Supporting Information for

Cu-Catalyzed Controllable C−H Mono-/Di-/Triarylations of Imidazolium Salts for Ionic Functional Materials

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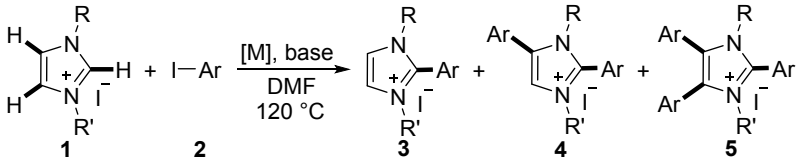
I. General remarks

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Cu_2O (97% purity) was directly used as purchased from Energy Chemical (China) Co., Ltd. All syntheses and manipulations were carried out under a N_2 atmosphere using standard Schlenk or vacuum line techniques. DMF was dried by refluxing over CaH_2. Analytical thin layer chromatography was performed on HG/T2354-92 GF254 plates (Qingdao Haiyang Chemical Co., Ltd.). The (benz)imidazolium substrates[1] are prepared by *N*-quaternizing of aryl alkyl or alkyl alkyl substituted (benz)imidazoles with iodomethane, iodoethane, and 1-iodobutane, 1,3-diphenylimidazolium tetrafluoroborate[2] 2-ethylimidazo[1,5-*a*]pyridin-2-ium iodide,[3] 1,3-dibutyl-4,5-diphenyl-1*H*-imidazol-3-ium iodide,[4] (*E*)-(2-iodovinyl)benzene,[5] (iodoethynyl)benzene,[6] were prepared according to the literature procedures.

NMR spectra were obtained on a Bruker AV II-400 MHz. The ^1H NMR (400 MHz) chemical shifts were measured relative to $CDCl_3$ or DMSO-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm; DMSO-d_6: δ = 2.50 ppm). The ^{13}C NMR (100 MHz) chemical shifts were obtained using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm; DMSO-d_6: δ = 39.52 ppm). High-resolution mass spectra (HR-MS) were obtained on a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected.

II. General procedure for the C–H functionalization of imidazolium salts



1 **2** **3** **4** **5**

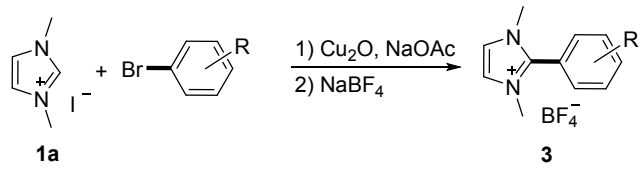
A Schlenk tube with a magnetic stir bar was charged with an imidazolium salt **1** (0.2 mmol, 1.0 equiv), an iodide **2** (2.0-5.0 equiv), Cu_2O (5.7 mg, 20 mol%), NaOAc (16 mg, 1.0 equiv) or K_2CO_3 (2.0-5.0 equiv) and DMF (1 mL). The reaction mixture was stirred at 120 °C for 24 h or 36 h in an oil bath under a N_2 atmosphere and then cooled down to room temperature. DMF was removed under reduced pressure, and the residue was passed through a silica gel column eluted with dichloromethane/methanol (v/v, 100/1−20/1) to afford the desired product.

Table S1. Screening of the catalyst[a]

Entry	Cat./ mol%	Base/ 1 equiv	Yield[b] **3aa**:**4aa**:**5aa**
1	Cu_2O/10	NaOAc	87:0:0
2	Cu_2O/5	NaOAc	65:0:0
3	Cu_2O/2	NaOAc	47:0:0
4	CuI/20	NaOAc	75:0:0
5	CuI/40	NaOAc	88:0:0

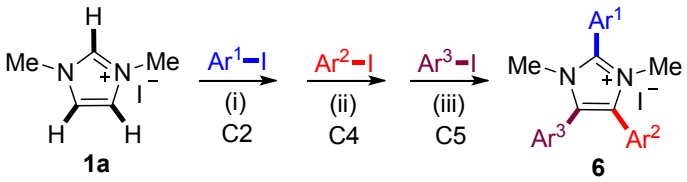
[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2 equiv), catalyst (x mol%) and NaOAc (1 equiv) in DMF (1 mL) at 120 °C for 24 h under a N_2 atmosphere. [b] Isolated yield.

General procedure for the C2-arylation of 1a with arylbromides



A Schlenk tube with a magnetic stir bar was charged with **1a** (0.2 mmol, 1.0 equiv), an aryl bromide (0.4 mmol, 2.0 equiv), Cu_2O (5.7 mg, 20 mol%), NaOAc (16 mg, 1.0 equiv) and DMF (1 mL). The reaction mixture was stirred at 120 °C for 24 h in an oil bath under a N_2 atmosphere. After the mixture was cooled down to room temperature, $NaBF_4$ (1 mol, 5 equiv) was added to stir for another 2 h. DMF was then removed under reduced pressure, and the residue was passed through a silica gel column eluted with dichloromethane/methanol (v/v, 50/1−20/1) to afford the desired product.

III. General procedure for the sequential C–H arylation of imidazolium salts

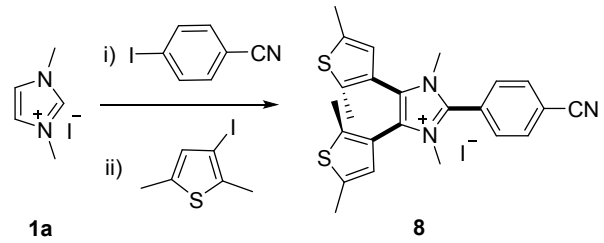


A Schlenk tube with a magnetic stir bar was charged with imidazolium salt **1a** (0.2 mmol, 1.0 equiv), an Ar^1I (0.2 mmol, 1.0 equiv), Cu_2O (5.7 mg, 20 mol%), NaOAc (0.2 mmol, 1.0 equiv) and DMF (1 mL). The reaction mixture was stirred at 120 °C for 24 h in an oil bath under a N_2 atmosphere. After the reaction was cooled down to room temperature, Cu_2O (2.9 mg, 10 mol%), an Ar^2I (0.2 mmol, 1.0 equiv) and KCO_3 (0.2 mmol, 1.0 equiv) were added under the protection of N_2. The reaction was stirred at 120 °C for another 24 h. After the reaction was cooled down to room temperature, Cu_2O (2.9 mg, 10 mol%), an Ar^3I (0.6 mmol, 3.0 equiv) and KCO_3 (0.6 mmol, 3.0 equiv) were added again under the protection of N_2. The

mixture was reacted at 120 °C for further 24 h. Finally, DMF was removed under reduced pressure after the mixture was cooled down to room temperature. The residue was passed through a silica gel column eluted with dichloromethane/methanol (v/v, 100/1−50/1) to afford the desired product.

IV. Synthesis of 7 and 8

2,2'-(1,4-Phenylene)bis(3-ethyl-1-phenyl-1*H*-benzo[*d*]imidazol-3-ium) diiodide (7). A Schlenk tube with a magnetic stir bar was charged with imidazolium salt **1i** (0.1 mmol), 1,4-diiodobenzene (0.1 mmol), Cu_2O (5.7 mg, 40 mol%), NaOAc (16 mg, 2.0 equiv) and DMF (1 mL). The reaction mixture was stirred at 120 °C for 30 h in an oil bath. After the volatiles were removed under reduced pressure, the residue was passed through a silica gel column eluted with dichloromethane/methanol (v/v, 50/1−10/1) to afford **7** as a light yellow solid (65 mg, 84% yield). M.p.: > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.45 (t, J = 7.2 Hz, 6H), 4.49 (q, J = 7.2 Hz, 4H), 7.46–7.52 (m, 8H), 7.58–7.63 (m, 4H), 7.76 (t, J = 8.0 Hz, 2H), 7.85 (t, J = 8.0 Hz, 2H) , 7.95 (s, 4H), 8.35 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.4, 41.8, 113.3, 114.0, 125.4, 127.2, 127.3, 127.7, 130.0, 130.6, 130.7, 131.4, 132.1, 132.6, 148.9 ppm. HRMS (ESI): calcd for $C_{36}H_{32}IN_4^+$ ([M−I$^-$]$^+$) 647.1666, found 647.1669.



