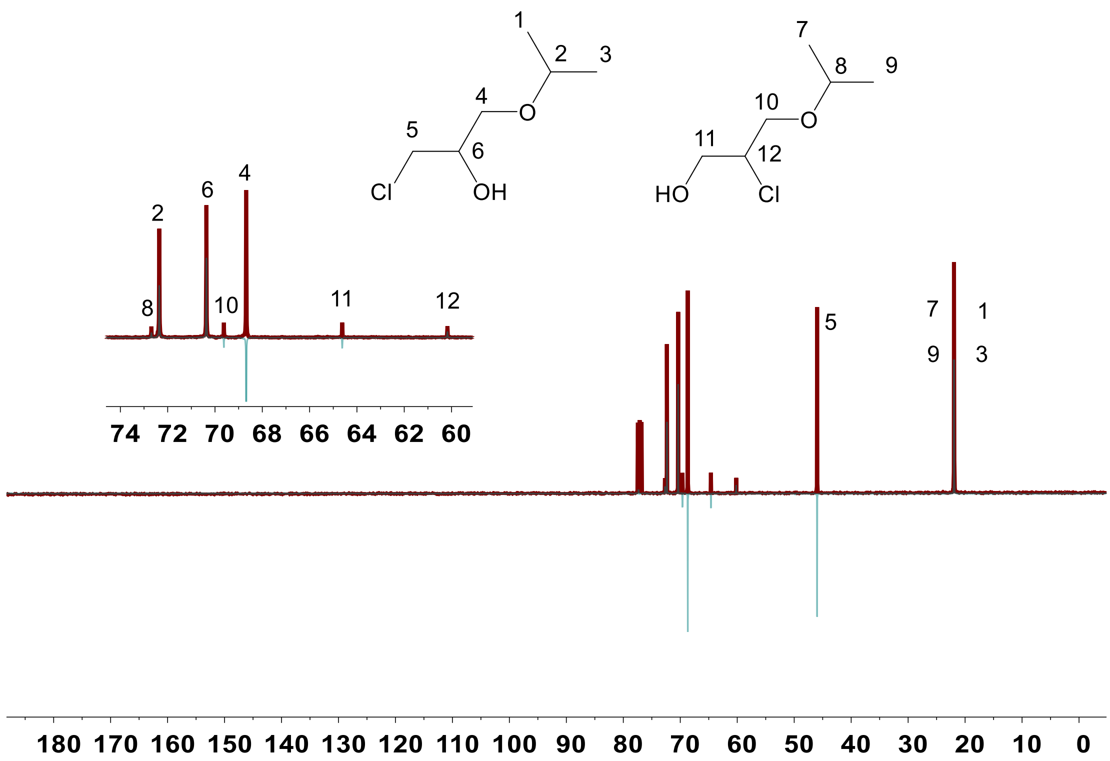


Fig. S17 [13]C NMR of 2b+2c.

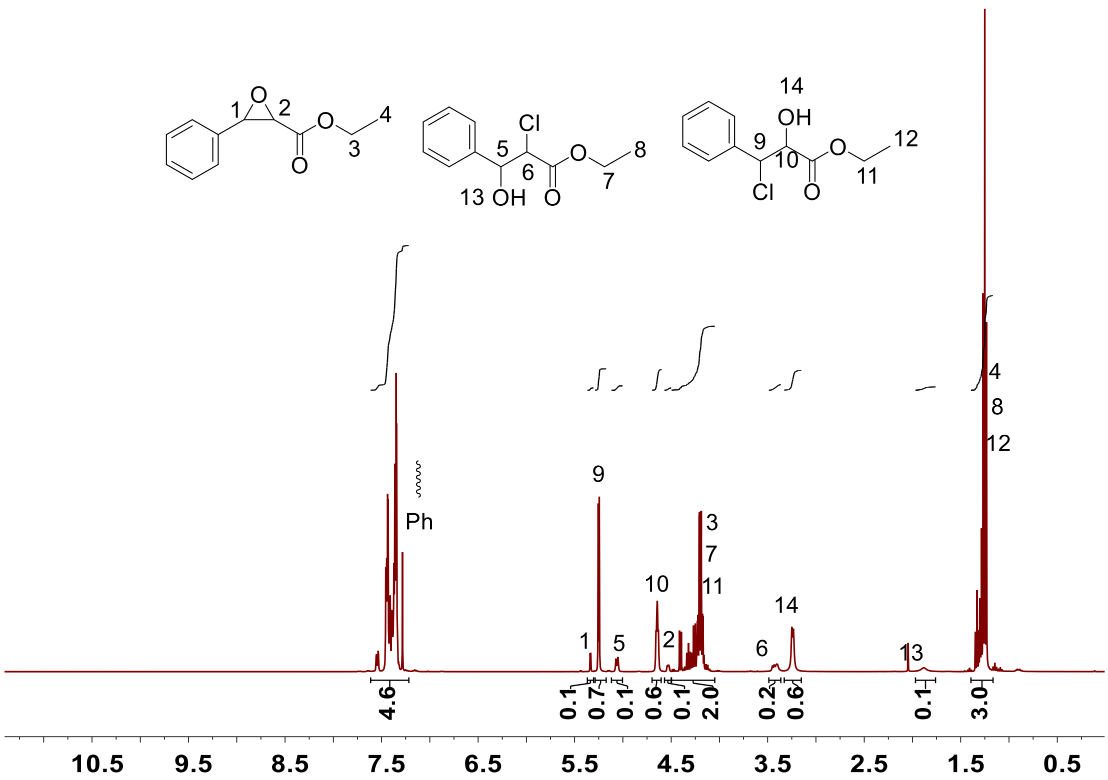


Fig. S18 ^{1}H NMR of 3a+3b+3c.

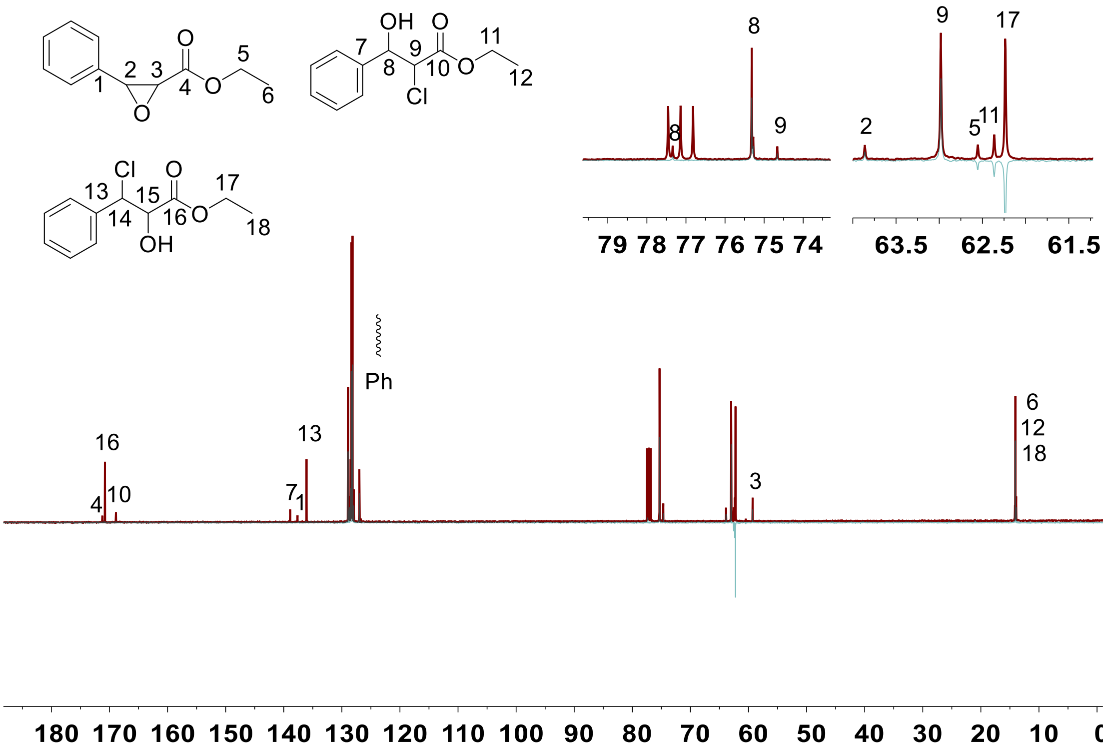


Fig. S19 ^{13}C NMR of 3a+3b+3c.

