Supporting Information

Sponge-like quaternary ammonium-based poly (ionic liquid)s: toward high CO_2 capture and efficient cycloaddition at mild conditions

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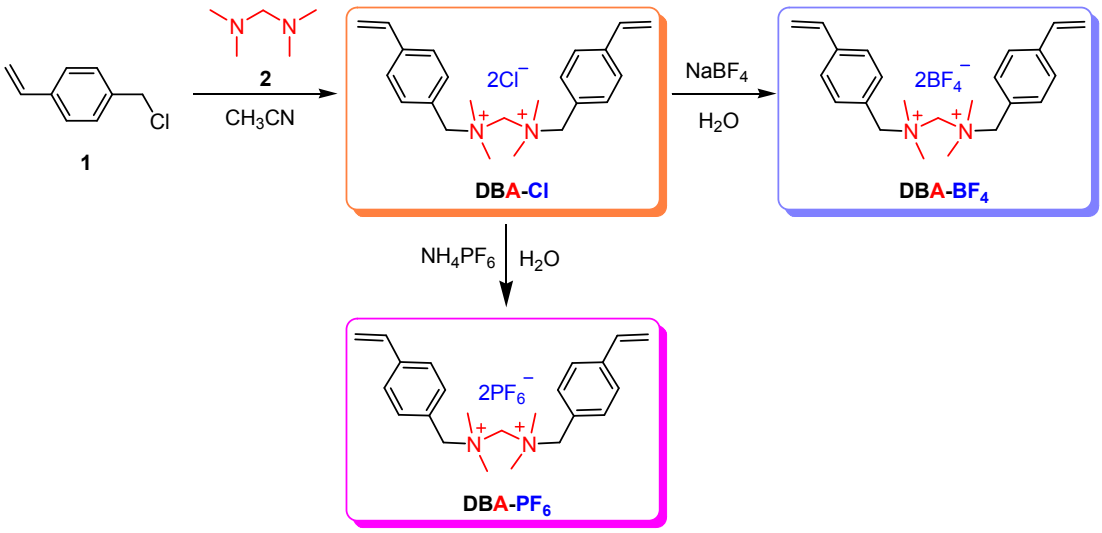
S1. Experimental

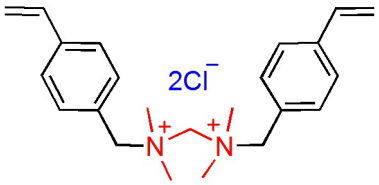
S1.1 General

All reagents were commercially available and were directly used without further purification. ^{1}H and ^{13}C spectra were acquired on a Bruker DPX 500 spectrometer at ambient temperature by using DMSO as the solvent and TMS (tetramethylsilane) as internal reference. The IR spectra were recorded on a Nicolet 330 infrared spectrometer (Thermo Electron Corporation, USA). The textural properties were analyzed by N_2 adsorption and desorption method (ASAP 2020, Micromeritics, USA). The specific surface areas were evaluated using the Brunauer-Emmett-Teller (BET) method and the pore distribution was calculated by the BJH method from desorption branches of isotherms. Thermogravimetric (TG) analysis was carried out on a NETZSCH TG 209F1 instrument by heating the samples from 35 to 800 °C in flowing air stream (20 $mL \cdot min^{-1}$) with a heating rate of 10 $°C \cdot min^{-1}$. The SEM images were recorded using a Zeiss SIGMA microscope. The TEM images were recorded using a JEOL-JEM-1400 microscope after the specimens were dispersed in ethanol and placed on holey copper grids. CO_2 adsorption were analyzed by CO_2 adsorption and desorption method (ASAP 2020, Micromeritics, USA) at 273 K. The resulting reaction mixture was analyzed by GC-mass spectrometry (GC-MS) for product identification, which was performed on an Agilent 6890 instrument equipped with an Agilent 5973 mass selective detector. The conversion and selectivity of products were quantified on an Agilent 7890A GC equipped with a flame ionization detector and a DB-5 column (30 m × 0.25 mm × 0.25 μm) using dodecane as internal standard.

S1.2 Synthesis of dicationic crosslinkers

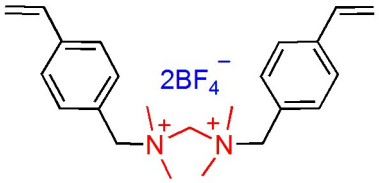


Scheme S1. Synthesis of the quaternary ammonium-based dicationic crosslinkers.



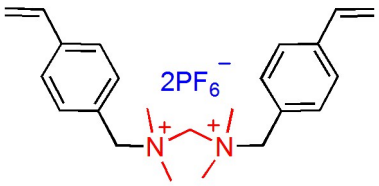
DBA-Cl. In fact, Matyjaszewski et al.[1] reported the preparation of **DBA-Cl** through the quaternization reaction of tetramethylethylenediamine with 4-vinylbenzyl chloride in the mixture solvent of methanol and H_2O. The regents in the quaternization reaction were water-insoluble, leading to a low conversion (24% according to ^1H NMR measurement of the reaction solutions). Furthermore, pure DBA-Cl could not be produced according to the reported method. In this work, an improved method was proposed. **DBA-Cl** was prepared from the quaternization reaction of 4-vinylbenzyl chloride (compound **1**) with tetramethylethylenediamine (compound **2**). Compound **1** (30.10 g, 200 mmol) was dissolved in acetonitrile (50 mL), followed with addition of compound **2** (10.52 g, 100 mmol). The mixture was stirred under N_2 at 50 °C for 48 h. After reaction, the precipitated salt was generated and washed by addition of 3×150 mL anhydrous ethyl acetate. After filtration, the residue was dried in a vacuum at 80 °C for 12 h to give the high purity product as brown solid in quantitative yield: ^1H

NMR (500 M, DMSO) δ (ppm) = 3.157(s, 12H), 4.288(s, 2H), 4.805(s, 4H), 5.380(d, J = 11.5 Hz, 2H), 5.958(d, J = 17.5 Hz, 2H), 6.803(dd, J = 11.0, 17.5 Hz, 2H), 7.639(dd, J = 9.0, 27.0 Hz, 8H). ^{13}C NMR (125 M, DMSO) δ (ppm) = 49.38, 55.54, 66.70, 116.35, 126.58, 127.04, 133.58, 135.86, 139.05.



DBA-BF$_4$

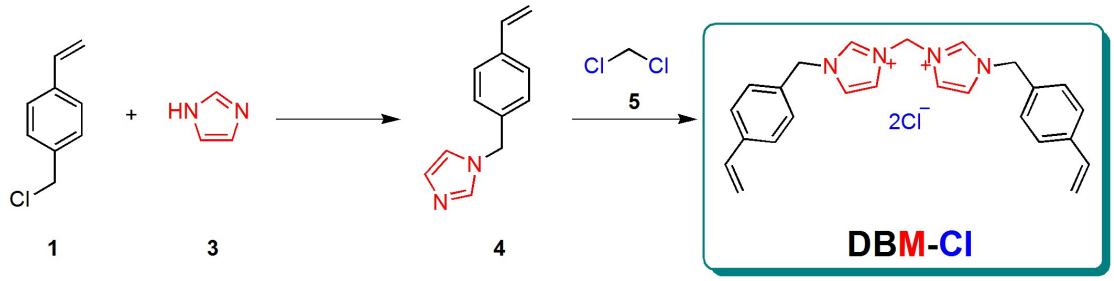
DBA-BF$_4$ was prepared from the anion exchange of **DBA-Cl** with BF_4^-. **DBA-Cl** (16.28 g, 50 mmol) was dissolved in water (50 mL), followed with addition of $NaBF_4$ (4.20 g, 60 mmol). The mixture was stirred at room temperature for 12 h. After reaction, the precipitated salt was washed with 3×150 mL distillation water. After filtration, the residue was dried in a vacuum at 80 °C for 12 h to give the product as gray solid with quantitative yield. ^{1}H NMR (500 M, DMSO) δ (ppm) = 3.057(s, 12H), 3.931(s, 2H), 4.591(s, 4H), 5.405(d, J = 11.5 Hz, 2H), 5.976(d, J = 17.5 Hz, 2H), 6.821(dd, J = 11.0, 17.5 Hz, 2H), 7.615(dd, J = 9.0, 32.0 Hz, 8H). ^{13}C NMR (125 M, DMSO) δ (ppm) = 49.38, 55.54, 66.70, 116.35, 126.58, 127.04, 133.58, 135.86, 139.05.



DBA-PF$_6$

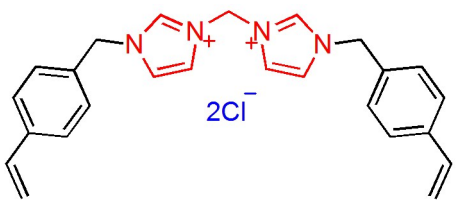
DBA-PF$_6$ was prepared from the anion exchange of **DBA-Cl** with PF_6^-. **DBA-Cl** (16.28 g, 50 mmol) was dissolved in water (50 mL), followed with addition of NH_4PF_6 (5.85 g, 60 mmol). The mixture was stirred at room temperature for 12 h. After reaction, the precipitated salt was washed with 3×150 mL distillation water. After filtration, the residue was dried in a vacuum at 80 °C for 12 h to give the

product as gray solid with quantitative yield. ^{1}H NMR (500 M, DMSO) δ (ppm) = 3.058(s, 12H), 3.931(s, 2H), 4.592(s, 4H), 5.403(d, J = 11.5 Hz, 2H), 5.975(d, J = 17.5 Hz, 2H), 6.821(dd, J = 11.0, 18.0 Hz, 2H), 7.615(dd, J = 9.0, 32.5 Hz, 8H). ^{13}C NMR (125 M, DMSO) δ (ppm) = 49.60, 55.47, 67.47, 116.51, 126.66, 126.70, 133.47, 135.78, 139.27.



Scheme S2. Synthesis route of imidazolium-based dication monomer DBM-Cl.

N-(4-vinylbenzyl)-imidazole (Compound **4**). The intermediate compound **4** was prepared according to the reported method.[2] Imidazole (compound **3**, 3.58 g, 50 mmol) in 50 mL THF was added dropwise into NaOH (3.16 g, 50 mmol) suspension of THF; the system reflexed for 2 h. After cooling the mixture to room temperature, 1-(chloromethyl)-4-vinylbenzene (compound **1**, 8.03 g, 50 mmol) was added dropwise, and allowed to react at room temperature for overnight. The resulting mixture was poured into 100 mL of water and extracted with 3×50 mL methylene chloride (CH_2Cl_2). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum to give 9.02 g (98 % yield) intermediate compound **4** as a dark red viscous oil. ^{1}H NMR (400 M, $CDCl_3$) δ (ppm) = 5.102(s, 2H), 5.277(dd, J = 0.8, 10.8 Hz, 1H), 5.755(dd, J = 0.8, 17.6 Hz, 1H), 6.698(dd, J = 10.8, 17.6 Hz, 1H), 6.899(t, J = 1.2 Hz, 1H), 7.086-7.125 (m, 3H), 7.390(d, J = 8.0 Hz, 2H), 7.547(s, 1H). ^{13}C NMR (100 M, $CDCl_3$) δ (ppm) =50.86, 114.97, 119.57, 127.07, 127.84, 130.10, 135.83, 136.33, 137.7, 137.97.



DBM-Cl

DBM-Cl. Imidazolium-based dicationic crosslinker **DBM-Cl** was obtained according to the reported method.[3] Intermediate compound **4** (7.37 g, 40 mmol) and CH_2Cl_2 (3.48 g, 20 mmol) were dissolved in 5 mL THF. After stirring at room temperature for 1 h, the mixture was solvothermally treated at 100 °C for 24 h in a Teflon-lined stainless steel autoclave. After cooling to room temperature, the obtained crude salt was washed with diethyl ether (5 × 100 mL) and dried under vacuum, giving the light yellow powder product 1,1'-bis(4-vinylbenzyl)-3,3'-methylenediimidazolium chloride **DBM-Cl**. ^{1}H NMR (500 M, DMSO) δ (ppm) = 5.314(d, J = 11.0 Hz, 2H), 5.478(s, 4H), 5.884(d, J = 18.0 Hz, 2H), 6.744(s, 2H), 6.751(dd, J = 11.0, 18.0 Hz, 2H), 7.434-7.542 (m, 8H), 7.891(t, J = 1.5 Hz, 2H), 8.161(t, J = 1.5 Hz, 2H), 9.792(s, 2H). ^{13}C NMR (125 M, DMSO) δ (ppm) = 52.56, 58.66, 115.84, 123.07, 123.56, 127.11, 129.46, 133.95, 136.35, 138.22, 138.28

S1.3 Preparation of PIL alcogels

The poly(ionic liquid)s (PILs) were synthesized through free radical self-polymerization of dicationic crosslinkers induced by AIBN in distilled water or dimethylsulfoxide, which was chosen based on the solubility of different crosslinkers..