2-(4-Cyanophenyl)-4,5-bis(2,5-dimethylthiophen-3-yl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (8). A Schlenk tube with a magnetic stir bar was charged with imidazolium salt **1a** (0.2 mmol, 1 equiv), 4-iodobenzonitrile (0.2 mmol, 1 equiv), Cu_2O (5.7 mg, 20 mol%), NaOAc (16 mg, 1 equiv) and DMF (1 mL). The reaction mixture was stirred at 120 °C for 24 h in an oil bath. The reaction was cooled down to room temperature, and 3-iodo-2,5-dimethylthiophene (0.6 mmol, 3 equiv), Cu_2O (2.9 mg, 10 mol%), K_2CO_3 (83 mg, 3 equiv) were added under the protection of N_2. Then the mixture was reacted at 120 °C for another 24 h. The volatiles were then removed under reduced pressure after the mixture was cooled down to room temperature. The residue was passed through a silica gel column eluted with

dichloromethane/methanol (v/v, 100/1−50/1) to afford **8** as a white solid (51 mg, 47% yield). M.p.: 245–247 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.97 (s, 4H), 2.21 (s, 2H), 2.42 (s, 6H), 3.49 (s, 6H), 6.62 (s, 0.8H), 6.89 (s. 1.2H), 8.12 (d, J = 6.8 Hz, 2H) , 8.28 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.5, 14.9, 34.2, 114.9, 118.0, 121.6, 126.5, 127.7, 132.0, 133.3, 137.5 ppm. HRMS (ESI): calcd for $C_{24}H_{24}N_3S_2^+$ ([M−I$^-$]$^+$) 418.1406, found 418.1401.

V. Electrochromism of 7

Fabrication of an electrochromic device: Two pieces of FTO coated glasses using as the electrodes were spaced with two pieces of parafilm (thickness of about 50 μm). The two closed glasses were pressed to stick together with parafilm for several minutes by two spring clips. After removal of the spring clips, the device was used as described. The acetonitrile solutions of **7** without any supporting electrolyte were injected into the space of the two pieces of FTO glasses by a syringe, respectively. The adding potential was output from an alkaline battery and the voltage was measured by a multimeter.

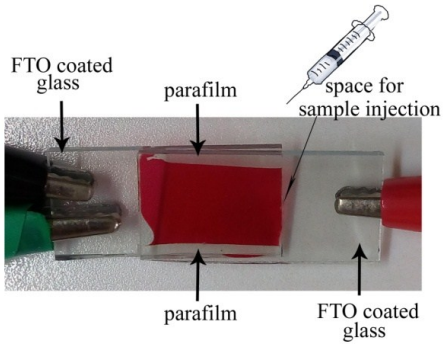


Figure S1. Diagram of the assembly of electrochromic device.

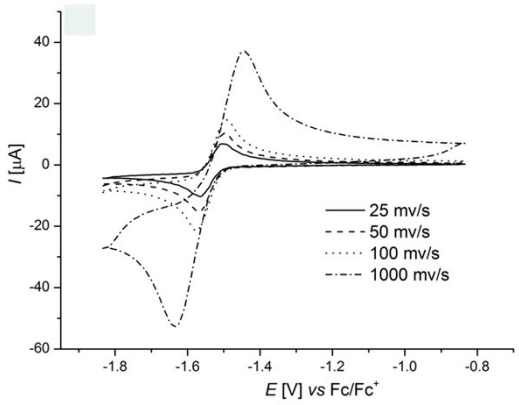


Figure S2. Cyclic voltammogram of **7** at different scan rates in DMF solution with [^{n}Bu$_4$N][PF$_6$] as supporting electrolyte (0.1 M), referenced to Fc/Fc$^+$.

VI. Photochromism of 8

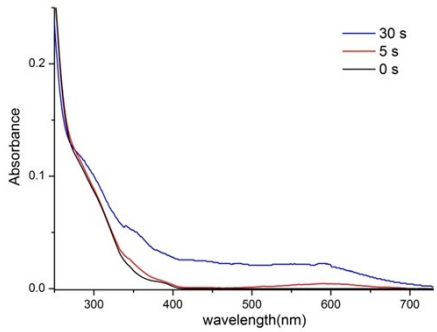
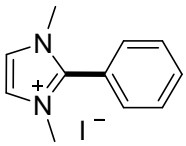
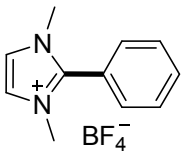


Figure S3. Absorption spectra of **8** in acetonitrile (10 μM) irradiated with an UV light (365 nm, 4 W).

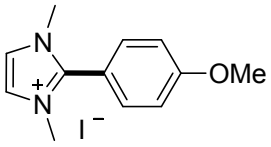
VII. Characterization of the products



1,3-Dimethyl-2-phenyl-1*H*-imidazol-3-ium iodide (3aa).[7] A white solid (57 mg, 95% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 6H), 7.69–7.78 (m, 5H), 7.88 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.7, 121.2, 123.2, 129.4, 130.6, 132.3, 144.1 ppm.

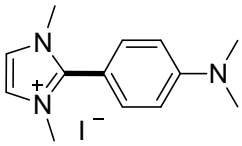


1,3-Dimethyl-2-phenyl-1*H*-imidazol-3-ium tetrafluoroborate (3aa-BF_4).[8] A white solid (35 mg, 67% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 6H), 7.69–7.78 (m, 5H), 7.88 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.7, 121.2, 123.2, 129.4, 130.6, 132.3, 144.1 ppm. ^{19}F NMR (DMSO-d_6, 376 MHz): δ= -148.35 (s), -148.29 (s) ppm.

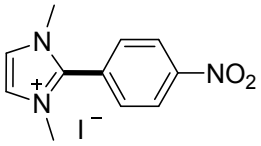


2-(4-Methoxyphenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ab). A light yellow solid (63 mg, 95%

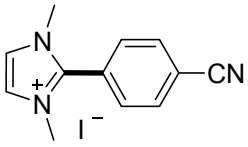
yield). M.p.: 55–57 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.84 (s, 6H), 3.89 (s, 3H), 7.13 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.8 Hz, 2H), 7.76 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 37.1, 55.9, 112.2, 115.5, 123.8, 132.8, 145.0, 162.8 ppm. HRMS (ESI): calcd for $C_{12}H_{15}N_2O^+$ ([M−I$^-$]$^+$) 203.1179, found 203.1180.



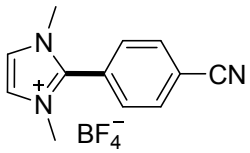
2-(4-(Dimethylamino)phenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ac). A white solid (50 mg, 72% yield). M.p.: 181–183 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.07 (s, 6H), 3.85 (s, 6H), 6.82 (d, J = 8.8 Hz, 2H), 7.44 (d, J = 8.8 Hz, 2H), 7.71 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 36.9, 40.2, 105.7, 112.2, 123.3, 131.7, 143.3, 152.7 ppm. HRMS (ESI): calcd for $C_{13}H_{18}N_3^+$ ([M−I$^-$]$^+$) 216.1495, found 216.1494.



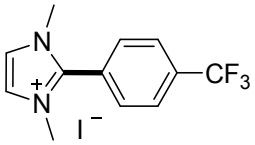
1,3-Dimethyl-2-(4-nitrophenyl)-1*H*-imidazol-3-ium iodide (3ad). A yellow solid (61 mg, 88% yield). M.p.: 148–150 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.72 (s, 6H), 7.94 (s, 2H), 8.11 (d, J = 8.4 Hz, 2H), 8.52 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.8, 123.8, 124.2, 127.3, 132.7, 142.2, 149.6 ppm. HRMS (ESI): calcd for $C_{11}H_{12}N_3O_2^+$ ([M−I$^-$]$^+$) 218.0924, found 218.0926.



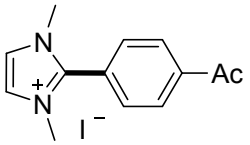
2-(4-Cyanophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ae). A yellow solid (60 mg, 92% yield). M.p.: 156–160 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.71 (s, 6H), 7.92 (s, 2H), 8.01 (d, J = 8.4 Hz, 2H), 8.21 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.8, 114.9, 117.9, 123.7, 125.7, 131.9, 133.2, 142.5 ppm. HRMS (ESI): calcd for $C_{12}H_{12}N_3^+$ ([M−I$^-$]$^+$) 198.1026, found 198.1028.



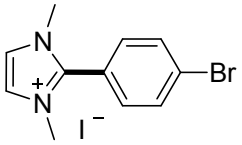
2-(4-Cyanophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium tetrafluoroborate (3ae-BF_4).[8] A light yellow solid (47 mg, 82% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 6H), 7.91 (s, 2H), 8.00 (d, J = 8.4 Hz, 2H), 8.20 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.8, 114.9, 117.9, 123.7, 125.7, 131.8, 133.2, 142.5 ppm. ^{19}F NMR (DMSO-d_6, 376 MHz): δ= -148.43 (s), -148.38 (s) ppm.