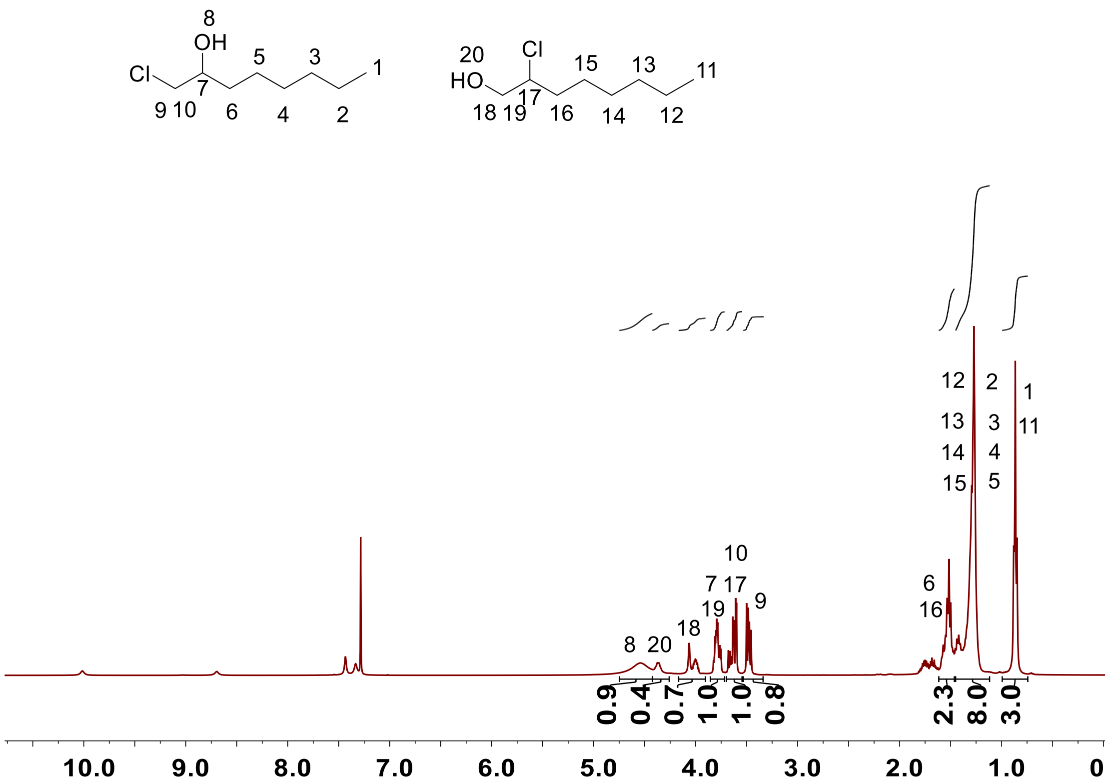


Fig. S20 ^{1}H NMR of 4b+4c.

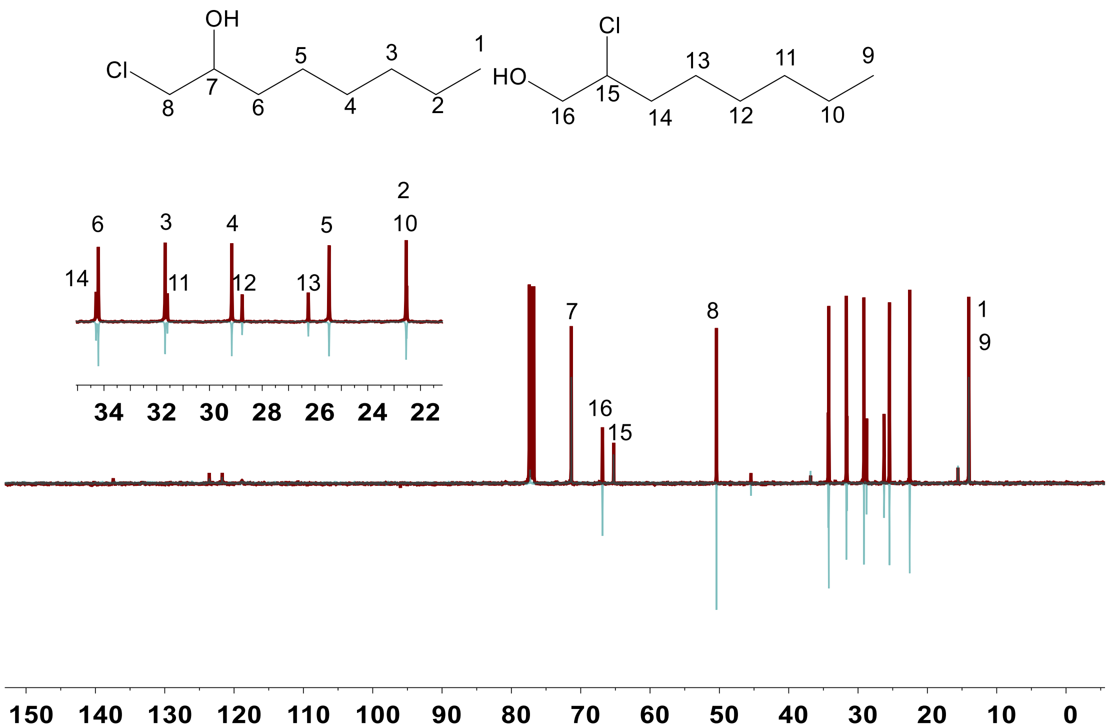


Fig. S21 ^{13}C NMR of 4b+4c.

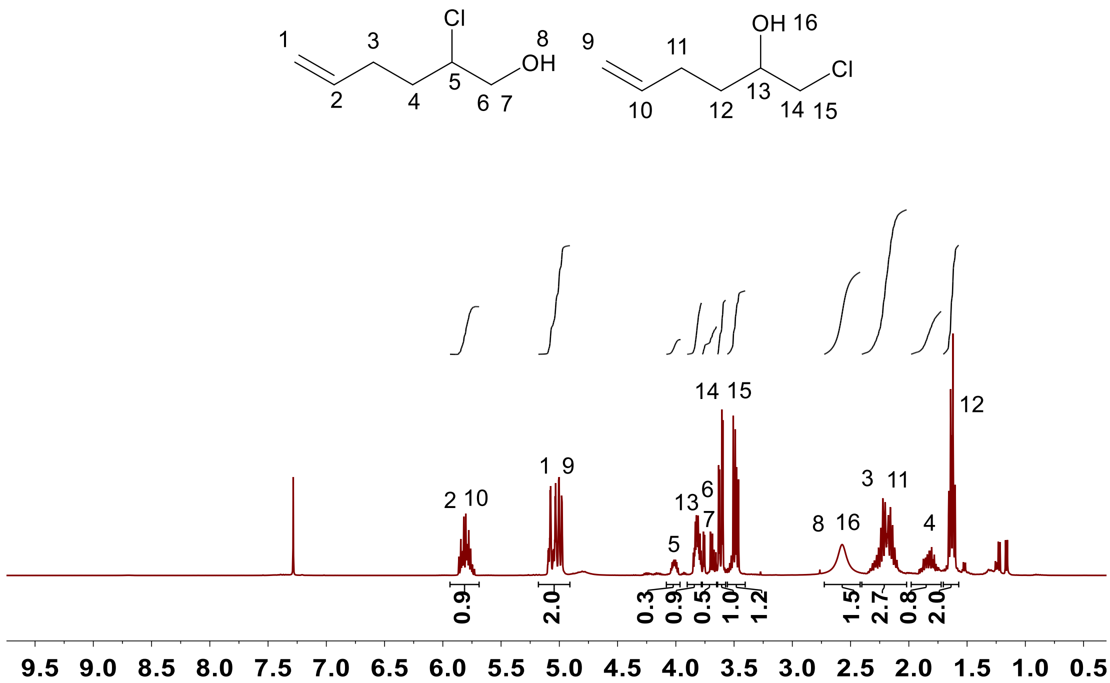


Fig. S22 ^{1}H NMR of 5b+5c.

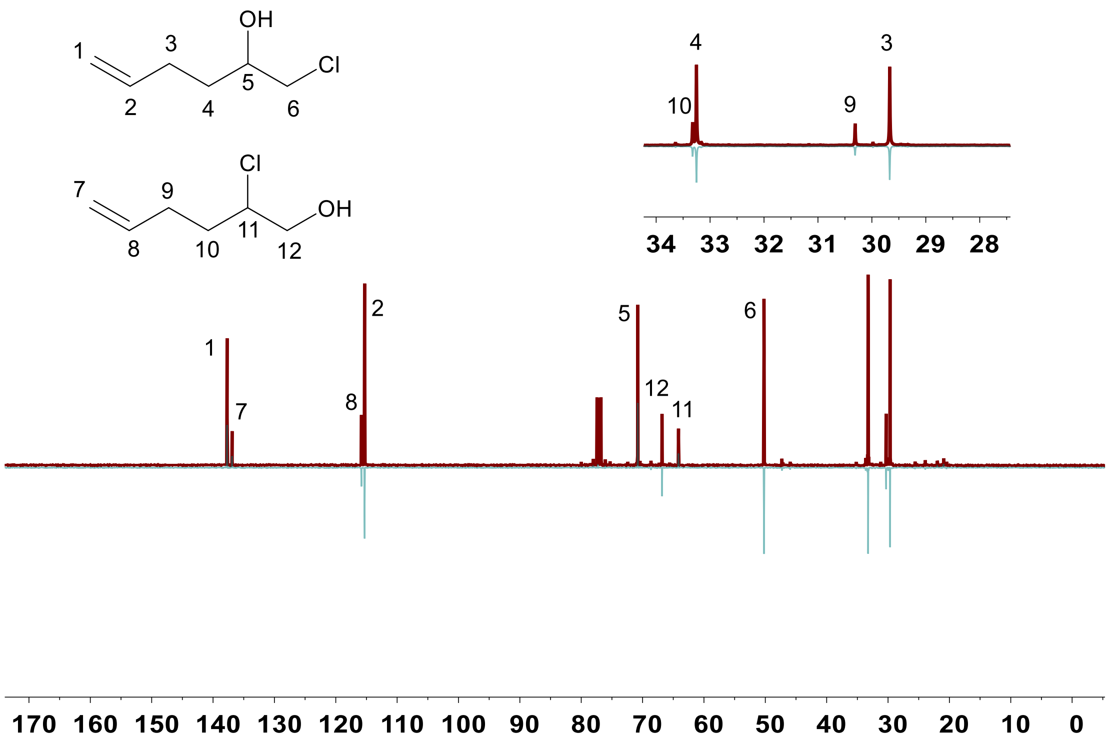


Fig. S23 ^{13}C NMR of 5b+5c.