PDBA-Cl alcogel. The dicationic crosslinker **DBA-Cl** (8.03 g, 25 mmol) was dissolved in distilled H_2O (100 mL), followed with addition of AIBN (0.08 g, 10 wt%). The mixture was stirred under N_2 at 50 °C for 12 h. After reaction, a bulk gel was generated. Then, the obtained gel was purified by distilled water firstly, and then turned into the alcogel by using ethanol to replace the water within the network of the gel.

PDBA-BF_4 alcogel. The dicationic crosslinker **DBA-BF_4** (12.75 g, 25 mmol) was dissolved in DMSO (100 mL), followed with addition of AIBN (0.08 g, 10 wt%). The mixture was stirred under N_2 at 50 °C for 12 h. After reaction, a bulk gel was generated. Then, the obtained gel was purified by distilled water firstly, and then turned into the alcogel by using ethanol to replace the water within the network of the gel.

PDBA-PF_6 alcogel. The dicationic crosslinker **DBA-PF_6** (15.66 g, 25 mmol) was dissolved in DMSO (100 mL), followed with addition of AIBN (0.08 g, 10 wt%). The mixture was stirred under N_2 at 50 °C for 12 h. After reaction, a bulk gel was generated. Then, the obtained gel was purified by distilled water firstly, and then turned into the alcogel by using ethanol to replace the water within the network of the solgels.

S1.4 Drying process

Three different drying methods (ambient pressure drying, AD; vacuum pressure drying, VD; supercritical CO_2 drying, SCD) were used to prepare different samples. Among them, SCD method was described in detail[4] as follows.

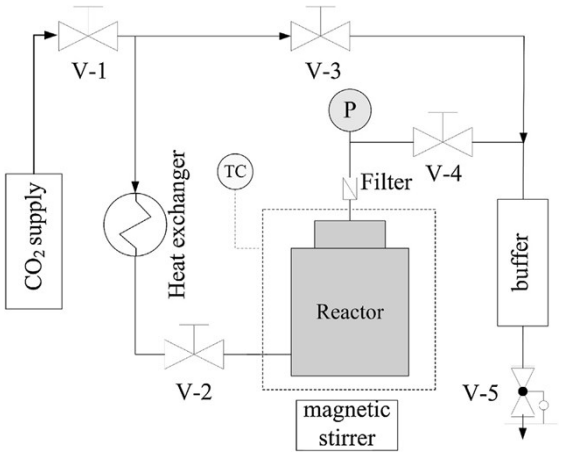
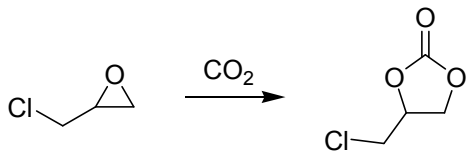


Figure S1. Schematic apparatus of the SCD process.

Figure S1 shows the schematic apparatus used for the SCD to prepare mesoporous poly (ionic liquid)s (MPILs) samples. There are three main parts: gas supply (with pressure control), reaction system (reactor, water bath, magnetic stirrer), and gas discharge (filter, buffer, reducing valve V-5). The SCD process was implemented at 60.0 °C and 15.0 MPa. Before the drying process, the obtained **PDBA-Cl** alcogel was placed in the reactor. Then, CO_2 was continuously charged through the reactor with a flow rate of about 1 NL/min for a period of time (2 h) until complete removal of ethanol in the **PDBA-Cl** alcogel. Finally, the CO_2 in the reactor was discharged slowly (<0.5 MPa/min) to obtain the MPIL sample **PDBA-Cl-SCD**. Other three MPILs (**PDBA-BF_4-SCD**, **PDBA-PF_6-SCD**, **PDBM-Cl-SCD**) were also obtained.

S1.5 Typical procedure of catalytic cycloaddition



Scheme S3. CO_2 cycloaddition to epichlorohydrin

The catalytic cycloaddition of CO_2 into cyclic carbonates was carried out using a 100 mL stainless-steel autoclave. In a typical catalytic cycloaddition (**Scheme S3**), epichlorohydrin (0.934 g, 10 mmol) and catalyst **PDBA-Cl-SCD** (100 mg, 2.4 mol%, according to the amount of ionic liquid monomer) were placed in autoclave equipped with a magnetic stirrer. The autoclave was carefully flushed thrice with CO_2. The reaction was carried out at specified temperature and 1 atm of CO_2 pressure for a desired period of time. After the reaction stopped, the reactor was cooled in an ice-water bath and slowly depressurized. The reaction mixture was centrifuged to remove the solid catalyst. The qualitative analysis of product was determined by GC-MS and quantitative analysis by GC using dodecane as internal standard. The recyclability test

was conducted as follows: After the reaction stopped, **PDBA-Cl-SCD** was separated by centrifugation. And then it was washed by ethyl acetate twice and anhydrous ethanol twice. After being dried by SCD, it can be directly used in the next catalytic reaction.

S2. Results

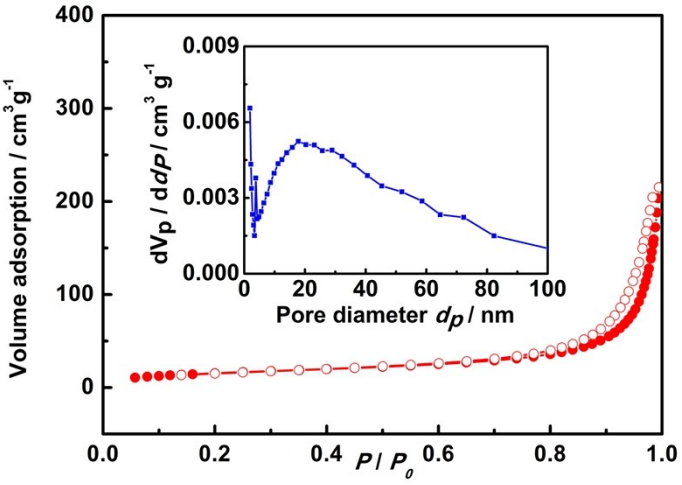


Figure S2. N_2 sorption isotherms curve of **PDBA-Cl-VD**.

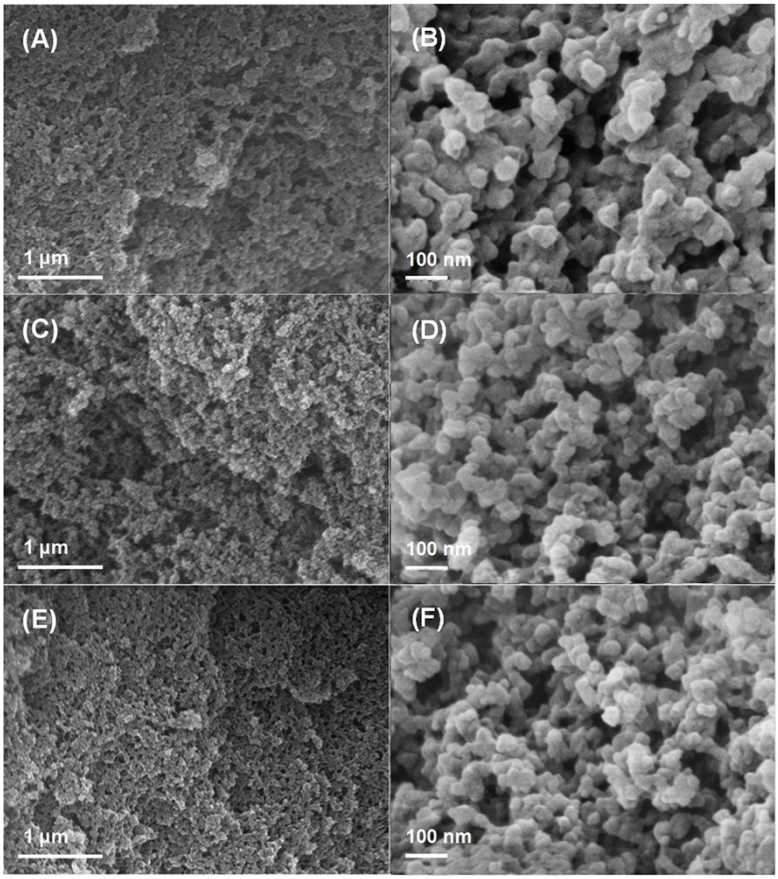


Figure S3. SEM images of PDBA-BF_4-SCD (A, B), PDBA-PF_6-SCD (C, D), and PDBM-Cl-SCD (E, F)

Table S1. Comparison of CO_2 adsorption in this work and some literature reports

Year	PILs	CO_2 adsorption [a] / mmol·g^{-1}	Ref.
2012	mpPIL	0.46	[5]
2013	P(CMVImTf_2N)	0.61	[6]
2013	PS-CC-film/VBTMACl/ PMVPMACl/M/20%	0.57	[1]
2014	Poly-VI-C6	0.50	[7]
2015	PDMBr	1.02	[3]
2017	PIL-8.1.BF_4	0.56	[8]
2017	PDBA-BF_4-SCD	1.23	This study

[a] 273 K and 1 atm.

Table S2. Optimization of reaction conditions of CO_2 cycloaddition[a]

Entry [b]	Pressure / atm	Temp. / °C	time / h	Cat. / mg	Con. [c] / %	Sel. [c] / %	Yield / %
1	10	100	6	100	100.0	99.9	99.9
2	1	100	6	100	100.0	99.8	99.8
3	1	90	6	100	99.4	99.9	99.3
4	1	80	6	100	73.5	99.8	73.4
5	1	90	8	100	100.0	99.8	99.8
6	1	90	4	100	85.3	99.6	85.0
7	1	90	6	150	99.5	99.8	99.3
8	1	90	6	50	78.6	89.7	70.5
9 [d]	1	120	12	100	94.6	96.5	91.3

[a] Epichlorohydrin 10 mmol. [b] **PDBA-Cl-SCD** was used as catalyst. [c] Determined by GC.

[d] From reference[3].

Table S3. Catalytic activity of different heterogeneous catalysts for cycloaddition of CO_2 with epichlorohydrin.

Entry	Catalyst	Solvent	Co-catalyst	CO_2 / MPa	Temp. / °C	Time / h	Yield / %	Ref.
1	Adenine-modified Ti-SBA-15 solid catalyst	CH_3CN	--	0.69	120	4	82.8	[9]
2	CO_2 adducts of *N*-heterocyclic carbene	CH_2Cl_2	--	2	120	8	98	[10]
3	Imidazolium salt-modified porous polymer (POM3-IM)	C_2H_5OH	--	1.0	120	8	90.0	[11]
4	$CaBr_2$	DMF	DBU	0.1	100	12	87	[12]
5	Zn-based bimetallic MOF	--	TBAB	1.2	23	60	99	[13]
6	Gd-MOF	--	TBAB	2	80	5	99.1	[14]
7	Metalporphyrin-based porous organic polymer (HUST-1-Co)	--	TBAB	0.1	RT	48	94.7	[15]

Table S4. Catalytic activity of different PILs for cycloaddition of CO_2 with epichlorohydrin.

Entry	Catalyst	CO_2 / MPa	Temp. / °C	Time / h	Yield / %	Ref.
1	Cross-linked-polymer-supported IL (PVBIMCl)	6	110	3	95.8	[16]
2	Cross-linked imidazolium-based PIL	3	140	5	98	[17]
3	Mesoporous zwitterionic PIL	1	150	8	97	[18]
4	Fluoro-functionalized PIL	1	120	9	93	[19]
5	Hydroxyl-functionalized phosphonium-based ionic liquid (PNPs-HPIL-3)	2.0	140	5	97.0	[20]
6	Porous cationic polymers (PCP-Cl)	3.0	100	12	98.0	[21]
7	Hierarchical porous poly(ionic liquid)s (AE-PIL-Cl)	1	140	6	93	[22]
8	Phosphonium-based porous ionic polymers (p5b)	2.5	130	15	99	[23]
9	Imidazolinium based porous hypercrosslinked ionic polymer	1	25	96	96	[24]
10	Imidazolium based meso-macroporous hierarchical polymer (PDMBr)	0.1	120	12	91.3	[3]
11	Imidazolium-based ionic polymer (IP3)	0.1	100	24	99	[25]
12	quaternary ammonium-based MPIL (PDBA-Cl-SCD)	0.1	90	6	99.3	This study

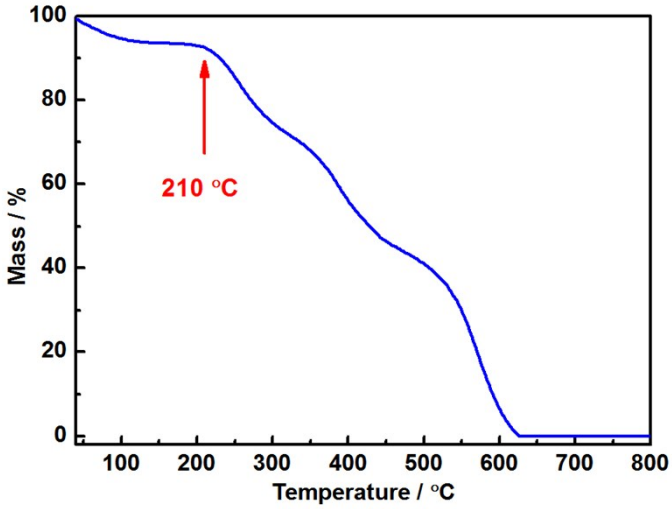


Figure S4. TG curves of **PDBA-Cl-SCD**.