1,3-Dimethyl-2-(4-(trifluoromethyl)phenyl)-1*H*-imidazol-3-ium iodide (3af). A light yellow solid (66 mg, 89% yield). M.p.: 56–58 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.87 (s, 6H), 7.86 (s, 2H), 7.91 (d, J = 8.0 Hz, 2H), 8.09 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 37.4, 110.1, 123.3 (q, $^1J_{C\text{-}F}$ = 271.6 Hz), 124.5, 126.9 (q, $^3J_{C\text{-}F}$ = 3.7 Hz), 132.4, 134.6 (d, $^2J_{C\text{-}F}$ = 33.0 Hz), 143.3 ppm. HRMS (ESI): calcd for $C_{12}H_{12}F_3N_2^+$ ([M−I$^-$]$^+$) 241.0947, found 241.0947.

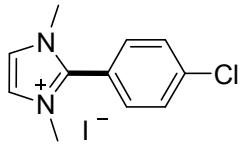


2-(4-Acetylphenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ag). A yellow solid (61 mg, 90% yield). M.p.: 148–150 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.69 (s, 3H), 3.71 (s, 6H), 7.91 (s, 2H), 7.95 (d, J = 8.4 Hz, 2H), 8.22 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 27.1, 35.8, 123.5, 125.2, 128.8, 131.2, 139.3, 143.2, 197.6 ppm. HRMS (ESI): calcd for $C_{13}H_{15}N_2O^+$ ([M−I$^-$]$^+$) 215.1179, found 215.1179.

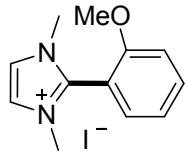


2-(4-Bromophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ah). A white solid (63 mg, 83% yield). M.p.: 144–146 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.69 (s, 6H), 7.74 (d, J = 8.4 Hz, 2H), 7.88 (s,

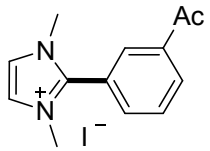
2H), 7.94 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.7, 120.4, 123.4, 126.5, 132.5, 132.8, 143.2 ppm. HRMS (ESI): calcd for $C_{11}H_{12}BrN_2^+$ ([M−I$^-$]$^+$) 251.0178, found 251.0151.



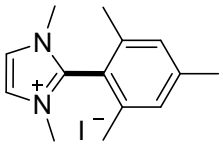
2-(4-Chlorophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium (3ai). A white solid (60 mg, 90% yield). M.p.: 166–168 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.69 (s, 6H), 7.79–7.84 (m, 4H), 7.89 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.8, 120.0, 123.4, 129.6, 132.7, 137.4, 143.1 ppm. HRMS (ESI): calcd for $C_{11}H_{12}ClN_2^+$ ([M−I$^-$]$^+$) 207.0684, found 207.0680.



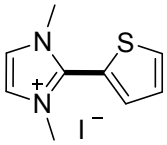
2-(2-Methoxyphenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3aj). A light yellow solid (54 mg, 82% yield). M.p.: 196–198 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.63 (s, 6H), 3.86 (s, 3H), 7.25 (t, J = 7.6 Hz, 1H), 7.37 (d, J = 8.8 Hz, 1H), 7.65 (d, J = 6.8 Hz, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.90 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.4, 56.2, 109.1, 112.6, 121.2, 123.3, 132.0, 134.7, 142.1, 157.6 ppm. HRMS (ESI): calcd for $C_{12}H_{15}N_2O^+$ ([M−I$^-$]$^+$) 203.1179, found 203.1180.



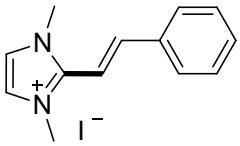
2-(3-Acetylphenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3ak). A light yellow solid (55 mg, 81% yield). M.p.: 195–197 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.66 (s, 3H), 3.70 (s, 6H), 7.86 (t, J = 7.6 Hz, 1H), 7.90 (s, 2H), 8.03 (d, J = 7.6 Hz, 1H), 8.28 (d, J = 8.0 Hz, 1H), 8.34 (s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 27.0, 35.7, 121.8, 123.3, 130.0, 130.6, 131.6, 135.0, 137.5, 143.3, 197.2 ppm. HRMS (ESI): calcd for $C_{13}H_{15}N_2O^+$ ([M−I$^-$]$^+$) 215.1179, found 215.1175.



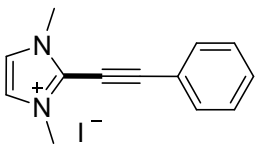
2-Mesityl-1,3-dimethyl-1*H*-imidazol-3-ium iodide (3al). A light yellow solid (42 mg, 62% yield). M.p.: 102–104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.03 (s, 6H), 2.38 (s, 3H), 3.75 (s, 6H), 7.07 (s, 2H), 8.15 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.0, 21.5, 36.1, 110.1, 116.9, 124.3, 129.7, 138.9, 143.9 ppm. HRMS (ESI): calcd for $C_{14}H_{19}N_2^+$ ($[M-I^-]^+$) 215.1543, found 215.1537.



1,3-Dimethyl-2-(thiophen-2-yl)-1*H*-imidazol-3-ium iodide (3am). A yellow solid (55 mg, 90% yield). M.p.: 104–106 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.92 (s, 6H), 7.34 (dd, *J* = 5.2 Hz, 3.6 Hz, 1H), 7.83 (dd, *J* = 5.2 Hz, 1.2 Hz, 1H), 7.88–7.90 (m, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 37.4, 118.5, 124.7, 129.0, 133.1, 136.3, 139.5 ppm. HRMS (ESI): calcd for $C_9H_{11}N_2S^+$ ($[M-I^-]^+$) 179.0637, found 179.0638.

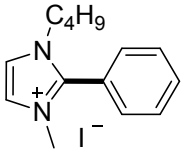


(*E*)-1,3-Dimethyl-2-styryl-1*H*-imidazol-3-ium iodide (3an). A gray solid (40 mg, 62% yield). M.p.: 182–184 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.95 (s, 6H), 7.29 (d, *J* = 16.8 Hz, 1H), 7.49–7.52 (m, 3H), 7.58 (d, *J* = 16.8 Hz, 1H), 7.76 (s, 2H), 7.83 (d, *J* = 6.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 36.1, 108.1, 123.4, 128.0, 129.0, 130.4, 134.6, 142.0, 142.4 ppm. HRMS (ESI): calcd for $C_{13}H_{15}N_2^+$ ($[M-I^-]^+$) 199.1230, found 199.1225.

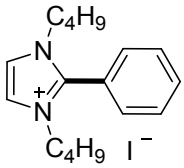


1,3-Dimethyl-2-(phenylethynyl)-1*H*-imidazol-3-ium iodide (3ao). A light brown solid (21 mg, 32% yield). M.p.: 156–158 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.96 (s, 6H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 7.2 Hz, 2H), 7.87 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 36.0,

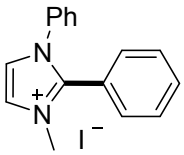
70.2, 105.0, 118.3, 124.2, 129.2, 131.7, 132.4 ppm. HRMS (ESI): calcd for $C_{13}H_{13}N_2^+$ ([M−I$^-$]$^+$) 197.1073, found 197.1069.



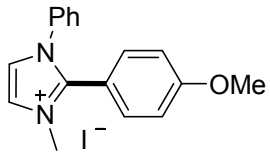
1-Butyl-3-methyl-2-phenyl-1*H*-imidazol-3-ium iodide (3ba). Light yellow oil (62 mg, 91% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, *J* = 7.6 Hz, 3H), 1.22–1.31 (m, 2H), 1.73–1.80 (m, 2H), 3.85 (s, 3H), 4.08 (t, *J* = 7.6 Hz, 2H), 7.64–7.74 (m, 6H), 7.90 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.5, 19.6, 32.1, 37.1, 49.3, 121.0, 122.3, 124.5, 130.1, 131.0, 132.9, 144.5 ppm. HRMS (ESI): calcd for $C_{14}H_{19}N_2^+$ ([M−I$^-$]$^+$) 215.1543, found 215.1541.