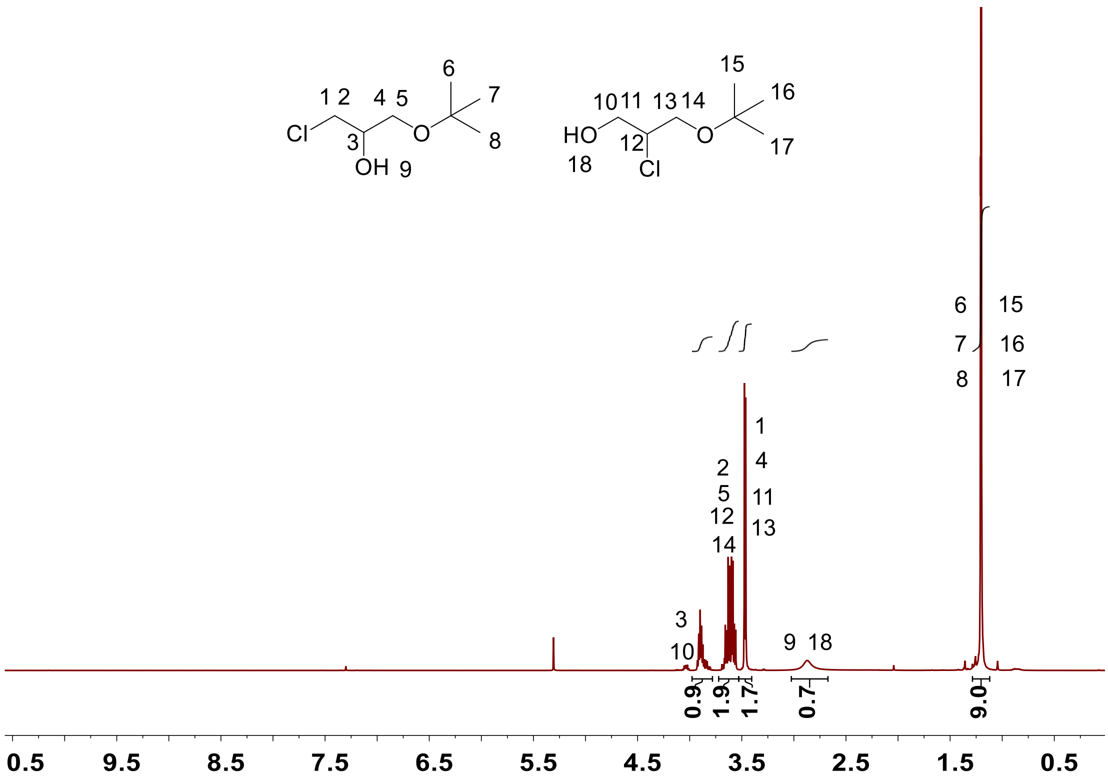


Fig. S24 [1]H NMR of 6b+6c.

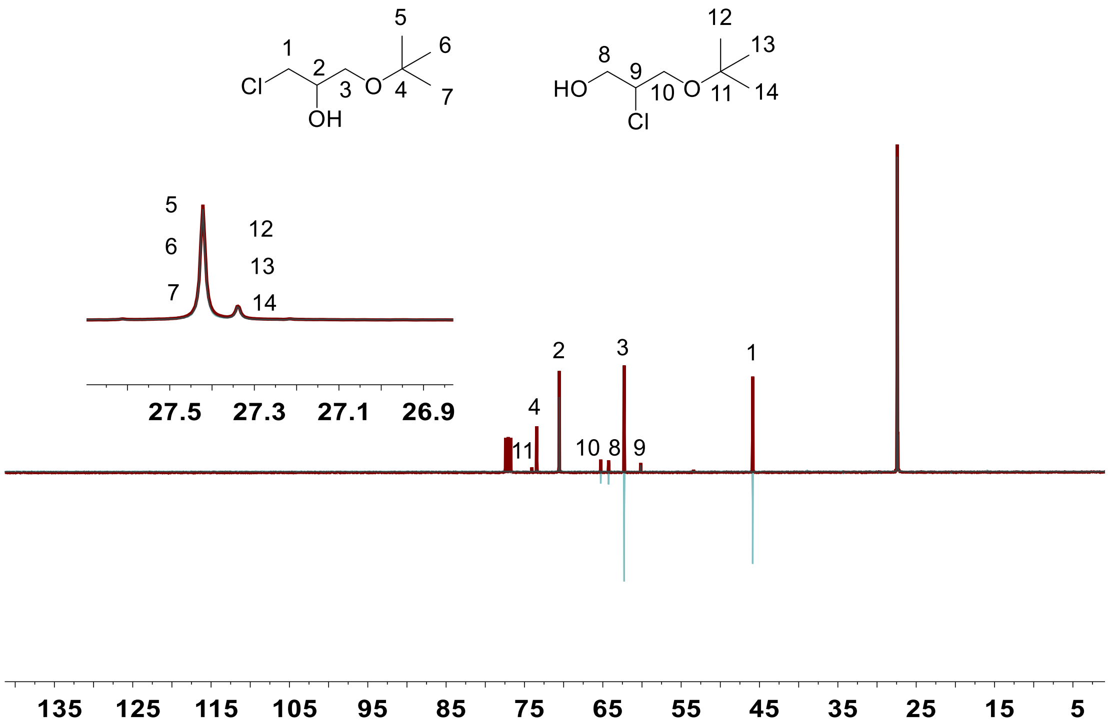


Fig. S25 [13]C NMR of 6b+6c.

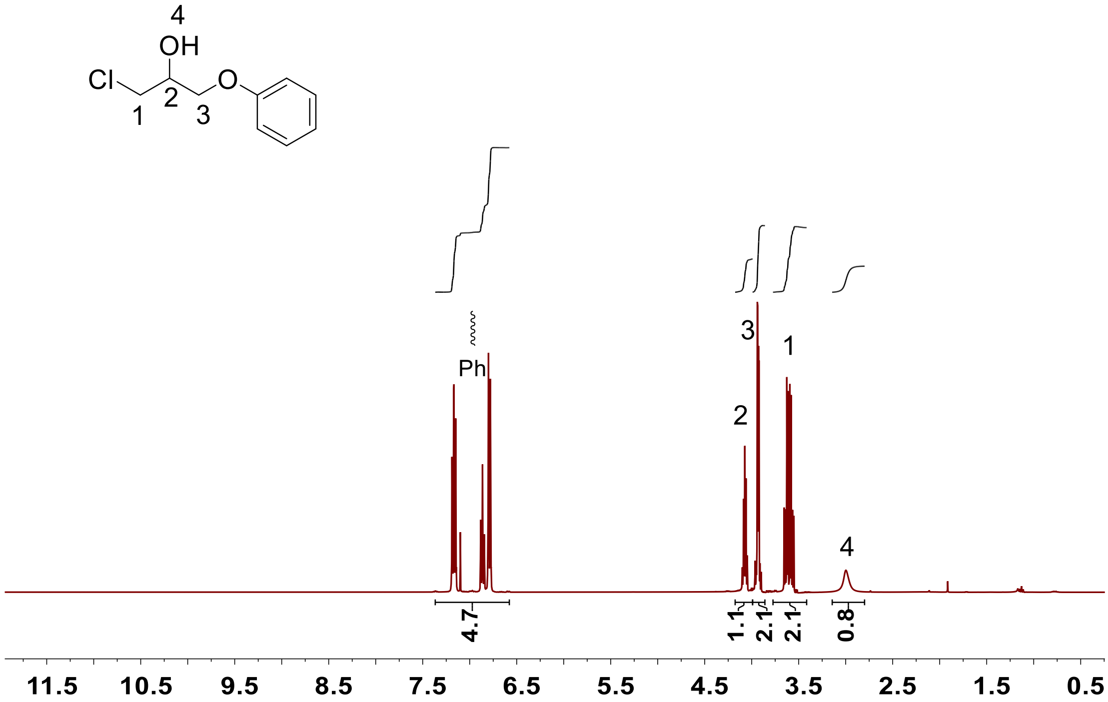


Fig. S26 [1]H NMR of 7b.