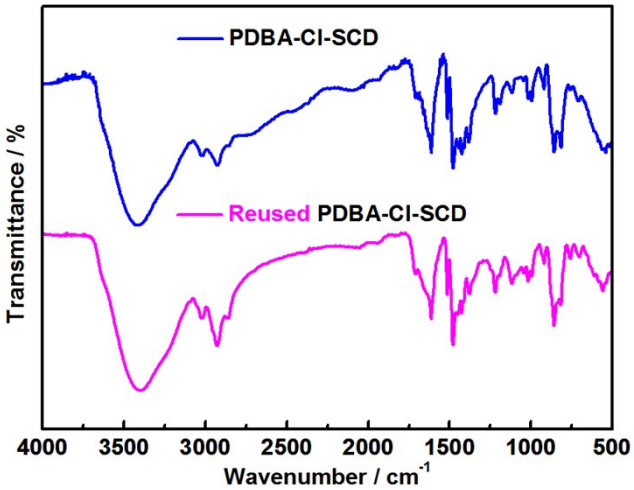


Figure S5. FT-IR spectra of PDBA-Cl-SCD and Reused-PDBA-Cl-SCD.

Table S5. Catalytic performance of **PDBM-Cl-SCD** for the cycloaddition of CO_2 with epichlorohydrin at different temepratures [a].

Catalyst	Temp. / °C	Con. [b] / %	Sel. [b] / %	Yield [b] / %
PDBM-Cl-SCD	90	77.2	63.2	48.8
PDBM-Cl-SCD	100	85.3	81.2	69.3
PDBM-Cl-SCD	110	93.0	89.4	83.1
PDBM-Cl-SCD	120	98.7	98.4	97.2
PDBM-Cl-SCD	130	99.3	95.6	94.9
PDBA-Cl-SCD	90	99.4	99.9	99.3

[a] Reaction conditions: epichlorohydrin 10 mmol, catalyst 2.4 mol% (according to the amount of ionic liquid monomer), CO_2 1 atm, 6 h. [b] Conversion and selectivity were determined by GC using dodecane as internal standard.

Table S6. Recycled experiments of CO_2 cycloaddition to epichlorohydrin. [a]

Run	**Conversion [b] / %**	**Selectivity [b] / %**	**Yield / %**
1	99.4	99.9	99.3
2	100.0	98.2	98.2
3	99.8	99.5	99.3
4	99.2	99.0	98.2
5	99.8	98.8	98.6

[a] Reaction conditions: epichlorohydrin 10 mmol, **PDBA-Cl-SCD** 100 mg (2.4 mol%), CO_2 1 atm, reaction temperature 90 °C, reaction time 6 h. [b] Determined by GC using dodecane as internal standard.

Table S7. Textural properties of **PDBA-Cl-SCD** and **Reused-PDBA-Cl-SCD**.

Entry	**Catalyst**	**S_{BET} [a] / ($m^2 \cdot g^{-1}$)**	**V_P [b] / ($cm^3 \cdot g^{-1}$)**	**D_{as} [c] / (nm)**
1	PDBA-Cl-SCD	211.0	1.24	21.6
2	Reused-PDBA-Cl-SCD	198.3	1.15	17.3

[a]BET surface area. [b]Pore volume. [c]Average pore size.

S3. Computational Details

All calculations were carried out with the Gaussian 09 program. The geometries of all the species were fully optimized by using density functional theory (DFT) of the CAM-B3LYP functional[26]. The CAM-B3LYP functional combined the hybrid qualities of B3LYP and the long range correction reported by Tawada et al.[27] The 6-31G(d,p)[28] basis set was used for all atoms. Vibrational analyses were performed at the same theoretical level to confirm each stationary point to be either a local minimum or a transition state (TS). The transition states were verified by intrinsic reaction coordinate (IRC)[29] calculations to be connected with the appropriate precursors and intermediates. Solvent effect of epichlorohydrin (ε =22.6) was modeled by using the SMD-flavor[30] of self-consistent reaction field (SCRF) theory.[31] The **PDBA-Cl-SCD** and **PDBM-Cl-SCD** were simplified as the monomers **DBA-Cl** and **DBM-Cl** (**Figure S6**), respectively.

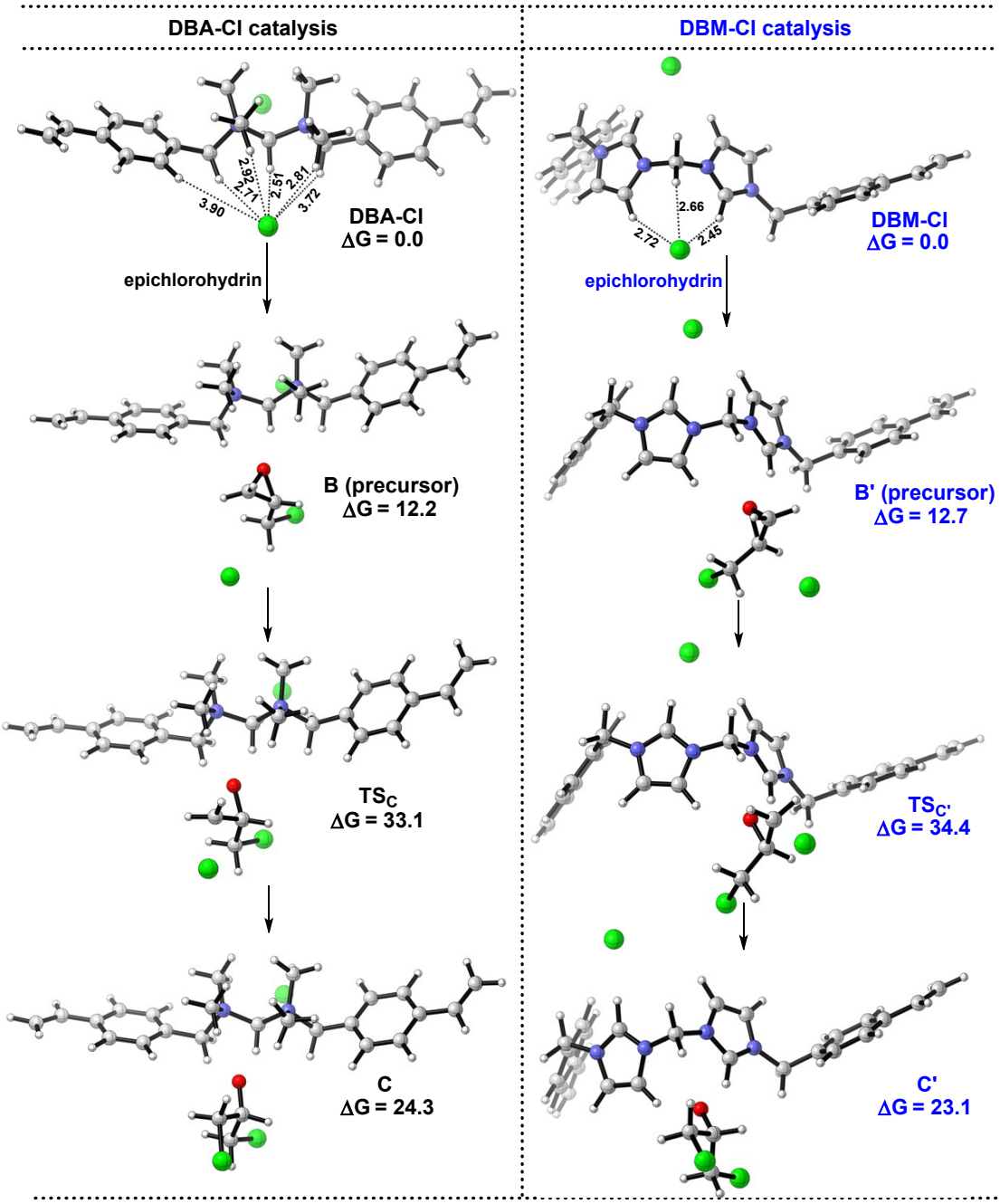


Figure S6. Computed structures and reaction energy profiles for the ring-opening processes of epichlorohydrin catalyzed by **DBA-Cl** (black)/**DBM-Cl** (blue). Relative free energies (ΔG, in kcal/mol) of key intermediates and transition states were computed at the SMD-CAM-B3LYP/6-31G(d,p) level of theory in epichlorohydrin solvent at 298 K.

The leaving ability of chloride can be quickly assessed by computing the free-energy change of Rxns. **1** and **2**,

$DBA\text{-}Cl = DBA^{2+} + 2Cl^-$ $\Delta G//\Delta E = -0.4//13.7$ kcal/mol **(1)**

$DBM\text{-}Cl = DBM^{2+} + 2Cl^{-}$ $\Delta G//\Delta E = 3.5\ //15.7$ kcal/mol **(2)**

The predicted lower free-energy change of Rxn. **1** indicates the higher leaving ability (and higher mobility) of Cl^{-} in **DBA-Cl** than in **DBM-Cl**. Accordingly, the predicted activation free-energy required for the ring-opening of epichlorohydrin is by 1.3 kcal/mol lower in the **DBA-Cl** catalysis than in the **DBM-Cl** catalysis (33.1 vs. 34.4 kcal/mol, see **Figure. S6**). In summary, these model computations elucidates that the superior catalytic activity of the **PDBA-Cl-SCD** catalyst over the **PDBM-Cl-SCD** catalyst can be ascribed to the higher leaving ability of Cl^{-}.

References for Supporting Information

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Appendix

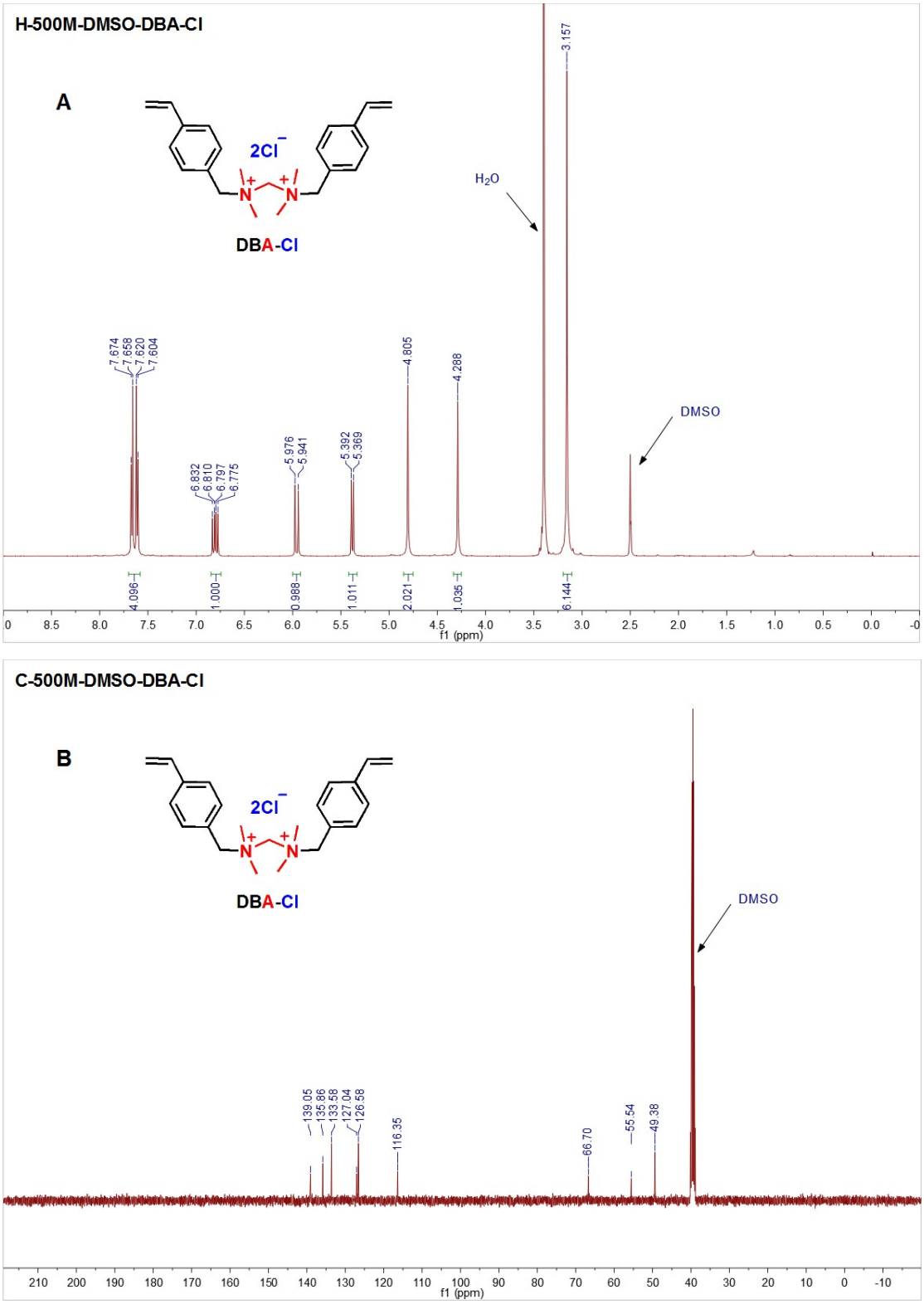


Figure S6. (A) ^{1}H NMR and (B) ^{13}C NMR of **DBA-Cl**.