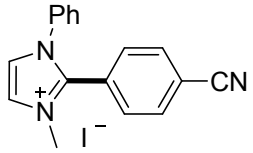
1,3-Dibutyl-2-phenyl-1*H*-imidazol-3-ium iodide iodide (3ca). Yellow oil (69 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.81 (t, *J* = 7.6 Hz, 6H), 1.20–1.29 (m, 4H), 1.71–1.77 (m, 4H), 4.07 (t, *J* = 7.6 Hz, 4H), 7.66–7.73 (m, 5H), 7.85 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.5, 19.6, 32.1, 49.2, 121.0, 122.7, 130.2, 130.8, 133.0, 144.2 ppm. HRMS (ESI): calcd for $C_{17}H_{25}N_2^+$ ([M−I$^-$]$^+$) 257.2012, found 257.2016.



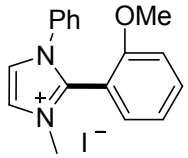
3-Methyl-1,2-diphenyl-1*H*-imidazol-3-ium iodide (3da). A light yellow solid (69 mg, 96% yield). M.p.: 170–172 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.79 (s, 3H), 7.40–7.60 (m, 10H), 8.13 (s, 1H), 8.18 (s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.9, 121.4, 123.5, 123.7, 126.2, 129.0, 129.6, 130.1, 130.9, 132.0, 135.0, 144.3 ppm. HRMS (ESI): calcd for $C_{16}H_{15}N_2^+$ ([M−I$^-$]$^+$) 235.1230, found 235.1227.



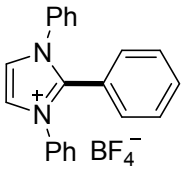
2-(4-Methoxyphenyl)-3-methyl-1-phenyl-1*H*-imidazol-3-ium iodide (3db). A yellow semisolid (74 mg, 95% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.80 (s, 3H), 4.01 (s, 3H), 6.93 (d, *J* = 8.8 Hz, 2H), 7.39–7.43 (m, 5H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.57 (t, *J* = 0.8 Hz, 1H), 8.03 (t, *J* = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 37.7, 55.7, 112.5, 115.1, 123.4, 124.8, 126.4, 130.1, 130.4, 133.2, 135.2, 144.9, 162.5 ppm. HRMS (ESI): calcd for $C_{17}H_{17}N_2O^+$ ($[M-I^-]^+$) 265.1335, found 265.1334



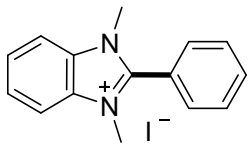
2-(4-Cyanophenyl)-3-methyl-1-phenyl-1*H*-imidazol-3-ium iodide (3de). A yellow solid (71 mg, 92% yield). M.p.: 96–98 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.04 (s, 3H), 7.36–7.47 (m, 3H), 7.50 (d, *J* = 7.6 Hz, 2H), 7.67 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 2H), 8.11 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 38.0, 116.2, 117.4, 124.2, 125.5, 126.5, 128.6, 128.9, 130.3, 131.0, 133.0, 134.6, 142.7 ppm. HRMS (ESI): calcd for $C_{17}H_{14}N_3^+$ ($[M-I^-]^+$) 260.1182, found 260.1181.



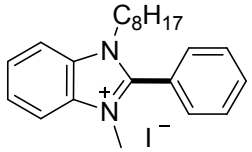
2-(2-Methoxyphenyl)-3-methyl-1-phenyl-1*H*-imidazol-3-ium iodide (3dj). A brown solid (63 mg, 81% yield). M.p.: 92–94 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.71 (s, 3H), 3.92 (s, 3H), 6.95 (d, *J* = 8.4 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 7.32–7.41 (m, 5H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.65 (s, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 8.20 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 37.2, 56.0, 109.6, 111.6, 121.8, 123.5, 125.1, 125.5, 129.9, 130.4, 133.5, 134.8, 135.2, 142.5, 157.7 ppm. HRMS (ESI): calcd for $C_{17}H_{17}N_2O^+$ ($[M-I^-]^+$) 265.1335, found 265.1333.



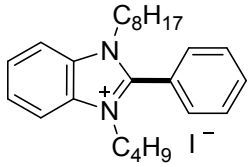
1,2,3-Triphenyl-1*H*-imidazol-3-ium tetrafluoroborate (3ea). A white solid (68 mg, 88% yield). M.p.: 236–238 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.33 (t, J = 7.6 Hz, 2H), 7.40–7.43 (m, 3H), 7.48–7.54 (m, 10H), 8.42 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 121.6, 124.0, 126.4, 128.6, 129.7, 130.3, 131.2, 131.8, 135.0, 144.5 ppm. ^{19}F NMR (DMSO-d_6, 376 MHz): δ= -148.32 (s), -148.27 (s) ppm. HRMS (ESI): calcd for $C_{21}H_{17}N_2^+$ ([M−BF_4^-]$^+$) 297.1386, found 297.1382.



1,3-Dimethyl-2-phenyl-1*H*-benzo[*d*]imidazol-3-ium iodide (3fa).[9] A white solid (61 mg, 87% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.90 (s, 6H), 7.78–7.87 (m, 5H), 7.91 (d, J = 6.8 Hz, 2H), 8.14 (t, J = 3.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ = 32.8, 113.4, 121.0, 126.6, 129.4, 130.7, 131.7, 132.9, 150.3 ppm.

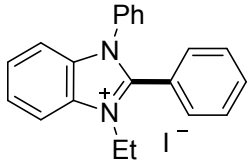


1-Butyl-3-methyl-2-phenyl-1*H*-benzo[*d*]imidazol-3-ium iodide (3ga). A semisolid (88 mg, 98% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, J = 7.2 Hz, 3H), 1.16–1.23 (m, 10H), 1.79–1.87 (m, 2H), 3.99 (s, 3H), 4.34 (t, J = 7.6 Hz, 2H), 7.67–7.69 (m, 2H), 7.72–7.80 (m, 4H), 7.88 (t, J = 5.6 Hz, 1H), 7.93 (d, J = 7.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.2, 22.6, 26.6, 28.8, 29.0, 29.4, 31.7, 34.4, 47.3, 113.5, 114.1, 120.7, 127.71, 127.74, 130.2, 131.0, 131.1, 132.3, 133.5, 150.1 ppm. HRMS (ESI): calcd for $C_{22}H_{29}N_2^+$ ([M−I^-]$^+$) 321.2325, found 321.2321.

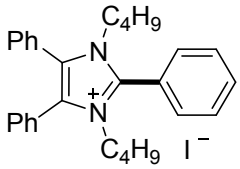


3-Butyl-1-octyl-2-phenyl-1*H*-benzo[*d*]imidazol-3-ium iodide (3ha). A semisolid (95 mg, 97% yield).

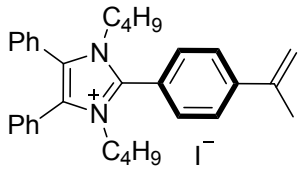
^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.79–0.84 (m, 6H), 1.15–1.31 (m, 12H), 1.79–1.84 (m, 4H), 4.32–4.38 (m, 4H), 7.67–7.71 (m, 2H), 7.73–7.81 (m, 3H), 7.84–7.90 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.5, 14.2, 20.0, 22.6, 26.6, 28.8, 29.0, 29.4, 31.4, 31.7, 47.3, 47.5, 113.9, 114.0, 120.9, 127.7, 130.3, 130.6, 131.3, 133.5, 149.8 ppm. HRMS (ESI): calcd for $C_{25}H_{35}N_2^+$ ([M−I$^-$]$^+$) 363.2795, found 363.2772.



3-Ethyl-1,2-diphenyl-1*H*-benzo[*d*]imidazol-3-ium iodide (3ia). A gray solid (83 mg, 98% yield). M.p.: 188–190 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.45 (t, J = 7.2 Hz, 3H), 4.45 (q, J = 7.2 Hz, 2H), 7.53–7.67 (m, 9H), 7.71–7.85 (m, 4H), 8.33 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.3, 41.6, 113.2, 113.8, 121.4, 126.9, 127.4, 127.6, 129.1, 130.0, 130.5, 130.6, 132.5, 132.7, 150.3 ppm. HRMS (ESI): calcd for $C_{21}H_{19}N_2^+$ ([M−I$^-$]$^+$) 299.1543, found 299.1540.

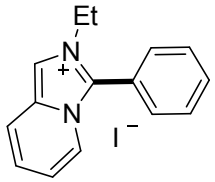


1,3-Dibutyl-2,4,5-triphenyl-1*H*-imidazol-3-ium iodide (3ja). A yellow solid (100 mg, 93% yield). M.p.: 128–130 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.54 (t, J = 7.6 Hz, 6H), 0.92–1.01 (m, 4H), 1.37–1.44 (m, 4H), 3.96 (t, J = 8.0 Hz, 4H), 7.37–7.38 (m, 6H), 7.63–7.65 (m, 4H), 7.70–7.72 (m, 3H), 8.10 (d, J = 7.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.0, 19.4, 31.6, 46.9, 122.0, 125.4, 129.0, 130.0, 130.1, 131.2, 131.3, 132.0, 132.6, 143.6 ppm. HRMS (ESI): calcd for $C_{29}H_{33}N_2^+$ ([M−I$^-$]$^+$) 409.2638, found 409.2648.