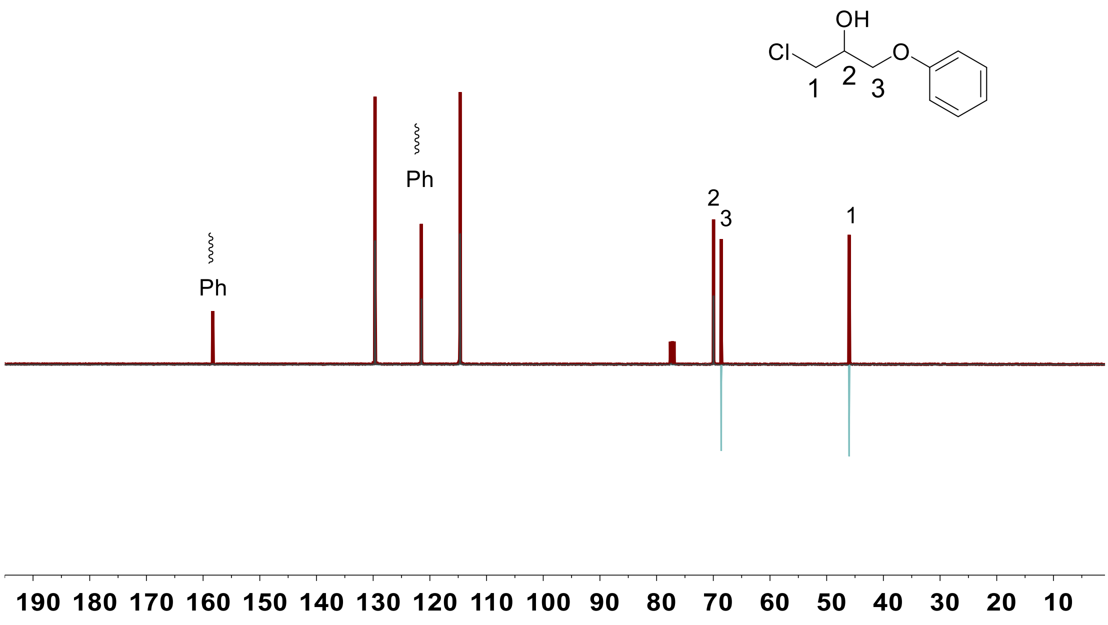


Fig. S27 [13]C NMR of 7b.

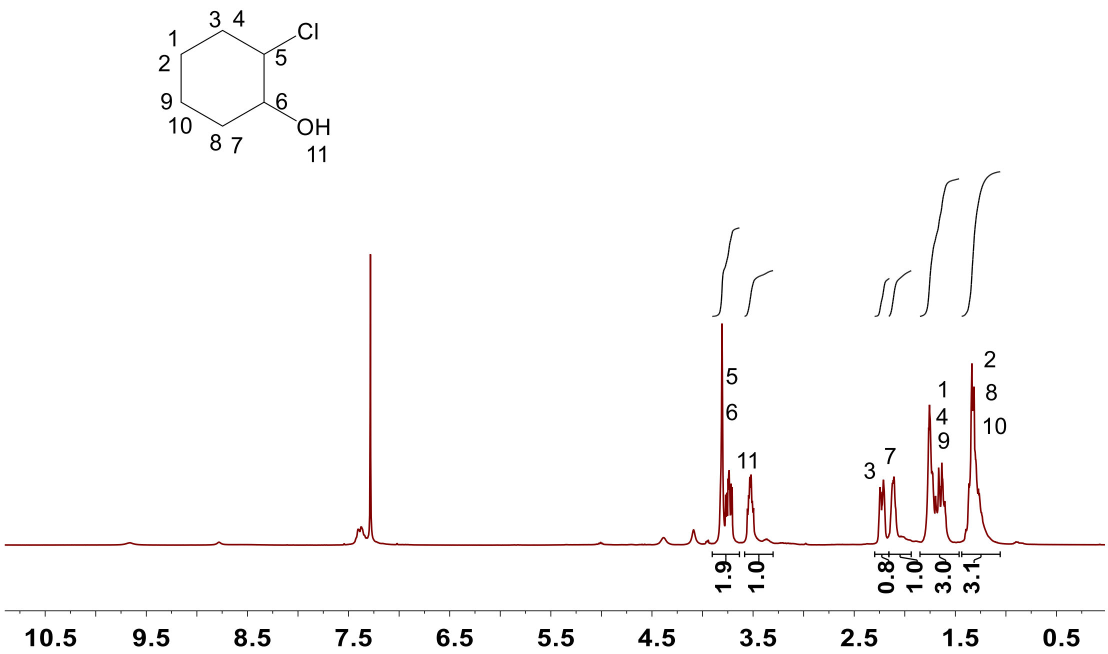


Fig. S28 ^{1}H NMR of 8b.

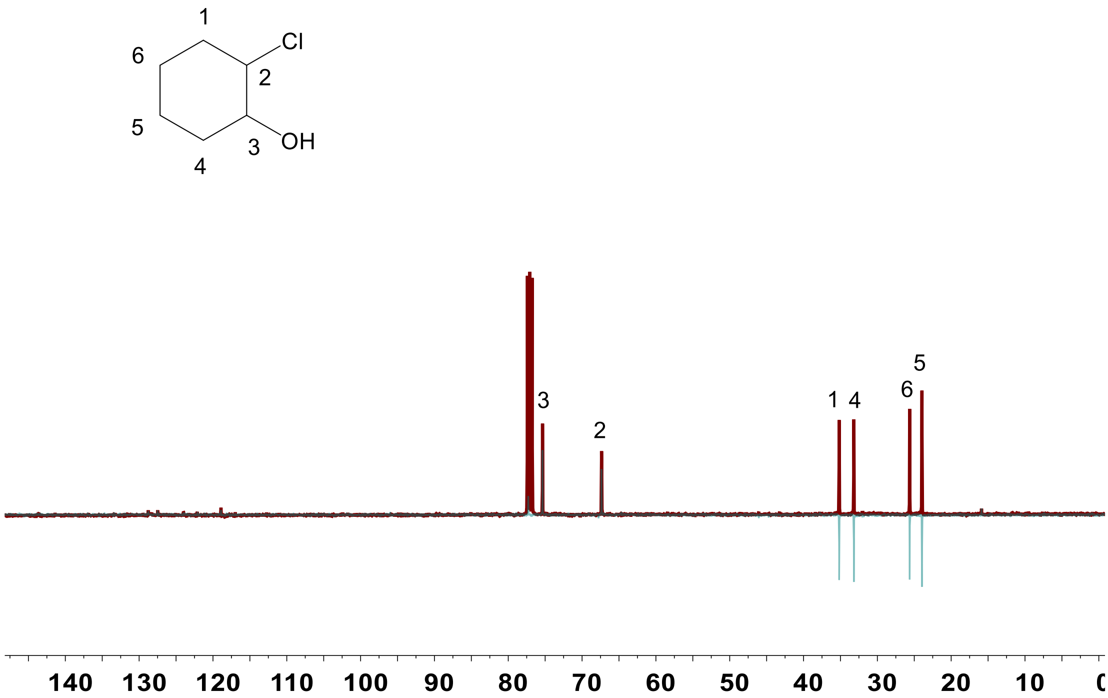


Fig. S29 ^{13}C NMR of 8b.

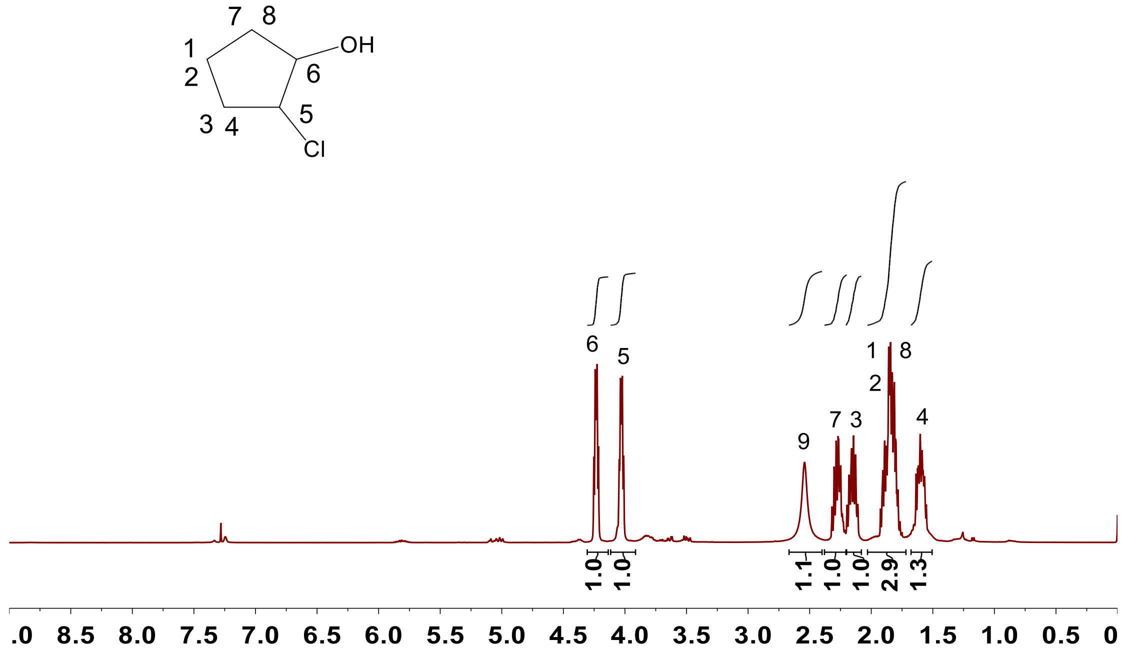


Fig. S30 ^{1}H NMR of 9b.