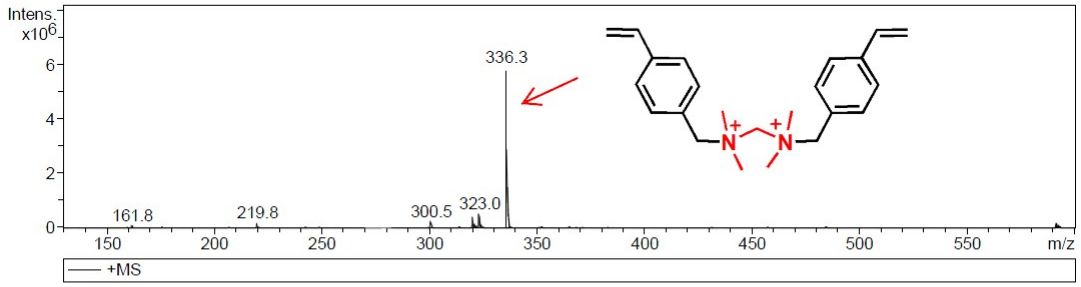
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\20170620\DBA-Cl.d	Acquisition Date	6/20/2017 10:24:18 AM
Method	pep-bodipy.m	Operator	bruker
Sample Name	DBA-Cl	Instrument	amaZon SL
Comment			

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	130 m/z	Scan End	600 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	48.6
Accumulation Time	492 µs	Averages	7 Spectra	Auto MS/MS	off



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1	219.8	208690
2	300.5	264590
3	300.9	198897
4	320.0	427447
5	321.0	154980
6	323.0	517432
7	336.3	5760905
8	337.2	1385388
9	338.1	136238
10	591.2	180337

Figure S7. Mass spectrum of **DBA-Cl**.

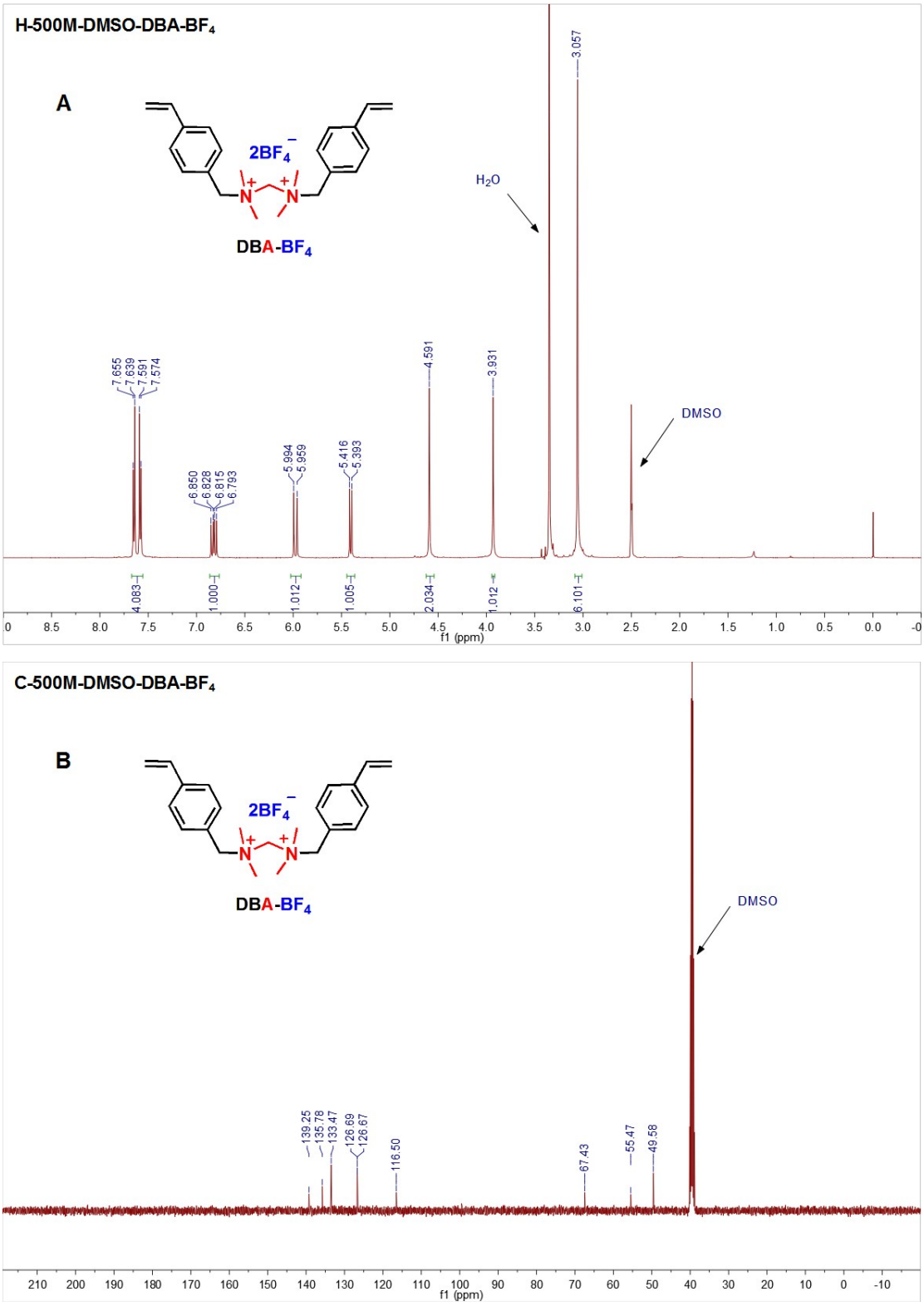


Figure S8. (A) ^{1}H NMR and (B) ^{13}C NMR of **DBA-BF$_4$**.

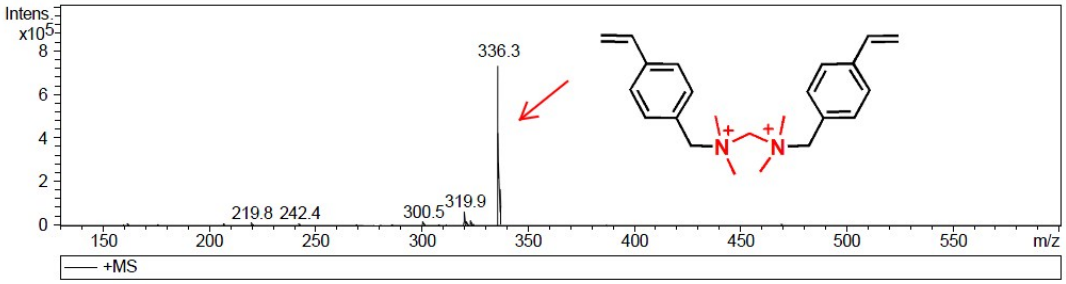
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\20170620\DBA-BF4.d	Acquisition Date	6/20/2017 10:31:52 AM
Method	pep-bodipy.m	Operator	bruker
Sample Name	DBA-BF4	Instrument	amaZon SL
Comment			

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	130 m/z	Scan End	600 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	48.6
Accumulation Time	288 µs	Averages	7 Spectra	Auto MS/MS	off



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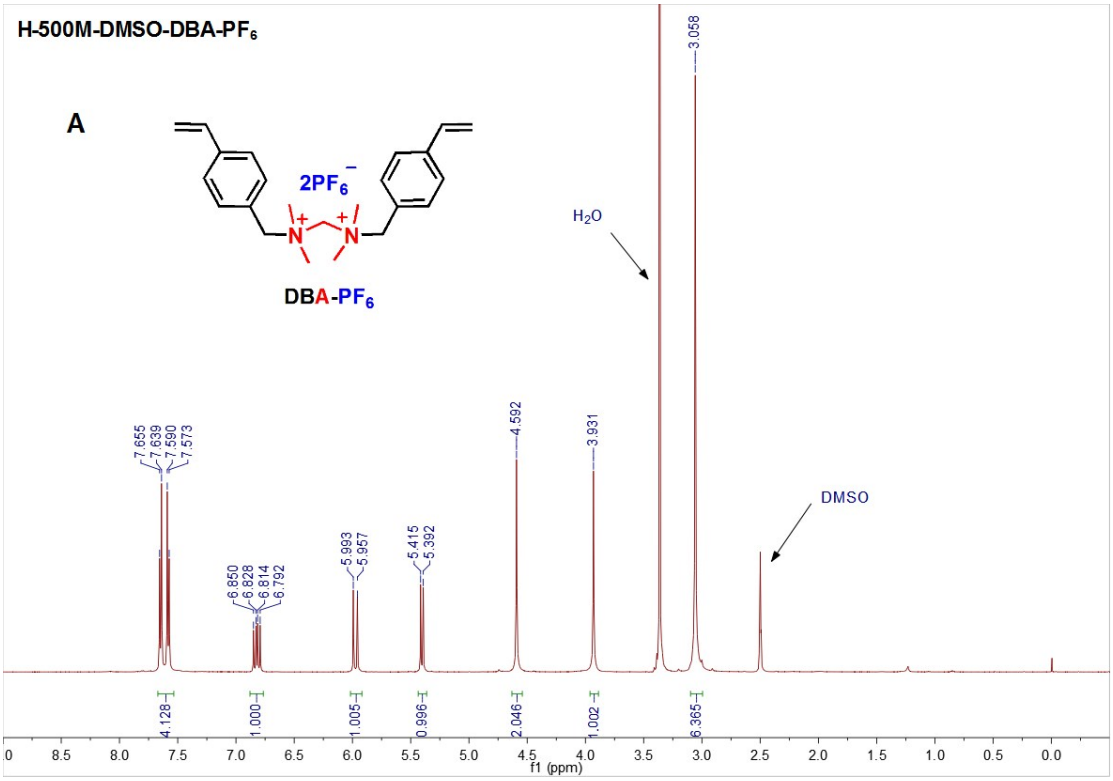
1	206.8	28371
2	219.8	12512
3	242.4	25451
4	300.5	73541
5	319.9	139225
6	321.0	49117
7	323.0	64324
8	336.3	7674523
9	337.2	1320657
10	338.1	228821

Figure S9. Mass spectrum of **DBA-BF_4**.