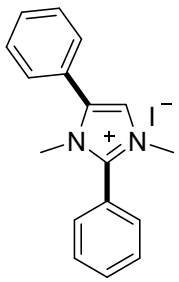


1,3-Dibutyl-4,5-diphenyl-2-(4-(prop-1-en-2-yl)phenyl)-1*H*-imidazol-3-ium iodide (3jp). A white solid (112 mg, 97% yield). M.p.: 131–133 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.56 (t, J = 7.6 Hz, 6H), 0.94–1.03 (m, 4H), 1.38–1.46 (m, 4H), 2.21 (s, 3H), 3.96 (t, J = 7.6 Hz, 4H), 5.27 (s, 1H), 5.56 (s, 1H),

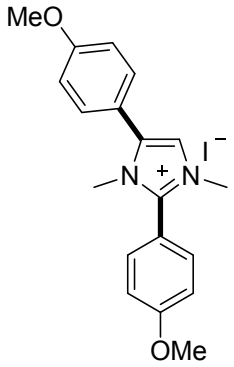
7.37–7.39 (m, 6H), 7.63–7.65 (m, 4H), 7.77 (d, J = 8.0 Hz, 2H), 8.07 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.1, 18.6, 20.7, 30.8, 46.1, 114.6, 119.8, 124.7, 125.9, 128.1, 129.3, 130.3, 130.5, 131.2, 140.9, 142.7, 144.3 ppm. HRMS (ESI): calcd for $C_{32}H_{37}N_2^+$ ([M−I$^-$]$^+$) 449.2957, found 449.2946.



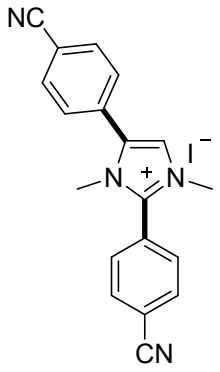
2-Ethyl-3-phenylimidazo[1,5-*a*]pyridin-2-ium iodide (3ka). A gray solid (54 mg, 77% yield). M.p.: 102–104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.59 (t, J = 7.2 Hz, 3H), 4.57 (q, J = 7.2 Hz, 2H), 7.04 (t, J = 6.8 Hz, 1H), 7.22 (t, J = 7.2 Hz, 1H), 8.07–8.18 (m, 6H), 8.28 (d, J = 9.2 Hz, 1H), 8.65 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 16.3, 45.9, 114.6, 118.9, 119.8, 120.5, 121.5, 124.9, 129.8, 130.7, 131.1, 133.2 ppm. HRMS (ESI): calcd for $C_{15}H_{15}N_2^+$ ([M−I$^-$]$^+$) 223.1230, found 223.1220.



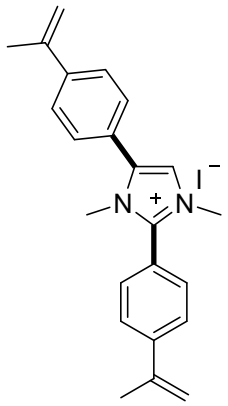
1,3-Dimethyl-2,5-diphenyl-1*H*-imidazol-3-ium iodide (4aa). A light yellow solid (65 mg, 87% yield). M.p.: 75–77 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.61 (s, 3H), 3.83 (s, 3H), 7.47 (br, 3H), 7.65–7.66 (m, 4H), 7.71 (d, J = 6.4 Hz, 2H), 7.93 (d, J = 6.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 35.1, 37.0, 121.3, 121.4, 125.3, 129.3, 130.0, 130.5, 130.6, 131.4, 132.8, 135.3, 145.1 ppm. HRMS (ESI): calcd for $C_{17}H_{17}N_2^+$ ([M−I$^-$]$^+$) 249.1386, found 249.1375.



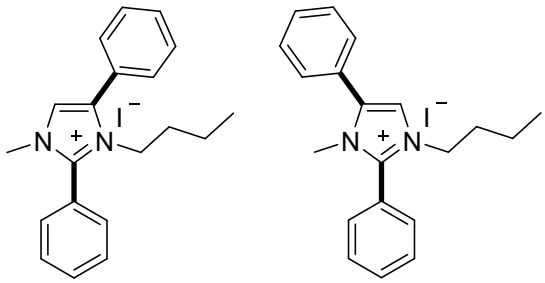
2,5-Bis(4-methoxyphenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (4ab). A light green solid (67 mg, 77% yield). M.p.: 176–178 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.60 (s, 3H), 3.80 (s, 3H), 3.82 (s, 3H), 3.88 (s, 3H), 6.97 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.55 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 34.9, 36.7, 55.6, 55.8, 112.9, 114.7, 115.4, 117.4, 120.6, 131.8, 133.0, 135.2, 145.1, 161.3, 162.8 ppm. HRMS (ESI): calcd for $C_{19}H_{21}N_2O_2^+$ ([M−I$^-$]$^+$) 309.1598, found 309.1584.



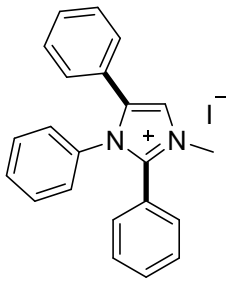
2,5-Bis(4-cyanophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (4ae). A yellow solid (35 mg, 41% yield). M.p.: 100–102 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.63 (s, 3H), 3.78 (s, 3H), 7.86 (d, *J* = 7.6 Hz, 2H), 8.06 (d, *J* = 7.2 Hz, 2H), 8.13 (d, *J* = 7.2 Hz, 2H), 8.26–8.29 (m, 3H), ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.0, 36.1, 112.7, 115.1, 117.9, 118.2, 122.8, 125.7, 130.0, 130.2, 131.9, 132.9, 133.2, 133.3, 143.9 ppm. HRMS (ESI): calcd for $C_{19}H_{15}N_4^+$ ([M−I$^-$]$^+$) 299.1291, found 299.1293.



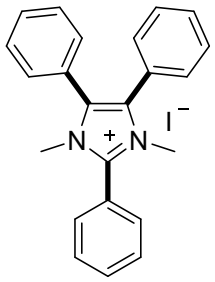
1,3-Dimethyl-2,5-bis(4-(prop-1-en-2-yl)phenyl)-1*H*-imidazol-3-ium iodide (4ap). A white solid (55 mg, 60% yield). M.p.: 191–193 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.14 (s, 3H), 2.19 (s, 3H), 3.65 (s, 3H), 3.87 (s, 3H), 5.16 (s, 1H), 5.26 (s, 1H), 5.42 (s, 1H), 5.52 (s, 1H), 7.57 (d, *J* = 6.8 Hz, 2H), 7.65 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.7, 21.8, 35.2, 37.1, 114.4, 115.8, 119.8, 121.4, 124.1, 126.4, 127.0, 130.3, 131.3, 135.3, 141.9, 142.3, 143.3, 145.2, 145.6 ppm. HRMS (ESI): calcd for $C_{23}H_{25}N_2^+$ ([M−I$^-$]$^+$) 329.2012, found 329.2011.



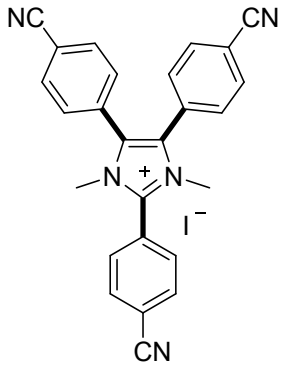
3-butyl-1-methyl-2,4-diphenyl-1*H*-imidazol-3-ium iodide (4ba) and **3-Butyl-1-methyl-2,5-diphenyl-1*H*-imidazol-3-ium iodide (4ba').** An inseparable mixture with an ratio of 1:2 as determined by ^{1}H NMR spectrum. Light yellow semisolid (55 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.54 (t, *J* = 7.2 Hz, 1.5H), 0.83 (t, *J* = 7.2 Hz, 3H), 0.92–0.99 (m, 1H), 1.29–1.32 (m, 3H), 1.76–1.84 (m, 2H), 7.49–7.50 (m, 4H), 7.58 (s, 1H), 7.62 (s, 0.5H), 7.67–7.74 (m, 8H), 7.89–7.94 (m, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.1, 13.5, 19.4, 19.7, 31.6, 32.0, 35.0, 37.1, 46.9, 49.3, 119.7, 121.5, 122.1, 125.3, 125.6, 129.4, 130.1, 130.48, 130.54, 130.6, 130.7, 131.2, 131.3, 132.9, 135.7, 144.9 ppm. HRMS (ESI): calcd for $C_{20}H_{23}N_2^+$ ([M−I$^-$]$^+$) 291.1856, found 291.1849.