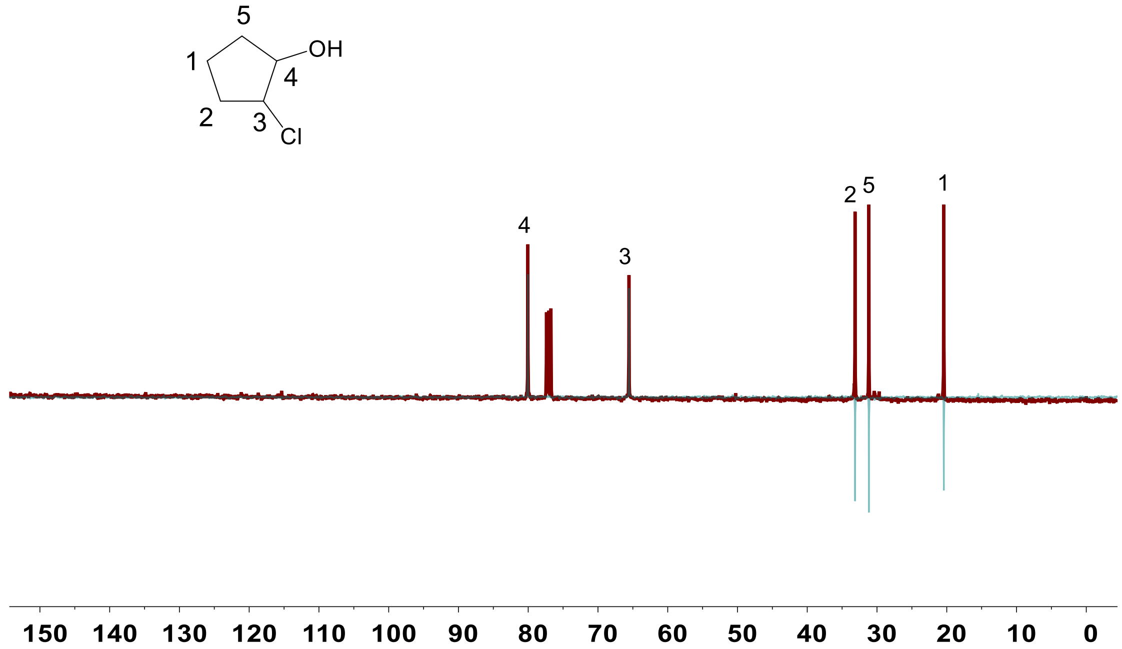


Fig. S31 ^{13}C NMR of 9b.

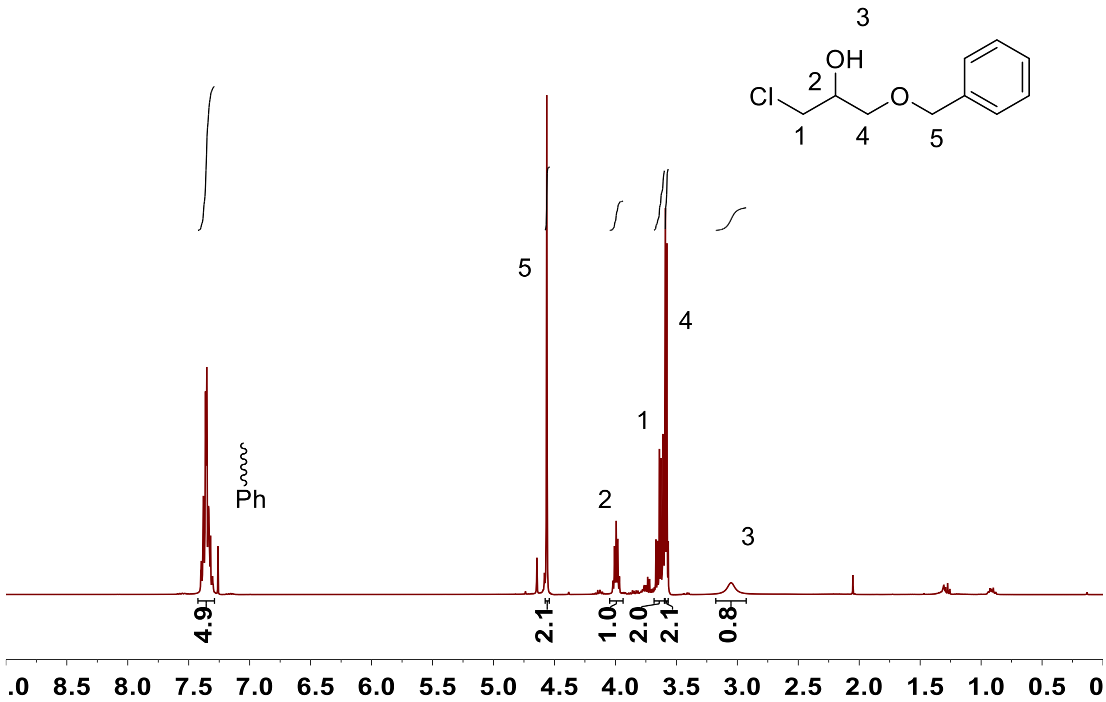


Fig. S32 ^{1}H NMR of 10b.

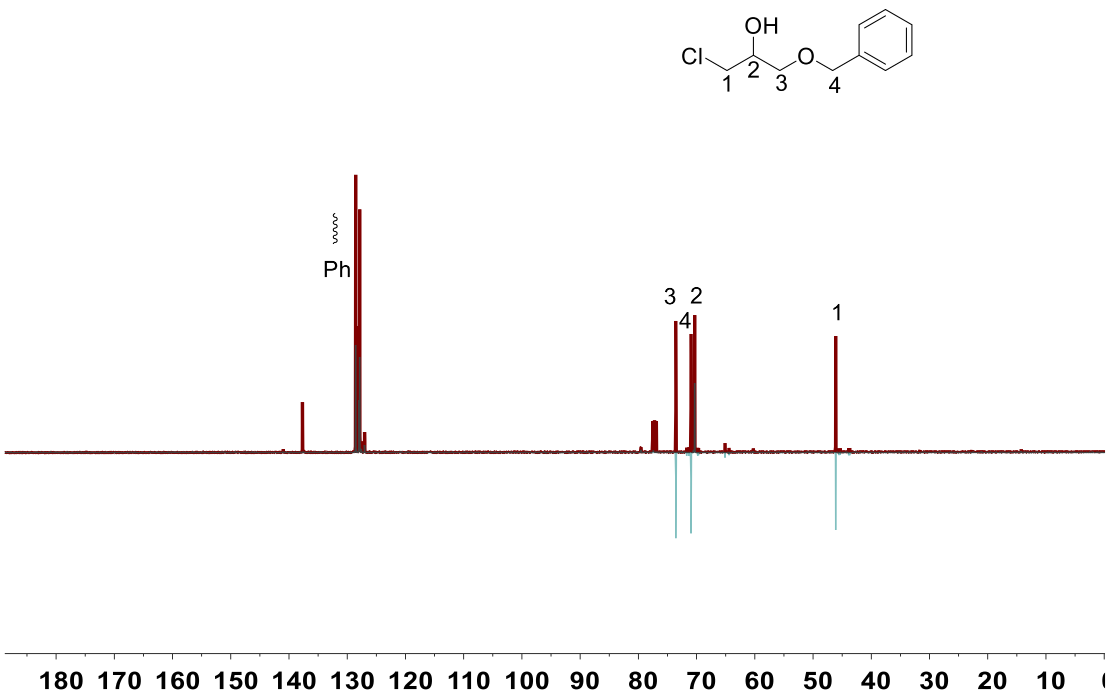


Fig. S33 ^{13}C NMR of 10b.