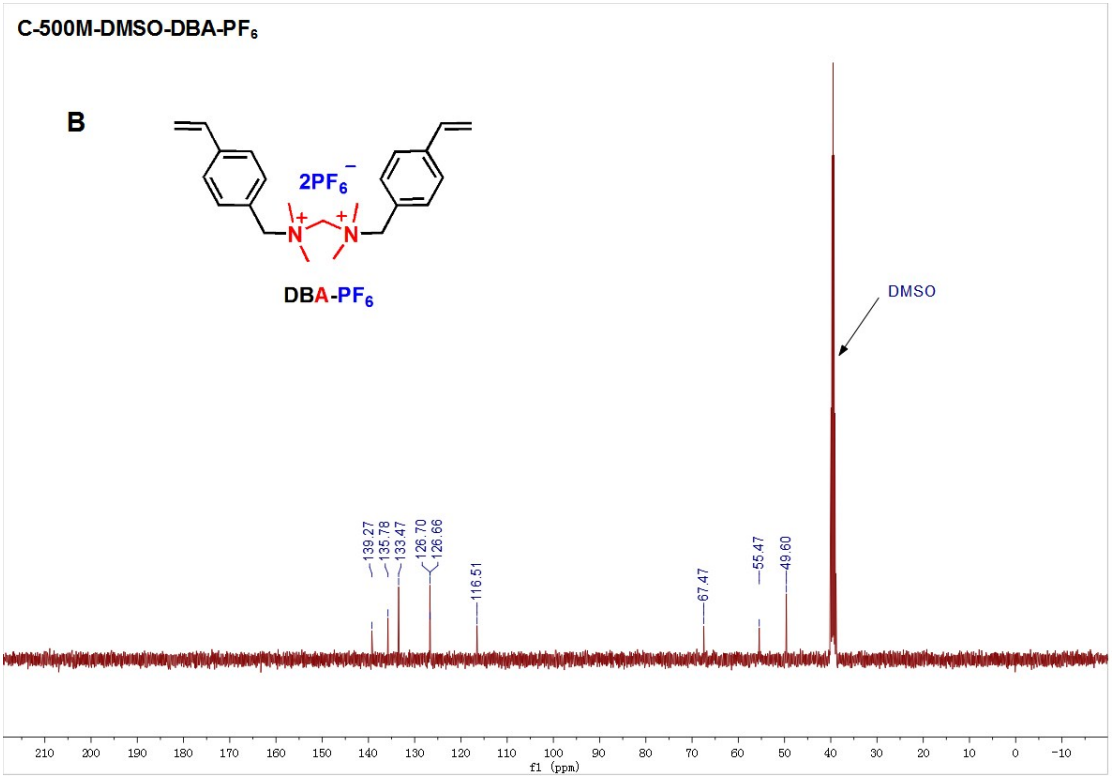


Figure S10. (A) ^{1}H NMR and (B) ^{13}C NMR of **DBA-PF$_6$**.

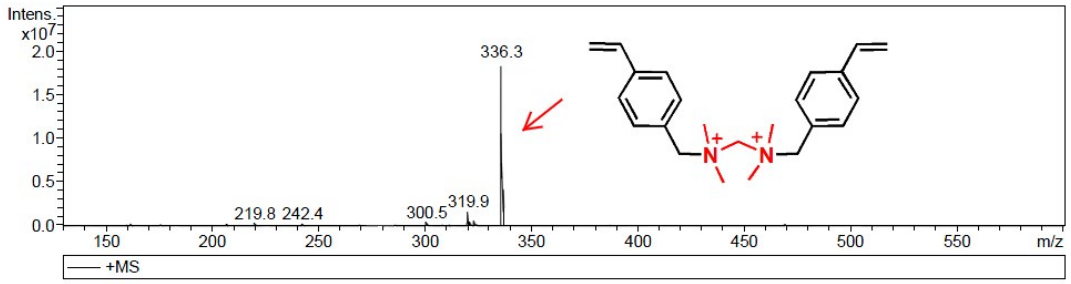
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\20170620\DBA-PF6.d	Acquisition Date	6/20/2017 10:28:08 AM
Method	pep-bodipy.m	Operator	bruker
Sample Name	DBA-PF6	Instrument	amaZon SL
Comment			

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	130 m/z	Scan End	600 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	48.6
Accumulation Time	220 µs	Averages	7 Spectra	Auto MS/MS	off



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2	219.8	328342
3	242.4	285251
4	300.5	473415
5	319.9	1639225
6	321.0	449117
7	323.0	564359
8	336.3	17774242
9	337.2	4390865
10	338.1	522867

Figure S11. Mass spectrum of **DBA-PF$_6$**.

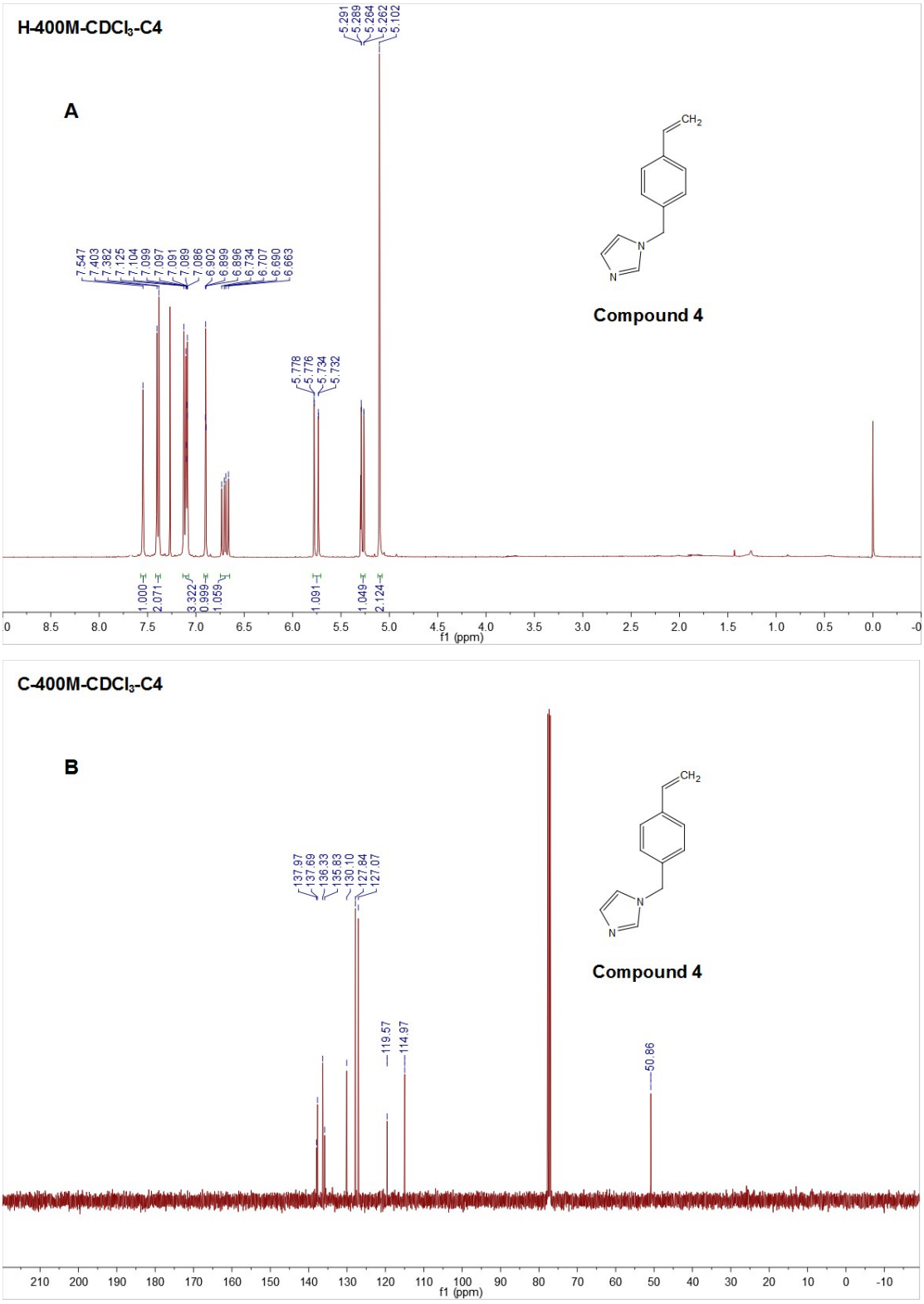


Figure S12. (A) ^{1}H NMR and (B) ^{13}C NMR of compound **4**.

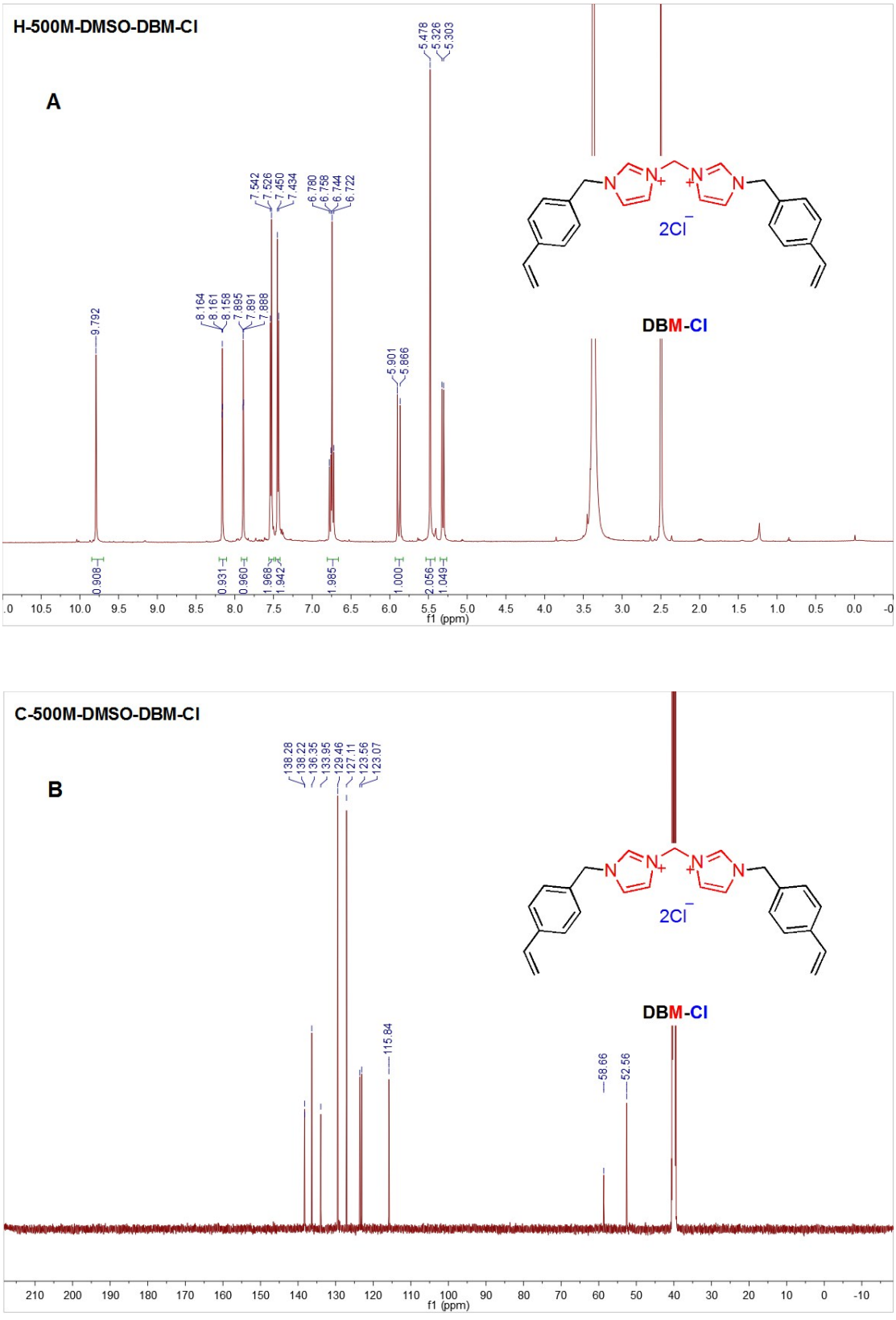


Figure S13. (A) ^{1}H NMR and (B) ^{13}C NMR of **DBM-Cl**.

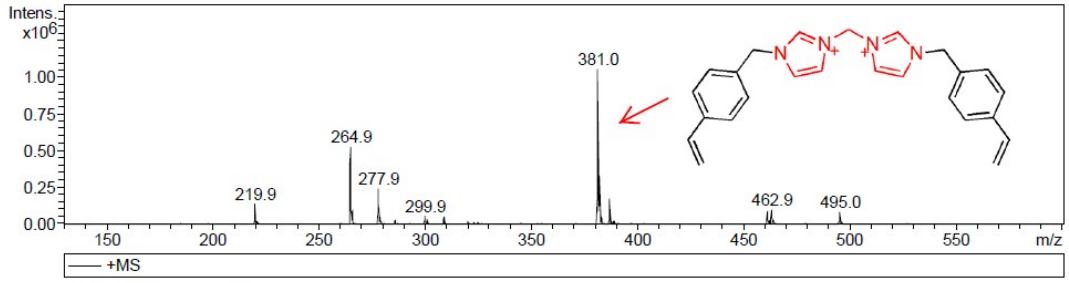
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\20170620\DBM-Cl.d	Acquisition Date	6/20/2017 10:31:39 AM
Method	pep-bodipy.m	Operator	bruker
Sample Name	DBM-Cl	Instrument	amaZon SL
Comment			

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	130 m/z	Scan End	600 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	48.6
Accumulation Time	3335 µs	Averages	7 Spectra	Auto MS/MS	off



#	m/z	I
1	219.9	139693
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3	265.9	95227
4	277.9	245408
5	381.0	1054974
6	382.0	335452
7	386.8	176635
8	460.9	88050
9	462.9	96603
10	495.0	86268

Figure S14. Mass spectrum of **DBM-Cl**.