3-Methyl-1,2,5-triphenyl-1*H*-imidazol-3-ium iodide (4da). A white solid (31 mg, 35% yield). M.p.: 108–110 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 3H), 7.48–7.59 (m, 8H), 7.62–7.66 (m, 5H), 7.76 (d, J = 6.8 Hz, 2H), 8.45 (s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.9, 121.6, 125.7, 128.3, 128.87, 128.91, 129.6, 129.7, 130.5, 130.9, 132.0, 133.4, 145.5 ppm. HRMS (ESI): calcd for $C_{22}H_{19}N_2^+$ ([M−I$^-$]$^+$) 311.1543, found 311.1537.

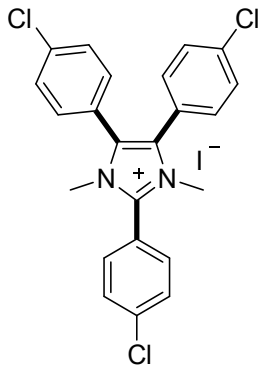


1,3-Dimethyl-2,4,5-triphenyl-1*H*-imidazol-3-ium iodide (5aa). A light yellow solid (80 mg, 89% yield). M.p.: 186–188 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.58 (s, 6H), 7.32–7.39 (m, 6H), 7.59 (d, J = 7.2 Hz, 4H), 7.65 (br, 3H), 8.12 (br, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 35.0, 122.0, 125.5, 129.1, 129.9, 130.2, 131.4, 131.7, 132.5, 132.7, 144.5 ppm. HRMS (ESI): calcd for $C_{23}H_{21}N_2^+$ ([M−I$^-$]$^+$) 325.1699, found 325.1691.

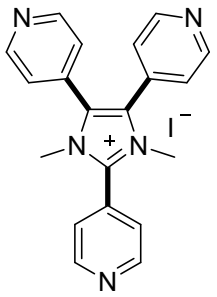


2,4,5-Tris(4-cyanophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (5ae). A light yellow solid (78 mg, 74% yield). M.p.: 185–187 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.58 (s, 6H), 7.66 (d, J = 7.2 Hz, 4H),

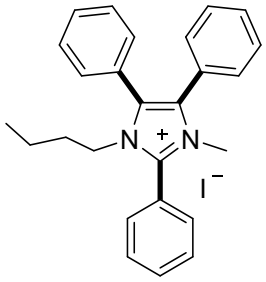
8.03 (d, J = 7.2 Hz, 4H), 8.13 (d, J = 6.4 Hz, 2H), 8.31 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 34.9, 113.1, 115.2, 117.9, 118.0, 125.9, 129.6, 130.9, 131.7, 132.1, 133.2, 133.5, 143.7 ppm. HRMS (ESI): calcd for $C_{26}H_{18}N_5^+$ ([M−I$^-$]$^+$) 400.1557, found 400.1558.



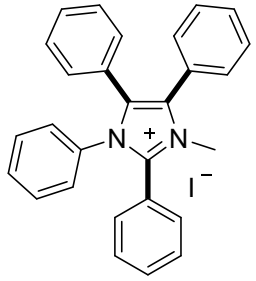
2,4,5-Tris(4-chlorophenyl)-1,3-dimethyl-1*H*-imidazol-3-ium iodide (5ai). A white solid (72 mg, 65% yield). M.p.: 140–142. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.56 (s, 6H), 7.35 (d, J = 7.2 Hz, 4H), 7.59 (d, J = 8.0 Hz, 4H), 7.63 (d, J = 7.2 Hz, 2H), 8.14 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 35.1, 120.1, 123.6, 129.6, 130.4, 131.9, 132.9, 133.3, 137.0, 139.6, 143.9 ppm. HRMS (ESI): calcd for $C_{23}H_{18}Cl_3N_2^+$ ([M−I$^-$]$^+$) 427.0530, found 427.0522.



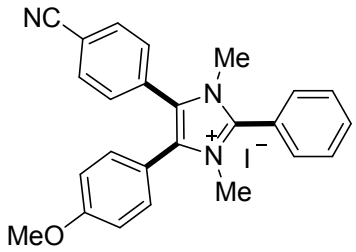
1,3-Dimethyl-2,4,5-tri(pyridin-4-yl)-1H-imidazol-3-ium iodide (5aq). A yellow solid (44 mg, 48% yield). M.p.: > 250 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.61 (s, 6H), 7.47 (d, J = 4.0 Hz, 4H), 7.94 (d, J = 4.0 Hz, 2H), 8.70 (br, 4H), 8.99 (d, J = 4.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 35.0, 125.0, 129.5, 130.3, 132.9, 143.2, 150.6, 151.0 ppm. HRMS (ESI): calcd for $C_{20}H_{18}N_5^+$ ([M−I$^-$]$^+$) 328.1557, found 328.1560.



1-Butyl-3-methyl-2,4,5-triphenyl-1*H*-imidazol-3-ium iodide (5ba). A light yellow solid (70 mg, 71% yield). M.p.: 79–81 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.53 (t, *J* = 7.2 Hz, 3H), 0.94–0.99 (m, 2H), 1.39–1.43 (m, 2H), 3.56 (s, 3H), 3.97 (t, *J* = 7.2 Hz, 2H), 7.35–7.39 (m, 6H), 7.61 (d, *J* = 5.2 Hz, 4H), 7.68 (br, 3H), 8.11 (d, *J* = 4.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.9, 19.4, 31.6, 34.9, 46.9, 122.0, 125.2, 125.6, 128.9, 129.0, 129.96, 130.04, 130.2, 131.30, 131.33, 131.4, 131.7, 132.6, 132.7, 144.0 ppm. HRMS (ESI): calcd for $C_{26}H_{27}N_2^+$ ([M−I$^-$]$^+$) 367.2169, found 367.2162.

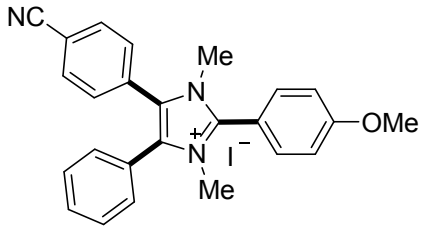


3-Methyl-1,2,4,5-tetraphenyl-1*H*-imidazol-3-ium iodide (5da). A white solid (45 mg, 44% yield). M.p.: 95–97 ºC. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.63 (s, 3H), 7.20–7.25 (m, 5H), 7.31 (br, 3H), 7.40 (br, 2H), 7.52 (br, 8H), 7.67 (d, *J* = 6.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 34.5, 122.1, 125.4, 125.5, 128.4, 128.5, 129.06, 129.14, 129.3, 129.7, 130.3, 130.8, 130.9, 131.0, 131.3, 131.9, 132.1, 133.4, 144.5 ppm. HRMS (ESI): calcd for $C_{26}H_{27}N_2^+$ ([M−I$^-$]$^+$) 367.2169, found 367.2176.

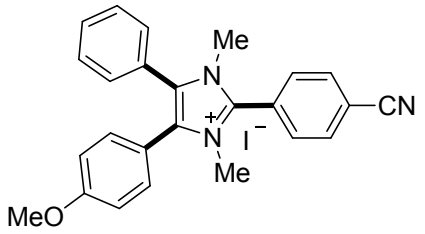


5-(4-Cyanophenyl)-4-(4-methoxyphenyl)-1,3-dimethyl-2-phenyl-1*H*-imidazol-3-ium iodide (6a). A yellow solid (58 mg, 57% yield). M.p.: 110–112 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.55 (s, 3H), 3.62 (s, 3H), 3.79 (s, 3H), 6.89 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.64–7.67 (m, 5H), 7.83 (d, *J* =

7.6 Hz, 2H), 8.11 (d, J = 6.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 34.9, 35.4, 55.5, 114.0, 114.9, 116.6, 118.1, 121.8, 130.0, 130.5, 130.6, 131.7, 132.4, 132.8, 132.86, 132.90, 133.4, 145.2, 161.3 ppm. HRMS (ESI): calcd for $C_{25}H_{22}N_3O^+$ ($[M-I^-]^+$) 380.1757, found 380.1752.