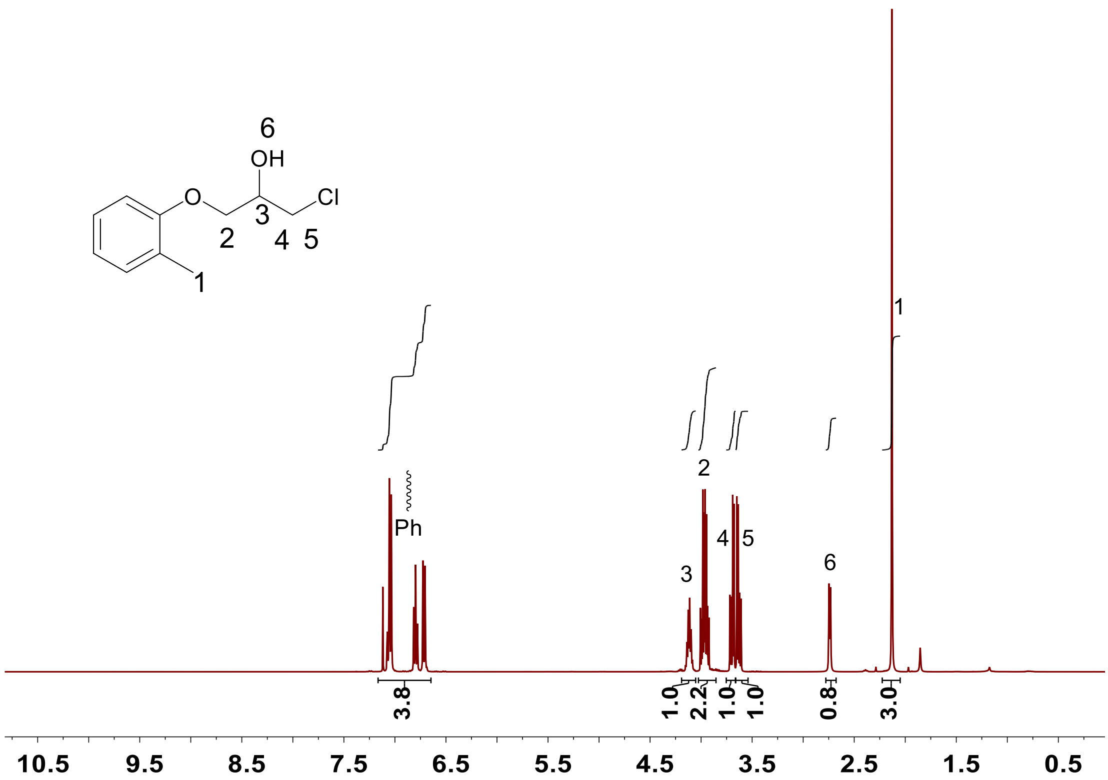


Fig. S34 ^{1}H NMR of 11b.

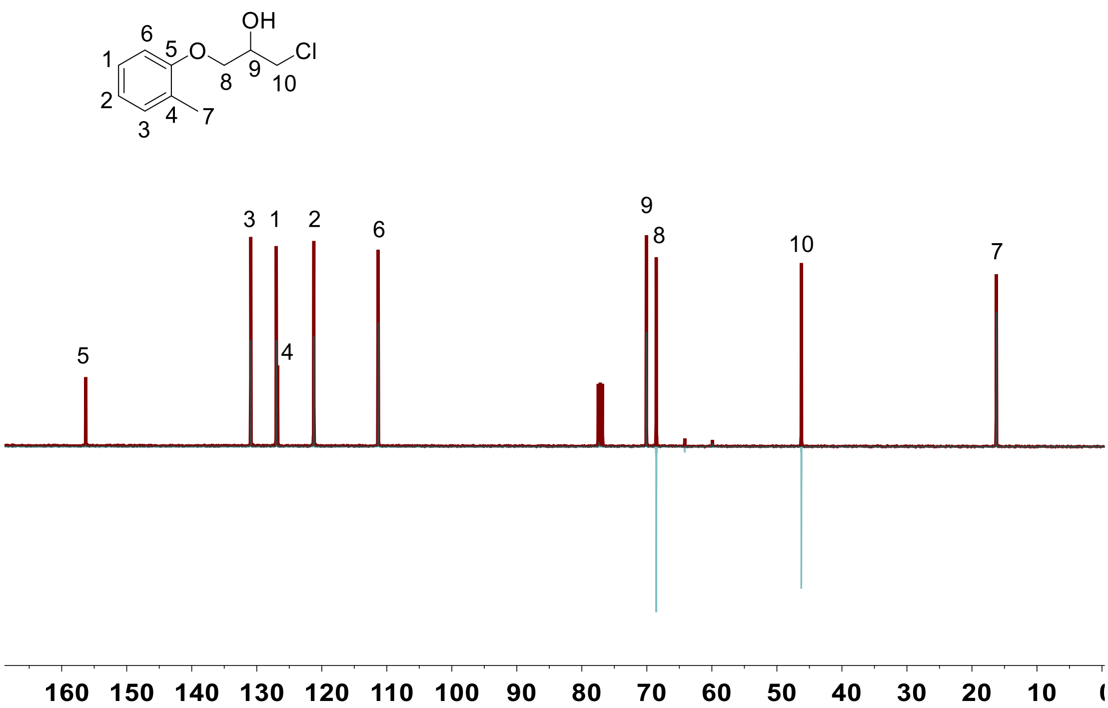


Fig. S35 ^{13}C NMR of 11b.

Determination of HCl Absorption

The whole absorption device consists of a water bath, two pressure sensors and two glass chambers whose volumes 190.45 cm^3 (V_1) and 41.81 cm^3 (V_2), respectively. The larger chamber is used to store the HCl, and the smaller chamber is equipped with a magnetic stirrer where the absorption reaction takes place. The temperature of the two chambers is controlled by a water bath with an accuracy of ±0.1K, and the pressure of the two chambers is monitored online by two pressure sensors with an error of ±0.2%. In a typical run, a known mass (ω) of DES was placed into the smaller chamber. Then the air in the two chambers was drained by a pump (<10Pa). the needle valves in the two chambers are closed, HCl was fed into the larger chamber, the pressure is recorded as P_1 and the small chamber was recorded to be P_0. The needle valve between the two chambers was turned on to let HCl enter from the large chamber to the small chamber. The sign of absorption balance is that the pressure of the two chambers does not change for at least 2 hours. The pressure of the large chamber was denoted as P_1', and P_2 for the small chamber. The partial pressure of HCl in the small chamber was $P_S=P_2–P_0$, and the absorption amount of HCl was calculated as follows.

$$n\ (P_s)= \rho_g(P_1,T)V_1 - \rho_g(P_1', T)\ V_1 - \rho_g(P_s,T)(V_2 - \omega/\rho_{IL})$$

Where ρ_g (P_i, T) represents the density of HCl in mol/cm^3 at P_i (i=1, S) and ρ_{IL} is the density of the DES in g/cm^3 at T. V_1 and V_2 represent the volumes in cm^3 of the two chambers. More HCl is then injected into the small chamber to achieve a new equilibrium and to measure solubility at different pressures.

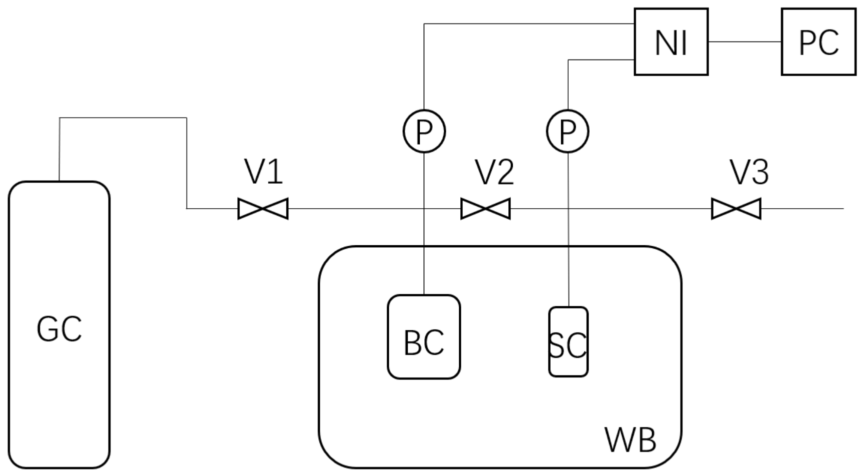


Fig. S36. The illustration of HCl solubility unit.

GC, gas cylinder; BC, big chamber; SC, small chamber; V1, V2, V3, valves; P, pressure transducer; NI, numerical instrument; PC, personal computer; WB: Water bath.

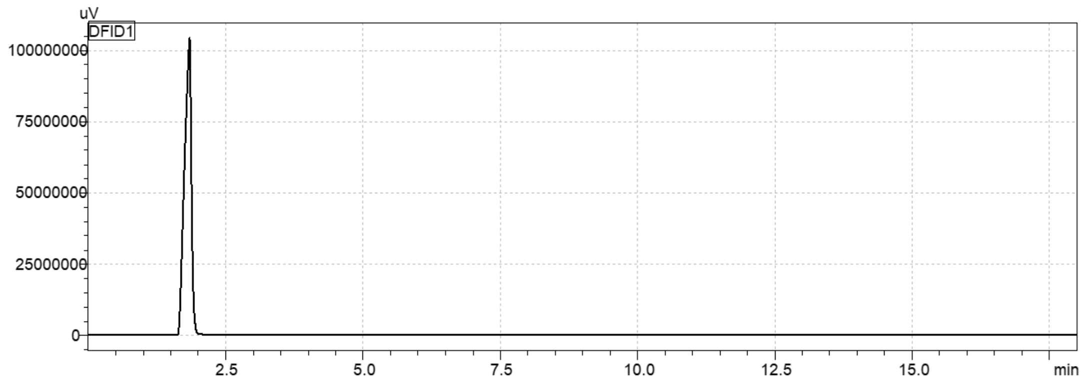


Fig. S37. GC result of the organic phase obtained from the DES aqueous extraction.