Molecular Geometries and Energies

CAM-B3LYP (SMD, epichlorohydrin) for **DBA-Cl/DBM-Cl** catalysis, Cartesian Coordinates and Energies in Hartree

epichlorohydrin

Number of imaginary freguencies: 0

C	0.02610800	1.07522500	0.00234200
C	1.48589400	1.06926900	0.00122100
O	0.76630700	2.29987600	0.00578200
H	-0.51125900	0.85714500	-0.91980500
H	-0.51351900	0.85072000	0.92209900
H	2.01243000	0.84487500	-0.92630000
C	2.25330800	0.80982800	1.26422800
H	3.20440500	1.34413100	1.27291100
Cl	2.65026300	-0.95036000	1.41881500
H	1.67308900	1.08996000	2.14378000

Energy (0K) = -652.6314818

Energy (0K) + ZPE = -652.552980

Enthalpy (298K) = -652.546874

Free Energy (298K) = -652.582171

DBA-Cl

Number of imaginary freguencies: 0

N	1.22229700	1.08112500	1.84461900
C	1.73799300	1.17086700	0.42137300
H	0.84532300	1.28143700	-0.19831000
H	2.27225100	0.23518600	0.24120000
N	2.69120400	2.26147600	-0.02888100
C	2.68056000	2.05267600	-1.57122000
H	1.63425700	2.17634400	-1.85722800
H	2.97728500	1.01359900	-1.71546600

C	0.53143900	-0.31357400	1.82353500
H	1.33092000	-1.01086100	1.56619800
H	-0.18300100	-0.25913400	1.00216300
C	3.56246500	2.96838800	-2.37135300
C	3.05412300	4.16325500	-2.89352700
C	4.87230300	2.60813100	-2.69425200
C	3.83790000	4.98564800	-3.68661900
H	2.02477400	4.44288700	-2.68957200
C	5.65688100	3.43321300	-3.48808500
H	5.27975600	1.66878800	-2.33220200
C	5.16035500	4.63978900	-3.99355900
H	3.40662900	5.89966700	-4.08087800
H	6.67331100	3.13408800	-3.72756300
C	-0.15509800	-0.73277200	3.09165800
C	-1.51273100	-0.47453900	3.29264700
C	0.53032400	-1.47829800	4.05755900
C	-2.15366700	-0.91742600	4.44111500
H	-2.07605900	0.06842300	2.53945400
C	-0.11025900	-1.91871800	5.20469400
H	1.57459800	-1.73090200	3.89894300
C	-1.46428200	-1.63483600	5.42492300
H	-3.21045000	-0.70694300	4.57853900
H	0.44781300	-2.50584100	5.92653700
C	6.03957900	5.47611800	-4.83083200
H	7.01708500	5.04230400	-5.03487900
C	-2.19088500	-2.06945100	6.63176000
H	-3.26881100	-1.92158300	6.59150000
C	5.76036300	6.67506800	-5.33839600
H	6.49183900	7.20147300	-5.94515500
H	4.81439500	7.18591300	-5.17990500

C	-1.66175800	-2.59298600	7.73574600
H	-2.29490900	-2.87737200	8.57156100
H	-0.59502300	-2.75459500	7.86616500
C	4.08435400	2.06381000	0.48074100
H	4.13154000	2.31502300	1.53571100
H	4.37896400	1.02518200	0.32676600
H	4.74309200	2.73793300	-0.06196100
C	2.23737200	3.64840500	0.28712200
H	2.34660400	3.82279000	1.35582500
H	2.88459700	4.34587900	-0.24053600
H	1.20405900	3.77163200	-0.03754100
C	2.28869600	1.08708700	2.88908600
H	1.83273300	0.82186100	3.84087200
H	3.05797800	0.36209700	2.62274300
H	2.69511600	2.09229400	2.97659200
C	0.20304900	2.12925900	2.16622500
H	0.69188600	3.08767800	2.31314800
H	-0.51749000	2.19082300	1.34996700
H	-0.28874400	1.85001400	3.09525800
Cl	-1.01974900	2.42528200	-1.42930500
Cl	3.80586100	-1.70261400	0.69473300

Energy (0K) = -1925.1136547

Energy (0K) + ZPE = -1924.595608

Enthalpy (298K) = -1924.565476

Free Energy (298K) = -1924.659477

DBA^{2+}

Number of imaginary freguencies: 0

N	1.25826900	1.04847400	1.85307500
C	1.75193600	1.16413300	0.42703600

H	0.85469200	1.23633600	-0.18216500
H	2.28941300	0.24268200	0.21257600
N	2.67113500	2.27548900	-0.03764700
C	2.62296900	2.09924100	-1.58597900
H	1.57906200	2.26465100	-1.85276100
H	2.87786500	1.05364600	-1.75982100
C	0.60628200	-0.36760200	1.84874400
H	1.42774800	-1.05121500	1.63831800
H	-0.08119800	-0.35890500	1.00283100
C	3.52097600	2.99892700	-2.38486800
C	3.05271000	4.22622100	-2.86708500
C	4.80725200	2.59093700	-2.74410700
C	3.85352800	5.03260900	-3.65933600
H	2.04167100	4.54603300	-2.63178400
C	5.60821700	3.39967500	-3.53735300
H	5.18285300	1.62818900	-2.40983200
C	5.15245900	4.63748200	-4.00484200
H	3.45387500	5.97315900	-4.02290000
H	6.60542400	3.06372200	-3.80643900
C	-0.11032700	-0.76996500	3.10509600
C	-1.47978700	-0.53799500	3.25055100
C	0.55844900	-1.46793000	4.11688600
C	-2.14972000	-0.96045300	4.38946700
H	-2.02855300	-0.03044300	2.46293300
C	-0.11179200	-1.88867800	5.25426800
H	1.61413200	-1.69755000	4.00507200
C	-1.47906300	-1.63145300	5.41821600
H	-3.21481400	-0.77019200	4.48462100
H	0.43439000	-2.43800700	6.01375100
C	6.04749000	5.45382600	-4.84493800

H	6.99562200	4.97911000	-5.09140600
C	-2.23883100	-2.04667400	6.61123800
H	-3.31655100	-1.91420300	6.53233800
C	5.81220000	6.67956100	-5.30860700
H	6.55003000	7.18801100	-5.92285700
H	4.89824300	7.23096900	-5.10443800
C	-1.73849500	-2.53688700	7.74346800
H	-2.39443400	-2.80922600	8.56553600
H	-0.67466100	-2.68189400	7.91149500
C	4.08127600	2.08831800	0.42941700
H	4.14848000	2.27234400	1.49690700
H	4.40831900	1.07627100	0.19401300
H	4.70774700	2.81345400	-0.08437000
C	2.21700600	3.65565400	0.31428800
H	2.36179000	3.82002700	1.37998800
H	2.83995700	4.36251600	-0.22925600
H	1.17332700	3.78314900	0.03004300
C	2.33531200	1.09148700	2.88832000
H	1.89643200	0.80571900	3.84201000
H	3.13162800	0.39769800	2.62184200
H	2.70489700	2.11027900	2.97577200
C	0.21406100	2.06796300	2.19166600
H	0.66806900	3.05020200	2.27678300
H	-0.55849200	2.06523600	1.42339500
H	-0.21557900	1.80367000	3.15485200

Energy (0K) = -1004.3652995

Energy (0K) + ZPE = -1003.847675

Enthalpy (298K) = -1003.822314

Free Energy (298K) = -1003.903958

Cl^-

Number of imaginary freguencies: 0

Cl	0.76670200	-4.80127500	-4.24504100

Energy (0K) = -460.3630631

Energy (0K) + ZPE = -460.363063

Enthalpy (298K) = -460.360703

Free Energy (298K) = -460.378086

A

Number of imaginary freguencies: 0

N	-0.80803300	0.65440400	1.54148000
C	-0.42105800	0.81580300	0.08357600
H	-1.35691200	1.03913800	-0.43683900
H	0.00107700	-0.13813900	-0.22387000
N	0.57521800	1.85580300	-0.38580200
C	0.40112100	1.76761600	-1.93295200
H	-0.64748300	2.01965200	-2.10404800
H	0.56421100	0.71696000	-2.17611100
C	-1.55381300	-0.71257400	1.50910000
H	-0.80320200	-1.43003300	1.17650600
H	-2.31059500	-0.60126400	0.73266700
C	1.30795600	2.64076600	-2.75183800
C	0.90530800	3.92448100	-3.13717500
C	2.52852600	2.15790400	-3.22874500
C	1.71163600	4.71218300	-3.94319900
H	-0.05985100	4.30436700	-2.81528200
C	3.33502400	2.94735200	-4.03597400
H	2.84702800	1.15062000	-2.97667400
C	2.94960000	4.24205800	-4.40032700
H	1.36306500	5.69818700	-4.23186200

H	4.28023100	2.55168200	-4.39627000
C	-2.18437900	-1.15663800	2.79731300
C	-3.51767600	-0.85185100	3.08006800
C	-1.48082700	-1.96507200	3.69698000
C	-4.11600000	-1.31344300	4.24357400
H	-4.09593500	-0.25679500	2.37945900
C	-2.07926800	-2.42473700	4.85930500
H	-0.45635700	-2.25092000	3.47661200
C	-3.40734300	-2.09682600	5.16118400
H	-5.15439400	-1.06637700	4.44483600
H	-1.50971000	-3.06140500	5.52822300
C	3.84867600	5.03969000	-5.25398300
H	4.71505300	4.49900900	-5.63136500
C	-4.08890800	-2.55075500	6.38697200
H	-5.16042300	-2.35955700	6.40902700
C	3.70718900	6.32191000	-5.58358500
H	4.43647200	6.81200000	-6.22253400
H	2.88144600	6.93847100	-5.23854100
C	-3.52532700	-3.13793200	7.44062000
H	-4.12564900	-3.43081600	8.29743900
H	-2.46079400	-3.34556300	7.50792800
C	1.98771600	1.51122900	-0.02906500
H	2.15492000	1.67823500	1.03048300
H	2.17961400	0.46924000	-0.28482700
H	2.65035000	2.16710200	-0.58888200
C	0.26655300	3.24784600	0.06111500
H	0.46742600	3.34006300	1.12604300
H	0.92745200	3.92874400	-0.47132200
H	-0.77417100	3.47495000	-0.16922700
C	0.33496800	0.56963000	2.49915200

H	-0.06227200	0.28539000	3.47150600
H	1.05099800	-0.17706200	2.15886500
H	0.80226400	1.54717200	2.59519000
C	-1.75486300	1.72387300	1.99723400
H	-1.21326500	2.65429200	2.14065800
H	-2.53708000	1.85217900	1.24826000
H	-2.17688900	1.42093500	2.95241600
Cl	-3.23626800	2.28658700	-1.42032500
Cl	3.32374400	-6.74719800	0.43472500
C	1.64335900	-3.06423300	-0.93781300
C	1.96364800	-3.13576200	0.48543700
H	2.44276100	-2.83415200	-1.63986600
H	2.98990200	-2.97449400	0.80838700
H	1.35352300	-3.74750800	1.14645000
O	1.30251800	-1.98285900	-0.06113800
C	0.50536000	-3.86088100	-1.48469700
H	0.85757300	-4.82108900	-1.86421200
H	-0.26986800	-4.02585400	-0.73657000
Cl	-0.28725400	-3.00768300	-2.87667100

Energy (0K) = -2577.7434116

Energy (0K) + ZPE = -2577.145175

Enthalpy (298K) = -2577.107861

Free Energy (298K) = -2577.222185

TS_B

Number of imaginary freguencies: 1

N	1.19343100	1.14520500	1.81629300
C	1.52217700	1.34557300	0.34951600
H	0.58299900	1.65213300	-0.11673600
H	1.88890700	0.37896200	0.00136500