5-(4-Cyanophenyl)-2-(4-methoxyphenyl)-1,3-dimethyl-4-phenyl-1*H*-imidazol-3-ium iodide (6b). A yellow solid (63 mg, 62% yield). M.p.: 126–128 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.62 (s, 3H), 3.83 (s, 3H), 3.89 (s, 3H), 6.97 (t, J = 7.6 Hz, 1H), 7.13 (d, J = 8.4 Hz, 2H), 7.49–7.68 (m, 8H), 7.87 (d, J = 8.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 35.0, 36.8, 55.8, 112.8, 114.1, 114.8, 115.4, 121.0, 125.5, 129.3, 130.0, 130.4, 130.6, 131.4, 133.0, 133.1, 145.5, 162.9 ppm. HRMS (ESI): calcd for $C_{25}H_{22}N_3O^+$ ($[M-I^-]^+$) 380.1757, found 380.1752.



2-(4-Cyanophenyl)-4-(4-methoxyphenyl)-1,3-dimethyl-5-phenyl-1*H*-imidazol-3-ium iodide (6c). A yellow solid (53 mg, 52% yield). M.p.: 113–115 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.60 (s, 6H), 3.77 (s, 3H), 6.87 (d, J = 7.6 Hz, 2H), 7.36–7.40 (m, 3H), 7.51 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 6.8 Hz, 2H), 7.97 (d, J = 8.0 Hz, 2H), 8.40 (d, J = 8.0 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 35.1, 35.2, 55.5, 114.7, 116.6, 116.9, 117.5, 125.3, 126.5, 129.2, 130.5, 131.0, 131.5, 132.9, 133.0, 133.4, 133.6, 142.1, 161.2 ppm. HRMS (ESI): calcd for $C_{25}H_{22}N_3O^+$ ($[M-I^-]^+$) 380.1757, found 380.1763.

VIII. References

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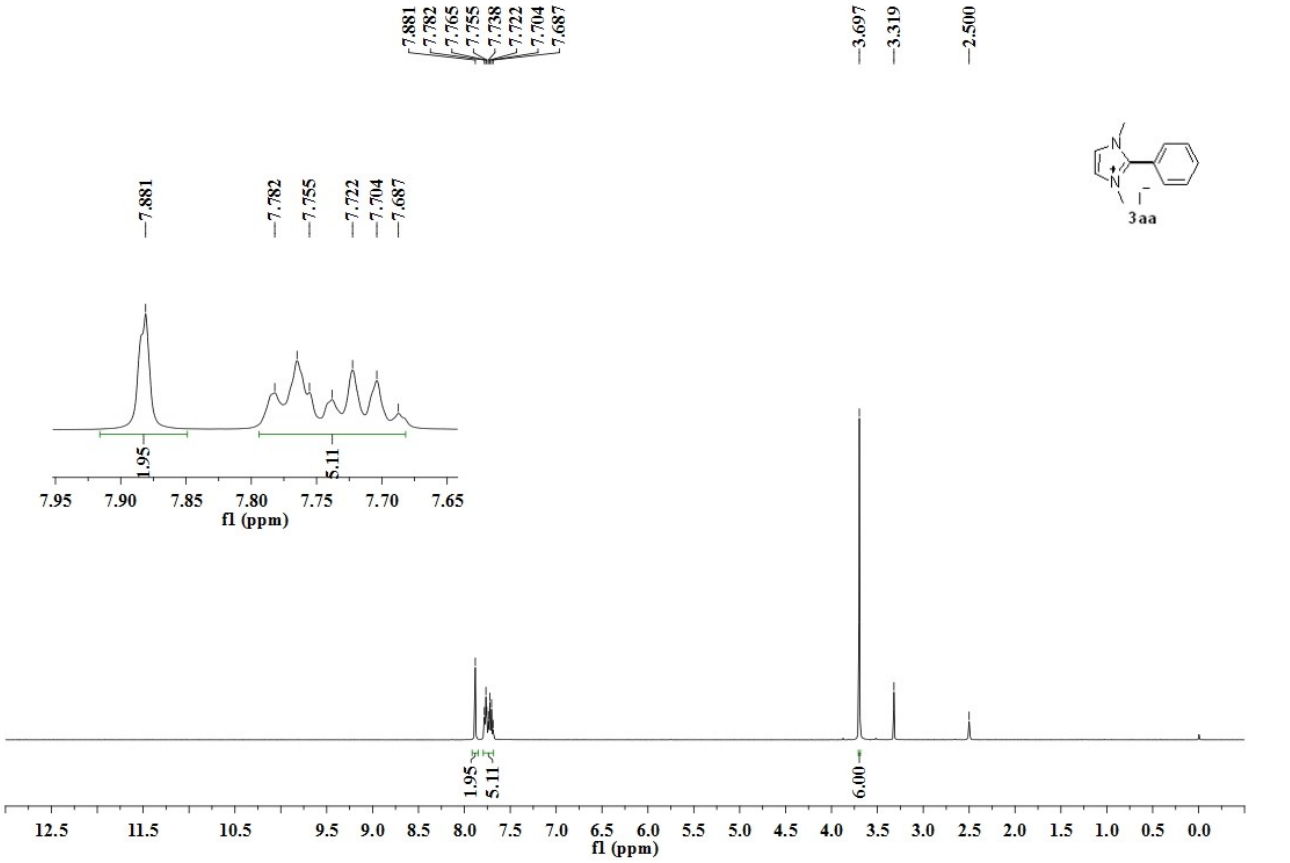
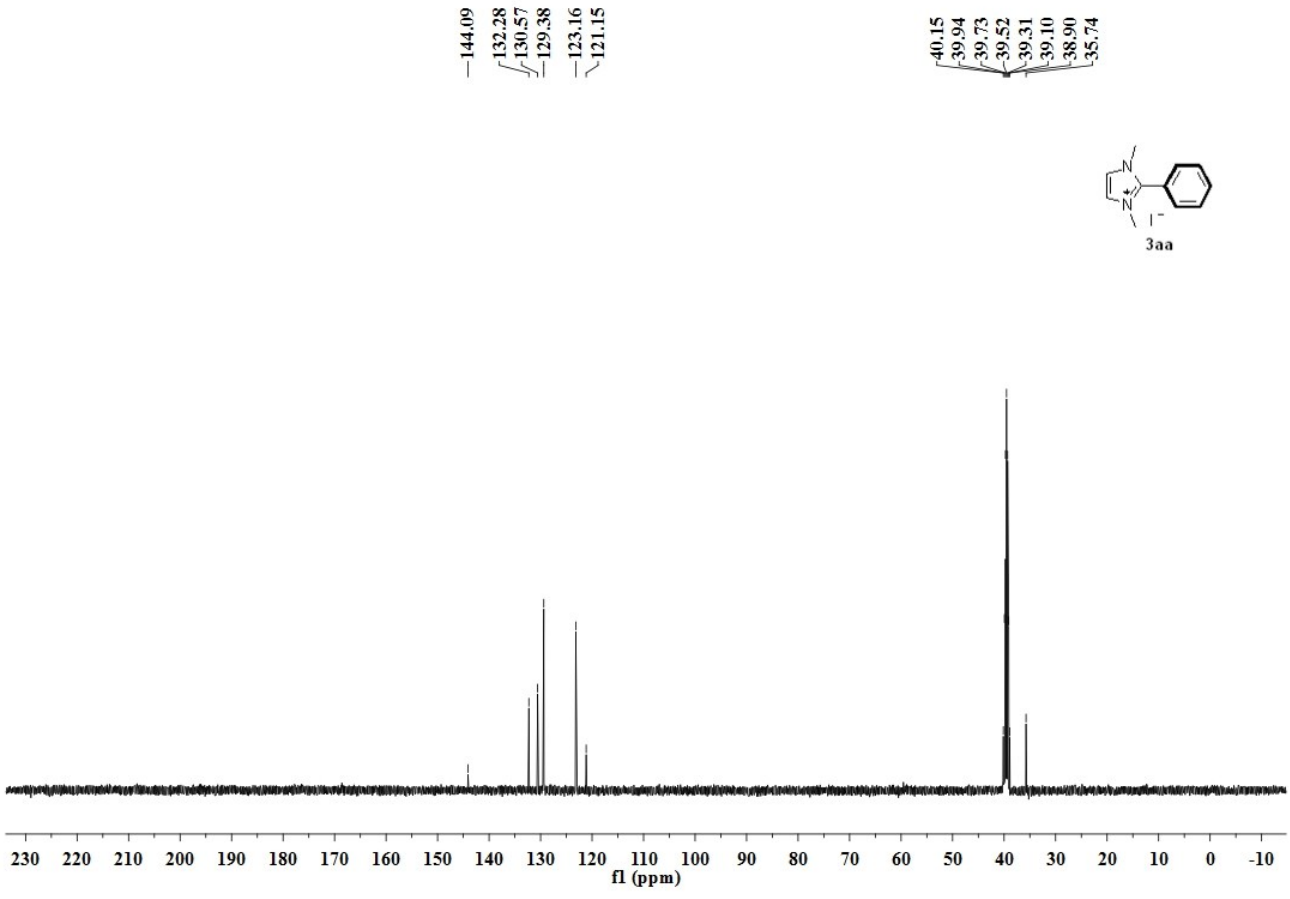
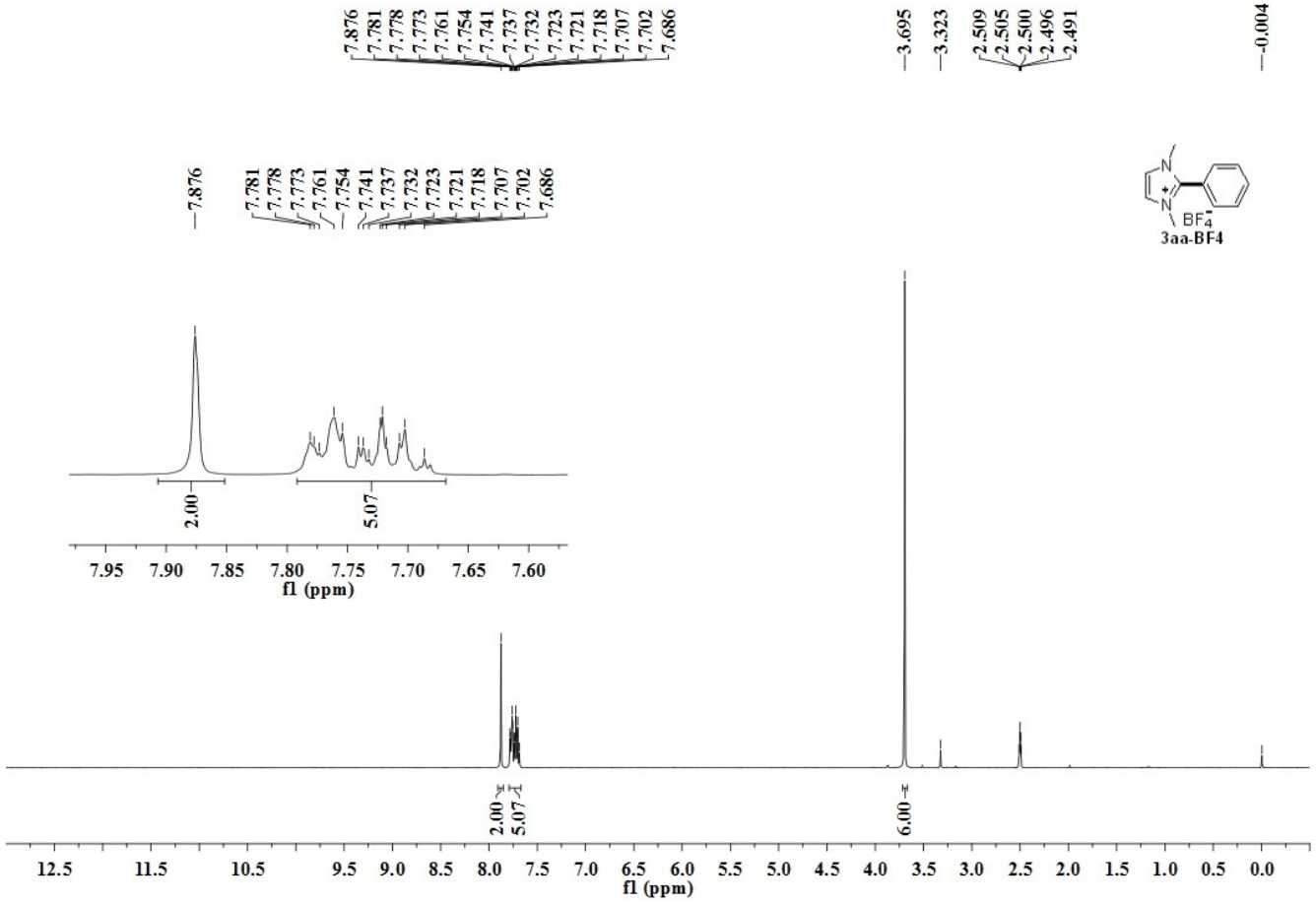
IX. Copies of ^{1}H and ^{13}C NMR spectra