Theoretical calculation method

All the structures were fully optimized with the DFT method including the dispersion corrections (B3LYP) method using the Empirical Dispersion = GD3BJ keyword [6]. 6–311++g(d,p) basis set was used for all atoms [abbreviation as B3LYP/6311++g(d,p)]. The influence of water solvent was investigated in condensed phase using the Polarizable Continuum Model (PCM) at B3LYP/6–311++g(d,p) method. Energy calculations and Zero–point energy (ZPE) correction have been done by using the same level of theory. The computed stationary points have been characterized as minima or transition states by diagonalizing the Hessian matrix and analyzing the vibrational normal modes. In this way, if the imaginary frequency is not displayed, the stationary point can be classified as minima, and if only one imaginary frequency is obtained, the stationary point can be classified as a transition state (TS). The particular nature of the transition states has been determined by analyzing the motion described by the eigenvector associated with the imaginary frequency. All calculations were performed with the Gaussian 09 suite of programs [7].

The coordinates of the optimized structures

	HCl		
H	0.00000000	0.00000000	–1.21800800
Cl	0.00000000	0.00000000	0.07164800

1a			
C	–1.59592800	0.60531500	–0.12283800
C	–2.59249300	–0.07602300	0.72009300
O	–2.48815700	–0.38252300	–0.67972500
C	–0.14675000	0.27041700	–0.07258600
C	0.79411600	1.30328500	–0.02930400
C	2.15628100	1.01617300	0.04616500
C	2.59060000	–0.30814300	0.06874800
C	1.65571400	–1.34324800	0.01428400
C	0.29507800	–1.05688800	–0.05579900
H	–1.82248200	1.62167300	–0.43456500
H	–3.49730800	0.44842700	1.01297300
H	–2.25910600	–0.86604600	1.38702700
H	0.45928100	2.33471100	–0.05615900
H	2.87615000	1.82565200	0.08033300
H	3.64930100	–0.53320900	0.12249600
H	1.98826200	–2.37485700	0.02318300
H	–0.42855000	–1.86150700	–0.11006100

EmimCl/Im

C	0.97153300	–0.41668000	–0.87218600
N	0.33713700	–1.58885300	–0.96494100
C	1.04435200	–2.53730800	–0.24784700
C	2.12854400	–1.90806900	0.28168400
N	2.06334900	–0.58612900	–0.12113200
C	–0.93882000	–1.81232400	–1.64996200
C	3.00220300	0.48772000	0.25603800
C	2.87393900	0.85427900	1.72869700
H	0.65194800	0.53155300	–1.28276000
H	0.72075900	–3.56111400	–0.18397100
H	2.93068600	–2.28183900	0.89284200
H	–1.18062700	–0.92815000	–2.23359600
H	–0.84449400	–2.67269600	–2.30979200
H	–1.71806400	–1.98557100	–0.90933700
H	2.76431200	1.33937300	–0.37940700
H	4.00650500	0.13989200	0.01322000
H	3.58910200	1.64486700	1.96346300
H	3.08700000	–0.00000600	2.37420800
H	1.87000200	1.22183000	1.94840400
C	–1.60851200	–0.02083400	1.33287800
N	–2.62600700	–0.85105000	1.49550400
C	–3.59433400	–0.42069600	0.60839300

C	–3.14284500	0.67303100	–0.08872800
N	–1.87553900	0.91754500	0.38693000
H	–0.67302700	–0.05596700	1.86875500
H	–4.54706700	–0.91946400	0.52281600
H	–3.59144500	1.27929700	–0.85730400
H	–1.23224700	1.64559900	0.04974000
Cl	0.26221900	2.93924000	–0.89091800

INT1			
C	1.88989200	0.37287100	1.14826200
N	0.84322400	0.23243100	1.96784700
C	–0.01848600	1.29857900	1.77588500
C	0.53527300	2.08833300	0.81676900
N	1.72708700	1.49315700	0.44013900
C	0.66584900	–0.84679600	2.94402300
C	2.66394500	1.99692700	–0.58452000
C	2.05715400	1.97083800	–1.98034900
H	2.70417900	–0.32152800	1.03535900
H	–0.93500300	1.39793200	2.32985700
H	0.19087100	3.00824100	0.37881300
H	1.38822000	–1.63088400	2.73105200

H	0.82630200	–0.45821800	3.94860600
H	–0.34176400	–1.24660800	2.85357200
H	3.54608800	1.36140400	–0.53158000
H	2.94886100	3.00681100	–0.28757500
H	2.77808300	2.38714800	–2.68657000
H	1.14734700	2.57200500	–2.03415000
H	1.83586800	0.94531400	–2.27837600
C	–1.06953900	–0.57033400	–1.03711400
N	–2.24476700	–0.79275600	–0.45036000
C	–2.16236200	–1.94157300	0.30707700
C	–0.89188400	–2.41717800	0.16419700
N	–0.23271700	–1.54495100	–0.67689900
H	–0.83810800	0.25258000	–1.68969200
H	–2.99797200	–2.31334600	0.87273300
H	–0.40744400	–3.28265200	0.57974000
H	0.77177100	–1.62092700	–0.96150500
Cl	2.76869500	–1.75015800	–1.33349200
H	–3.08372900	–0.17028400	–0.53773500
Cl	–4.66295500	1.08473700	–0.66727300

INT2			
C	–2.42288000	0.02288600	1.46644900
N	–1.29878200	–0.10959600	2.17987700
C	–0.92212200	–1.44114500	2.17723400
C	–1.84906100	–2.11189800	1.44138700
N	–2.77487100	–1.18011600	1.00657900
C	–0.60131800	0.96888400	2.88557500
C	–3.93389300	–1.45166600	0.13343700
C	–3.49788300	–1.85367500	–1.26840100
H	–2.94568300	0.94080300	1.25208700
H	–0.02533600	–1.78085100	2.66508700
H	–1.93164400	–3.15545100	1.19507700
H	–1.04572000	1.91941600	2.60171500
H	–0.70266100	0.82496300	3.96012600
H	0.45100700	0.95592400	2.60923300
H	–4.51851400	–0.53438100	0.10591200
H	–4.52462300	–2.23181400	0.61441300
H	–4.38518900	–2.01464200	–1.88358500
H	–2.92116900	–2.78043200	–1.25976100
H	–2.90261600	–1.06011700	–1.72158900
C	0.35477200	1.59315700	–0.34660500
N	1.42423500	2.21751500	0.14917200

C	1.09413100	3.52420300	0.44067500
C	–0.21850100	3.68293700	0.10832200
N	–0.65283600	2.46738400	–0.37868700
H	0.30795400	0.56550700	–0.66006300
H	1.81101000	4.21175800	0.85256400
H	–0.87017600	4.53577600	0.17362500
H	–1.62850500	2.26693100	–0.69772200
Cl	–3.60455100	1.98729200	–1.09223900
O	2.08242700	–2.17584200	1.45445700
C	1.57297600	–2.75050500	0.22576500
H	0.70972600	–3.39167900	0.37820500
C	2.84683200	–3.20348800	0.80192100
H	3.77919700	–2.86854400	0.35811500
H	2.37687800	1.81416500	0.30443800
C	1.47912300	–1.85764700	–0.96007600
C	2.49230200	–0.94515300	–1.27799300
C	0.34368800	–1.92357500	–1.77383000
C	2.37647200	–0.13164600	–2.40084700
H	3.35556800	–0.83814100	–0.63361300
C	0.22638300	–1.10556100	–2.89750400
H	–0.45145600	–2.61627000	–1.52535500
C	1.24647600	–0.21145700	–3.21724200

H	3.16333000	0.57746300	–2.62896900
H	–0.66183600	–1.16326800	–3.51526800
H	1.15636900	0.42880800	–4.08658200
H	2.88417700	–4.15394700	1.32590000
Cl	4.33698000	1.44568100	0.77766000

TS1			
C	–2.30525400	–1.05056100	1.06804200
N	–1.28592900	–0.52769400	1.75908500
C	–0.25605900	–1.45182400	1.81007700
C	–0.67602000	–2.54715400	1.11905000
N	–1.95502400	–2.27584500	0.66670600
C	–1.27233900	0.78995300	2.40526300
C	–2.77826900	–3.15419400	–0.18632600
C	–2.24939400	–3.20436600	–1.61405000
H	–3.25102500	–0.57947500	0.83798900
H	0.67542000	–1.22182100	2.30331300
H	–0.18303800	–3.48073000	0.91291700
H	–1.88355500	1.47842600	1.82619100
H	–1.66644900	0.70694200	3.41748900