N	2.56321100	2.34547300	-0.11279100
C	2.33865100	2.31973400	-1.65302600
H	1.30084000	2.63307100	-1.78284000
H	2.43869800	1.27153600	-1.93557800
C	0.36886000	-0.17393000	1.75980900
H	1.07886800	-0.91026500	1.37710000
H	-0.40449500	0.00919900	1.01366200
C	3.26470000	3.17162900	-2.47358400
C	2.93061100	4.49359000	-2.78896900
C	4.43445200	2.63574800	-3.01686100
C	3.75755300	5.26549600	-3.58952300
H	2.00228200	4.91665500	-2.41676500
C	5.26123500	3.40917300	-3.81931900
H	4.69656600	1.60044200	-2.81873100
C	4.94765100	4.74113300	-4.11054600
H	3.46290500	6.28290600	-3.82456700
H	6.16625700	2.97244400	-4.23168300
C	-0.25047400	-0.62343700	3.05252000
C	-1.55581800	-0.25451700	3.38560400
C	0.43017600	-1.49853000	3.90647100
C	-2.14722100	-0.71964000	4.55141300
H	-2.11921300	0.39483700	2.72194100
C	-0.16084800	-1.96235500	5.07121200
H	1.42932300	-1.83449400	3.64577800
C	-1.45877800	-1.57056100	5.42312500
H	-3.16373500	-0.42112600	4.79132000
H	0.38869900	-2.65319400	5.70219400
C	5.86716200	5.52262700	-4.95737500
H	6.66885500	4.94429700	-5.41370000
C	-2.12870100	-2.02567200	6.65496700

H	-3.19130700	-1.79468000	6.70795900
C	5.81436000	6.83202900	-5.19277000
H	6.54912300	7.30868100	-5.83560800
H	5.05923300	7.48407400	-4.76181000
C	-1.56230500	-2.65633900	7.68165500
H	-2.15197300	-2.94646600	8.54678500
H	-0.50444800	-2.90244700	7.71791100
C	3.96191700	1.90240000	0.19138000
H	4.19670300	2.11610300	1.22997400
H	4.04326500	0.83141200	-0.00244700
H	4.64474000	2.47136000	-0.43475900
C	2.34868400	3.73473900	0.39032400
H	2.57902200	3.77592300	1.45284100
H	3.03786300	4.39553800	-0.13173800
H	1.31733400	4.02973800	0.19533700
C	2.38098100	0.92830800	2.69645700
H	2.02059400	0.61703700	3.67495200
H	3.00925600	0.15302900	2.25826600
H	2.92174400	1.86539200	2.81601400
C	0.34568400	2.24625100	2.37089300
H	0.94853900	3.13669800	2.51993700
H	-0.46763800	2.45773700	1.67635800
H	-0.04176400	1.92822400	3.33598400
Cl	-1.23768200	3.17769000	-0.95215900
Cl	5.54229500	-4.55859100	0.57906700
C	3.54093500	-2.29330700	-0.37490900
C	4.25484800	-2.65729700	0.85196300
H	4.19848700	-2.00574800	-1.20934500
H	5.11788600	-2.06501700	1.11528100
H	3.68057900	-3.09490700	1.65533600

O	3.05606300	-1.24477100	0.38230800
C	2.52242300	-3.30824500	-0.84599700
H	2.99886700	-4.17967800	-1.29467000
H	1.86796100	-3.62130300	-0.03156000
Cl	1.44258200	-2.60168800	-2.12378000

Energy (0K) = -2577.7102225

Energy (0K) + ZPE = -2577.113789

Enthalpy (298K) = -2577.077285

Free Energy (298K) = -2577.188858

B

Number of imaginary freguencies: 0

N	-0.83442400	0.61658000	1.48758900
C	-0.49710400	0.80620100	0.02083400
H	-1.42876900	1.12260900	-0.45117400
H	-0.11910100	-0.17085800	-0.30901700
N	0.55680600	1.79836800	-0.43426600
C	0.34881800	1.75661400	-1.97406200
H	-0.68673700	2.06999000	-2.11999200
H	0.44997800	0.70487000	-2.24236200
C	-1.66682900	-0.69521700	1.42608400
H	-0.95636500	-1.42040200	1.01711600
H	-2.45595700	-0.49461000	0.70064600
C	1.28333500	2.59629200	-2.79844600
C	0.95850900	3.91712500	-3.12779500
C	2.45098400	2.04821100	-3.33403800
C	1.79228500	4.67630900	-3.93345300
H	0.03152200	4.34936600	-2.76287200
C	3.28483300	2.80876700	-4.14169400
H	2.70535800	1.01295400	-3.12550800

C	2.98048600	4.13980400	-4.44634700
H	1.50425400	5.69306000	-4.17939700
H	4.18809200	2.36242700	-4.54765600
C	-2.25919100	-1.16653900	2.72402400
C	-3.54525400	-0.78379500	3.11109700
C	-1.56885400	-2.07826400	3.53112200
C	-4.10793900	-1.27293800	4.28174900
H	-4.11764700	-0.10480500	2.48586200
C	-2.13136900	-2.56716000	4.69944200
H	-0.58336400	-2.42026800	3.22945300
C	-3.41184500	-2.16687400	5.10272000
H	-5.11007600	-0.96232100	4.56341400
H	-1.56981400	-3.27842700	5.29597800
C	3.90672000	4.90763600	-5.29834700
H	4.70527600	4.31984800	-5.74812600
C	-4.05807400	-2.65254000	6.33564100
H	-5.07673200	-2.29739100	6.48292900
C	3.86338700	6.21524500	-5.54551500
H	4.60239100	6.68109800	-6.19141200
H	3.11217000	6.87635400	-5.12156800
C	-3.52668200	-3.45357400	7.25706900
H	-4.10090500	-3.74702700	8.13140500
H	-2.51609700	-3.84834100	7.19375100
C	1.94805500	1.34064400	-0.11039000
H	2.19303500	1.61777900	0.91086900
H	1.98827600	0.25330400	-0.22838700
H	2.64083900	1.85165600	-0.77448600
C	0.34814000	3.19245500	0.05378800
H	0.56294900	3.23941200	1.11953300
H	1.05089700	3.84427200	-0.46192100

H	-0.67785600	3.49568600	-0.15703700
C	0.35390100	0.37958400	2.36192500
H	-0.00646200	0.07824400	3.34375200
H	0.95364900	-0.41075700	1.90464900
H	0.91070900	1.30800500	2.47568100
C	-1.67066000	1.72343200	2.04168400
H	-1.06204400	2.61019500	2.19110800
H	-2.48305000	1.94222000	1.34823800
H	-2.06238500	1.40962900	3.00673100
Cl	-3.23710500	2.69494600	-1.33747600
Cl	3.47810500	-4.78884700	0.04841900
C	1.53795900	-2.74835900	-0.47135600
C	2.42776200	-3.38868700	0.60797900
H	2.19683200	-2.52322700	-1.34112000
H	3.12169300	-2.63636100	0.98001400
H	1.82959800	-3.77170100	1.43646700
O	0.96947800	-1.65667700	0.09458500
C	0.52942300	-3.79674900	-0.95564500
H	1.00125800	-4.69535600	-1.35430800
H	-0.15819300	-4.06926200	-0.15273100
Cl	-0.50929000	-3.16117000	-2.30611400

Energy (0K) = -2577.7270791

Energy (0K) + ZPE = -2577.129463

Enthalpy (298K) = -2577.093117

Free Energy (298K) = -2577.202939

DBM-Cl

Number of imaginary freguencies: 0

C	1.50510000	0.36650500	-1.99260500
H	1.89652100	1.34305600	-2.26670800

C	0.99166700	-1.78312800	-2.13627500
H	0.93603800	-2.76353500	-2.59777200
C	0.55544800	-1.32098600	-0.94134800
H	0.04619800	-1.82362600	-0.13484900
N	0.89089900	0.01843700	-0.87100400
N	1.57903200	-0.70965000	-2.77979500
C	2.22401700	-0.73575200	-4.08554400
H	2.78951800	-1.65921500	-4.17325300
H	2.86268700	0.14391600	-4.16000400
C	0.85385800	0.49215100	-5.80667400
C	0.63190500	-1.71061300	-5.72795200
H	1.25802800	1.45372800	-5.51887500
C	-0.03169300	0.12230900	-6.76043400
H	0.72707600	-2.74847600	-5.40118700
H	-0.57236300	0.70816300	-7.48630000
N	1.25361900	-0.66767300	-5.16946600
N	-0.15807200	-1.25225000	-6.68932300
C	-1.01613800	-2.08307900	-7.55808800
H	-0.79582700	-1.79218200	-8.58641200
H	-0.69247700	-3.11442400	-7.41802900
C	0.56667800	0.92881800	0.24450000
H	-0.52117800	1.00301400	0.29235400
H	0.96268600	1.90683600	-0.03171200
C	-2.48795300	-1.93160000	-7.25648200
C	-3.27249100	-1.03107700	-7.98037100
C	-3.09506300	-2.69580000	-6.26056100
C	-4.62432200	-0.88532400	-7.70752700
H	-2.82231500	-0.44441200	-8.77626100
C	-4.44801500	-2.54956300	-5.98829300
H	-2.51017300	-3.41778200	-5.69754400

C	-5.23823200	-1.63961700	-6.70001700
H	-5.20706100	-0.18247800	-8.29396200
H	-4.90514500	-3.15583000	-5.21124900
C	1.12918400	0.46164400	1.56491000
C	2.49093600	0.57161400	1.84704100
C	0.28710100	-0.08331600	2.53562900
C	2.99301400	0.13768800	3.06507700
H	3.16654400	1.00517900	1.11524700
C	0.78971600	-0.51457900	3.75484600
H	-0.77789800	-0.16493300	2.33656800
C	2.15618100	-0.41720200	4.04145400
H	4.05583500	0.23281000	3.26945200
H	0.10521800	-0.92634100	4.48918900
C	-6.66977800	-1.52631000	-6.36543900
H	-7.01367800	-2.22652100	-5.60577900
C	2.74885500	-0.86277500	5.31617900
H	3.81460500	-0.66193000	5.41382500
C	-7.55051100	-0.67225700	-6.88307600
H	-8.58650200	-0.68118200	-6.55611000
H	-7.29394900	0.06529000	-7.63885900
C	2.12601500	-1.47267200	6.32275300
H	2.67132300	-1.75609800	7.21867900
H	1.06791200	-1.71990500	6.30917400
Cl	0.76670200	-4.80127500	-4.24504100
Cl	2.99052700	2.79372400	-3.90962100

Energy (0K) = -2107.2301705

Energy (0K) + ZPE = -2106.759481

Enthalpy (298K) = -2106.728599

Free Energy (298K) = -2106.830267

DBM^{2+}

Number of imaginary freguencies: 0

C	1.63297800	0.38381100	-1.78445400
H	2.18669100	1.27165300	-2.04739600
C	0.69139300	-1.61051900	-1.88962900
H	0.42101700	-2.56310600	-2.31651900
C	0.42724100	-1.08176300	-0.67317000
H	-0.12388100	-1.47981000	0.16390500
N	1.02760800	0.16024300	-0.62836500
N	1.44240900	-0.67544800	-2.57743900
C	1.98671800	-0.82794500	-3.92011000
H	2.43555500	-1.81398500	-4.00932200
H	2.72948500	-0.05008900	-4.07618700
C	0.31200500	0.46369700	-5.31241700
C	0.51302800	-1.69728900	-5.71702300
H	0.51496200	1.41200700	-4.84120400
C	-0.52822700	0.14252200	-6.32224900
H	0.84322800	-2.72306600	-5.66873600
H	-1.20769800	0.75355700	-6.89454100
N	0.95111200	-0.70339700	-4.93775900
N	-0.38781000	-1.21025500	-6.55605500
C	-1.08482900	-1.97409600	-7.61307000
H	-0.75643800	-1.56273000	-8.56891200
H	-0.72447300	-3.00075300	-7.54035500
C	0.95086600	1.11297000	0.49934000
H	-0.10010300	1.38346300	0.61311900
H	1.49923900	2.00209800	0.18607100
C	-2.58622100	-1.90628300	-7.48456300
C	-3.32894500	-1.08111900	-8.33086200
C	-3.26072500	-2.66356500	-6.52677400