H	–0.24214100	1.13943200	2.44035500
H	–3.78964700	–2.75170400	–0.15954900
H	–2.78142800	–4.14091800	0.27709100
H	–2.87749100	–3.87409300	–2.20451500
H	–1.22453800	–3.57916300	–1.64840900
H	–2.27882400	–2.21377000	–2.07154200
C	–1.58364500	1.49028300	–1.31556400
N	–0.76047800	2.50394600	–1.06080700
C	–1.49967600	3.53455700	–0.51918200
C	–2.79938800	3.11951800	–0.45219800
N	–2.82616900	1.83770100	–0.95909100
H	–1.30092400	0.54112000	–1.73693000
H	–1.04820600	4.46633800	–0.22671700
H	–3.68726300	3.61092700	–0.09570100
H	–3.65478900	1.20871400	–0.99531700
Cl	–5.14148900	–0.21379200	–0.76279500
O	1.75030700	2.35122900	–1.26474000
C	2.17340500	0.94104200	0.06243300
H	1.17939900	0.56334400	0.24990400
C	2.29828000	2.40042400	0.03948000
H	3.31332900	2.79876300	0.07155500
H	0.37001900	2.46654000	–1.19314300

C	3.12900800	0.00517300	–0.48915100
C	4.46192300	0.36275700	–0.75305100
C	2.70811000	–1.30987600	–0.75056100
C	5.34688700	–0.57496700	–1.26668000
H	4.80389300	1.36974200	–0.55259300
C	3.59588800	–2.24673700	–1.26264400
H	1.68126300	–1.58752700	–0.54449300
C	4.91732100	–1.87988800	–1.52166000
H	6.37348600	–0.29413100	–1.46806700
H	3.26282700	–3.25824600	–1.46075100
H	5.61259700	–2.60856800	–1.92136800
H	1.67284200	2.91129200	0.77612000
Cl	2.52091900	0.53185900	2.65709900

TS2			
C	2.87603400	–0.17349900	–0.89695300
N	2.08840500	–0.18938900	–1.97763100
C	2.11375100	–1.45787800	–2.53013400
C	2.94072200	–2.21160900	–1.75547000

N	3.40727300	–1.38997600	–0.74553600
C	1.32492000	0.94819800	–2.49770000
C	4.31180400	–1.78518800	0.35264600
C	3.57761500	–2.55799800	1.44006200
H	3.06862000	0.66039300	–0.23494000
H	1.55276500	–1.70510600	–3.41397700
H	3.23727700	–3.24225100	–1.83813300
H	1.59536600	1.83883300	–1.93652100
H	1.57373100	1.09468900	–3.54697900
H	0.25950100	0.75097600	–2.39211500
H	4.73726100	–0.86414600	0.74846300
H	5.11223300	–2.37547700	–0.09277700
H	4.29013100	–2.84972700	2.21381500
H	3.11378200	–3.46390800	1.04450900
H	2.80831800	–1.93542100	1.89883600
C	–0.03994500	1.73549100	0.60590400
N	–0.95436900	2.31816800	–0.16750800
C	–0.51515100	3.58383800	–0.49500900
C	0.69759600	3.76043000	0.10660200
N	0.96914400	2.59321500	0.78890300
H	–0.09283100	0.74119500	1.01407300
H	–1.09097400	4.24259000	–1.12071700

H	1.37635500	4.59464500	0.10861800
H	1.85278500	2.36715200	1.29147600
Cl	3.69664500	1.68601200	1.92409800
O	–2.98089800	1.18345300	–1.29558900
C	–4.49528200	0.48501600	–0.40989300
H	–5.26733200	0.75731700	–1.10785200
H	–4.44617300	1.00951500	0.52929200
C	–3.29206700	–0.15591800	–0.93606800
H	–3.46990100	–0.78814500	–1.81061500
H	–1.84737900	1.83392100	–0.56296600
C	–2.29831100	–0.80608000	–0.00755900
C	–2.39126900	–0.71809600	1.38390100
C	–1.20174800	–1.46879600	–0.57062600
C	–1.40178700	–1.27173500	2.19587200
H	–3.24114800	–0.23031100	1.84276600
C	–0.20964600	–2.01861700	0.23733400
H	–1.12927700	–1.55476800	–1.64985600
C	–0.30661300	–1.91911800	1.62527700
H	–1.48773300	–1.19862600	3.27354500
H	0.63037400	–2.53080700	–0.21490500
H	0.45920000	–2.35040800	2.25803300
Cl	–5.95927300	–1.18039500	0.52807500

Pro1			
C	–2.01515000	–0.85557700	1.11230700
N	–1.10120700	–0.35226400	1.95000800
C	–0.21658300	–1.35691600	2.30246100
C	–0.61333800	–2.48262300	1.64922000
N	–1.73751300	–2.14778100	0.91570600
C	–1.09261800	1.01831100	2.47282000
C	–2.50723000	–3.04531500	0.03134700
C	–1.73658300	–3.39226700	–1.23503900
H	–2.85319000	–0.33634100	0.66517900
H	0.61192700	–1.17703600	2.96350600
H	–0.19492400	–3.47308800	1.63794700
H	–1.55989700	1.67882700	1.74633500
H	–1.63664000	1.05441700	3.41591700
H	–0.06070400	1.32244800	2.63142300
H	–3.43259400	–2.52002900	–0.20290400
H	–2.74867200	–3.93658200	0.61076500
H	–2.35176200	–4.04186800	–1.86034100
H	–0.80941800	–3.92105900	–1.00681800
H	–1.50113200	–2.49088700	–1.80427200

C	–1.23186300	1.76724100	–1.54551100
N	–0.35740800	2.72036300	–1.25813800
C	–1.04433900	3.64896400	–0.50152000
C	–2.34410900	3.24021900	–0.33930300
N	–2.44504100	2.04272400	–1.01176700
H	–1.03205100	0.87877400	–2.12275800
H	–0.56600000	4.53857200	–0.12457600
H	–3.18102300	3.67804700	0.17738400
H	–3.27332800	1.43098000	–1.05164200
Cl	–4.78743400	–0.08467000	–0.82147800
O	2.37406100	2.45803800	–1.51585200
C	2.16965900	0.96882800	0.38406400
H	1.08719000	1.06262400	0.41865500
C	2.77095700	2.26479300	–0.17384600
H	3.86084200	2.21105500	–0.14838200
H	1.39257200	2.60218600	–1.51445800
C	2.55709000	–0.28280800	–0.34361200
C	3.89884200	–0.64217500	–0.51078700
C	1.56315600	–1.09091900	–0.89796900
C	4.23701300	–1.78800700	–1.22273200
H	4.68028300	–0.03045500	–0.07540200
C	1.89979300	–2.23532800	–1.61950600

H	0.52206800	–0.81737000	–0.77321700
C	3.23743600	–2.58648900	–1.78254600
H	5.27932200	–2.05854500	–1.34426600
H	1.12040000	–2.84906600	–2.05311100
H	3.50202300	–3.47648700	–2.34130800
H	2.45565200	3.09791500	0.46471900
Cl	2.66931400	0.85924500	2.17257700

Pro2			
C	–1.89340200	–1.64622300	0.66707200
N	–0.96128700	–2.59428700	0.80079100
C	–0.90075400	–3.32511600	–0.37103200
C	–1.82640900	–2.79766000	–1.21759500
N	–2.43450500	–1.74979600	–0.55063300
C	–0.11106200	–2.79573400	1.97951100
C	–3.50885200	–0.89068100	–1.08964400
C	–3.06469800	–0.14781100	–2.34062400
H	–2.17522400	–0.93654100	1.42661200
H	–0.21673700	–4.14586900	–0.49467200
H	–2.10317300	–3.07733700	–2.21807700
H	–0.59025200	–2.32807700	2.83597300

H	–0.01165400	–3.86471900	2.15608100
H	0.86266800	–2.33614500	1.80910800
H	–3.78042200	–0.18641700	–0.30484400
H	–4.36836800	–1.53251900	–1.28700600
H	–3.88646900	0.48194400	–2.68306100
H	–2.79918400	–0.83429000	–3.14702500
H	–2.20839000	0.49169700	–2.12661800
C	–0.69352400	1.36680000	0.93719000
N	0.06168100	0.82214100	1.88135300
C	–0.73363600	0.74388700	3.00698900
C	–1.97889400	1.25067500	2.72627900
N	–1.93290000	1.64377000	1.40754500
H	–0.38613500	1.56633100	–0.07596700
H	–0.36585200	0.33599700	3.93484500
H	–2.86406700	1.36967600	3.32747900
H	–2.72474800	2.04028700	0.87284700
Cl	–4.49638900	2.65178700	–0.10803900
O	2.37128400	–0.63774300	1.64744300
C	4.27913300	0.56970400	0.91173100
H	4.80144800	0.14949000	1.76627100
H	3.92103300	1.56687600	1.15707500
C	3.15717300	–0.37275800	0.48692400

H	3.61345300	–1.32508700	0.20026900
H	1.59554500	–0.01586200	1.68997300
C	2.29950000	0.10620000	–0.67104100
C	2.19922800	1.44766400	–1.04449700
C	1.53307500	–0.84110400	–1.35885100
C	1.35207200	1.83442000	–2.08365500
H	2.77683800	2.20625000	–0.53221600
C	0.68103400	–0.45935200	–2.38964400
H	1.60754600	–1.88618900	–1.07935600
C	0.58967600	0.88339100	–2.75772700
H	1.28719100	2.87983400	–2.36182700
H	0.09339700	–1.20674200	–2.90842500
H	–0.06932000	1.18473000	–3.56326300
Cl	5.53237300	0.76550800	–0.40345800

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