C	-4.70989000	-1.00755800	-8.22077900
H	-2.82098300	-0.49423700	-9.09110700
C	-4.64124600	-2.58700400	-6.41566900
H	-2.70690000	-3.32423200	-5.86554700
C	-5.39360500	-1.75843800	-7.25742600
H	-5.25733200	-0.35769000	-8.89557300
H	-5.15128000	-3.18507000	-5.66566100
C	1.50327900	0.55251500	1.78632500
C	2.87819900	0.42595700	1.98575000
C	0.63967000	0.16595800	2.81244800
C	3.37052200	-0.08083700	3.17935400
H	3.57298900	0.73280600	1.20921700
C	1.13325900	-0.33721400	4.00727700
H	-0.43352000	0.26742600	2.67715100
C	2.51110100	-0.47122700	4.21410100
H	4.44410300	-0.16971500	3.31987400
H	0.43345500	-0.62619700	4.78426200
C	-6.85846300	-1.72044500	-7.09349600
H	-7.24002100	-2.34843300	-6.29006100
C	3.09407800	-0.99433900	5.46367100
H	4.18073500	-1.06303200	5.46171600
C	-7.72869300	-1.01470800	-7.81283900
H	-8.79255200	-1.06624600	-7.59881300
H	-7.43705700	-0.36544700	-8.63405100
C	2.43903000	-1.37459800	6.55882800
H	2.98041800	-1.74529100	7.42471800
H	1.35710200	-1.33644100	6.65274600

Energy (0K) = -1186.478982

Energy (0K) + ZPE = -1186.008322

Enthalpy (298K) = -1185.982318

Free Energy (298K) = -1186.068511

A'

Number of imaginary freguencies: 0

C	1.00988200	0.04766100	1.12769000
H	1.31010000	1.06172900	0.89465600
C	0.65857900	-2.12884900	0.92543000
H	0.67227900	-3.09628800	0.43456600
C	0.17287700	-1.72903600	2.12347800
H	-0.31056900	-2.28641200	2.90966600
N	0.40685500	-0.37146400	2.23027100
N	1.17613700	-1.00056100	0.31616600
C	1.82673500	-0.96715300	-0.98651700
H	2.38180700	-1.89277500	-1.11091900
H	2.49532800	-0.11146400	-1.02306700
C	0.46577300	0.34547100	-2.66082200
C	0.24938700	-1.85866400	-2.68042600
H	0.85128500	1.29896600	-2.33049500
C	-0.41524900	0.01624800	-3.63301900
H	0.34782600	-2.90999800	-2.39761000
H	-0.95567600	0.63349900	-4.33258000
N	0.86693000	-0.84010700	-2.07346800
N	-0.53806700	-1.36033200	-3.62266200
C	-1.39324200	-2.15586700	-4.52788900
H	-1.16301100	-1.82954000	-5.54327900
H	-1.07567200	-3.19302800	-4.42121800
C	-0.00679400	0.48287300	3.36173700
H	-1.09642500	0.44498000	3.40618800
H	0.28801300	1.50030500	3.10262500
C	-2.86590000	-2.00590900	-4.23100600

C	-3.64058500	-1.07897400	-4.93157200
C	-3.48303700	-2.79668800	-3.26230700
C	-4.99291800	-0.93287700	-4.66142200
H	-3.18243500	-0.47167200	-5.70718000
C	-4.83655100	-2.65023900	-2.99302300
H	-2.90545100	-3.53954900	-2.71897700
C	-5.61689200	-1.71333400	-3.68042800
H	-5.56818000	-0.20904400	-5.22939000
H	-5.30187900	-3.27705700	-2.23744600
C	0.59709500	0.05395900	4.67656600
C	1.93587600	0.31021500	4.97333000
C	-0.18606000	-0.60060500	5.62872000
C	2.47438400	-0.08728100	6.18831900
H	2.56444800	0.83041000	4.25624500
C	0.35257100	-0.99468900	6.84486900
H	-1.23341800	-0.79815000	5.41790600
C	1.69624300	-0.74659200	7.14786400
H	3.51840900	0.12185800	6.40438800
H	-0.28442600	-1.49932400	7.56382500
C	-7.04934700	-1.59971600	-3.34975000
H	-7.40499900	-2.32663500	-2.62123900
C	2.32167300	-1.13961400	8.42400200
H	3.37716800	-0.88596400	8.50789300
C	-7.91788200	-0.71592300	-3.83720100
H	-8.95607100	-0.72733300	-3.51737600
H	-7.64845500	0.04985900	-4.55966900
C	1.73465700	-1.75339600	9.44949800
H	2.29923400	-1.99477600	10.34576500
H	0.68679000	-2.04156300	9.45223600
Cl	0.42491800	-5.00526400	-1.35780300

Cl	5.50155800	6.28529900	-0.53006700
C	3.17924300	3.22064400	-0.55598300
C	1.93965100	3.97262600	-0.38203400
H	3.79421700	3.00138600	0.31398300
H	3.70540700	3.25643200	-1.50706800
H	1.65397600	4.28179700	0.62169700
O	1.90478700	2.55307100	-0.59201800
C	1.42437100	4.81856500	-1.49891500
H	1.77401700	5.84628800	-1.39156900
H	1.72666900	4.42962300	-2.47105200
Cl	-0.38860800	4.87986200	-1.50246000

Energy (0K) = -2759.8593333

Energy (0K) + ZPE = -2759.308906

Enthalpy (298K) = -2759.270728

Free Energy (298K) = -2759.392205

$TS_{B'}$

Number of imaginary freguencies: 1

C	1.17798500	0.11618400	-1.86803400
H	1.43645400	1.14368400	-2.13510100
C	0.94497200	-2.07624400	-2.10026500
H	1.01227100	-3.03385200	-2.60247400
C	0.44165000	-1.72087300	-0.89526800
H	-0.00833600	-2.31561100	-0.11664600
N	0.60160100	-0.35276900	-0.76986800
N	1.39848800	-0.91207900	-2.69178500
C	2.04432900	-0.79488700	-3.99149800
H	2.65467200	-1.67855300	-4.15449200
H	2.63548700	0.11812000	-3.98871900
C	0.58319600	0.51413400	-5.56455900

C	0.51981100	-1.69600800	-5.73787300
H	0.92221600	1.45537400	-5.14495400
C	-0.28304100	0.19084900	-6.55293600
H	0.69482800	-2.75437200	-5.53100900
H	-0.87329000	0.81415700	-7.20520500
N	1.07007000	-0.68038400	-5.06701500
N	-0.30951400	-1.18908700	-6.64002300
C	-1.11489000	-1.97607300	-7.59521700
H	-0.92739700	-1.55657900	-8.58477300
H	-0.71796500	-2.99100200	-7.57385800
C	0.14925300	0.46174500	0.37434800
H	-0.93756100	0.37462700	0.42092800
H	0.39733900	1.49579200	0.13215800
C	-2.59006700	-1.96484100	-7.27310300
C	-3.44197000	-1.03612000	-7.87510400
C	-3.13143900	-2.88454200	-6.37567500
C	-4.79617400	-1.01536400	-7.57770600
H	-3.04183500	-0.32537400	-8.59276100
C	-4.48728300	-2.86383300	-6.07960100
H	-2.49182700	-3.62783100	-5.90760600
C	-5.34564300	-1.92925300	-6.66995600
H	-5.43090500	-0.28148500	-8.06351200
H	-4.89289300	-3.58956900	-5.38017600
C	0.77328400	0.04162200	1.68309900
C	2.10693400	0.33130700	1.97278400
C	0.01493700	-0.63983100	2.63637200
C	2.66417300	-0.05903700	3.18156900
H	2.71690900	0.87158900	1.25454200
C	0.57183200	-1.02631400	3.84692200
H	-1.02713600	-0.86740000	2.42939500

C	1.90968700	-0.74210800	4.14345500
H	3.70398800	0.17587600	3.39148000
H	-0.04485600	-1.55775900	4.56445700
C	-6.77737200	-1.95444000	-6.31801700
H	-7.05425600	-2.72789500	-5.60338600
C	2.55339700	-1.12337600	5.41403500
H	3.61732600	-0.89852600	5.46805900
C	-7.73075300	-1.14566900	-6.77639500
H	-8.75865800	-1.25827200	-6.44320600
H	-7.54401800	-0.34805100	-7.49049800
C	1.97229200	-1.69178400	6.46862600
H	2.55049700	-1.92953200	7.35715000
H	0.91520200	-1.94112900	6.50485000
Cl	0.94231900	-4.90424700	-4.61579400
Cl	5.47900000	4.65015900	-3.63391400
C	3.80341000	3.04636800	-3.70555300
C	2.50199100	3.59687700	-3.32117300
H	4.31452100	2.43234500	-2.97956600
H	3.97402900	2.84087000	-4.75224800
H	2.44402100	3.92649300	-2.27334500
O	2.04801100	2.31286300	-3.55885500
C	1.95850000	4.67212500	-4.23505100
H	2.46176100	5.62623900	-4.07992600
H	2.03416900	4.37889900	-5.28282200
Cl	0.19570600	4.96202500	-3.91214900

Energy (0K) = -2759.826933

Energy (0K) + ZPE = -2759.277894

Enthalpy (298K) = -2759.240701

Free Energy (298K) = -2759.357675

B'

Number of imaginary freguencies: 0

C	0.89461300	0.11939200	1.14061600
H	1.18775900	1.13258600	0.76753800
C	0.63452400	-2.08393600	1.03160400
H	0.69974600	-3.07163600	0.60366300
C	0.14508200	-1.66044900	2.21884600
H	-0.30125200	-2.20908600	3.03267400
N	0.31885900	-0.28857500	2.26593200
N	1.09356300	-0.95941400	0.37302000
C	1.73534300	-0.89646900	-0.93360100
H	2.28786600	-1.81681900	-1.09982600
H	2.36270300	-0.00438600	-0.92885800
C	0.28138000	0.52128100	-2.39720400
C	0.23350700	-1.66646500	-2.77942500
H	0.64196900	1.41546100	-1.88456600
C	-0.56889700	0.28741000	-3.42379100
H	0.43081000	-2.73938700	-2.71352700
H	-1.15277800	0.96541500	-4.02541700
N	0.76385500	-0.71544200	-2.00527200
N	-0.58480000	-1.07788000	-3.64350900
C	-1.36515700	-1.76338600	-4.69176700
H	-1.17406300	-1.22979500	-5.62403200
H	-0.95168800	-2.76720800	-4.78461800
C	-0.11975800	0.58395400	3.37032800
H	-1.20684900	0.50735500	3.43098800
H	0.13227800	1.60314100	3.07683900
C	-2.84482800	-1.81304600	-4.39301800
C	-3.70556600	-0.83992800	-4.90531300
C	-3.38281000	-2.83346400	-3.60951800

C	-5.06440500	-0.87440000	-4.63093200
H	-3.30871700	-0.04858900	-5.53505900
C	-4.74298400	-2.86744900	-3.33515500
H	-2.73706400	-3.61363000	-3.21584700
C	-5.61054000	-1.89031900	-3.83686800
H	-5.70398700	-0.10180900	-5.04505000
H	-5.14491100	-3.67142300	-2.72478900
C	0.51161100	0.22452900	4.69366800
C	1.84410700	0.53569200	4.96567000
C	-0.23685500	-0.42495600	5.67676900
C	2.41006600	0.19704000	6.18608400
H	2.44583800	1.05247700	4.22348600
C	0.32881200	-0.76039600	6.89843200
H	-1.27860800	-0.66697200	5.48501600
C	1.66620500	-0.45595000	7.17668400
H	3.44889700	0.44824800	6.38166900
H	-0.28142900	-1.26525800	7.64029700
C	-7.04684400	-1.98070500	-3.51547900
H	-7.31322500	-2.81458400	-2.86790000
C	2.31957400	-0.78453200	8.45699600
H	3.37188000	-0.51037600	8.51146500
C	-8.01690800	-1.16804900	-3.93006300
H	-9.04602200	-1.33600100	-3.62500600
H	-7.84465200	-0.31433800	-4.57999900
C	1.76061700	-1.36242300	9.51841500
H	2.34462200	-1.55700000	10.41361400
H	0.71725000	-1.66420200	9.55307500
Cl	0.79713600	-5.06076000	-2.52938000
Cl	4.89994900	4.58121400	-1.23144100
C	3.67177200	3.22600800	-1.36951300

C	2.56375900	3.22928600	-0.30326900
H	4.24637700	2.30549700	-1.27975800
H	3.25342100	3.29579700	-2.37506700
H	3.06503800	3.29230800	0.68778000
O	1.83772500	2.09611500	-0.48311800
C	1.73566900	4.50922200	-0.46080400
H	2.32801600	5.42082300	-0.38030700
H	1.19900200	4.50000700	-1.41132700
Cl	0.45933900	4.64893100	0.82620000

Energy (0K) = -2759.8465289

Energy (0K) + ZPE = -2759.296476

Enthalpy (298K) = -2759.259495

Free Energy (298K) = -2759.375581