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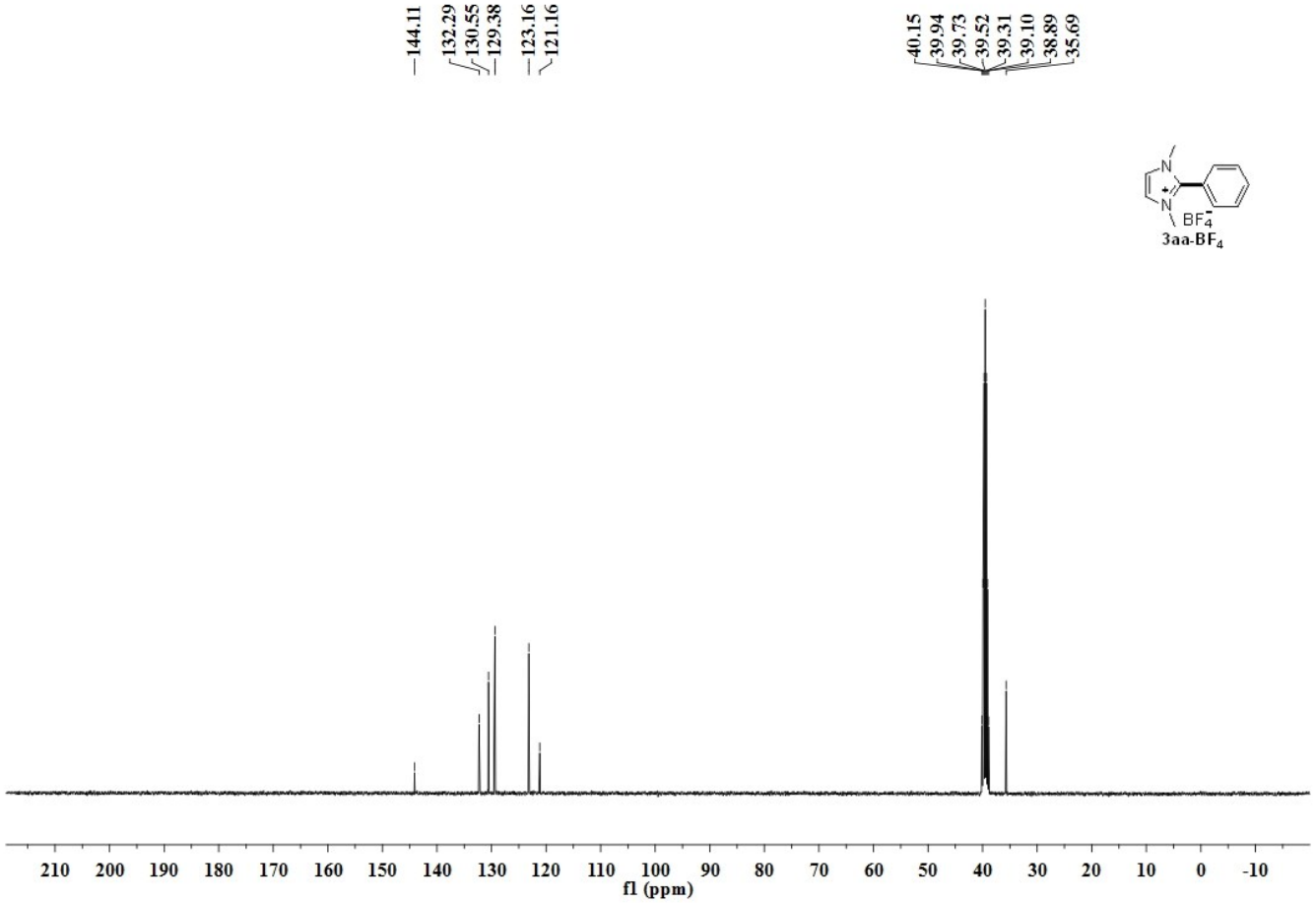
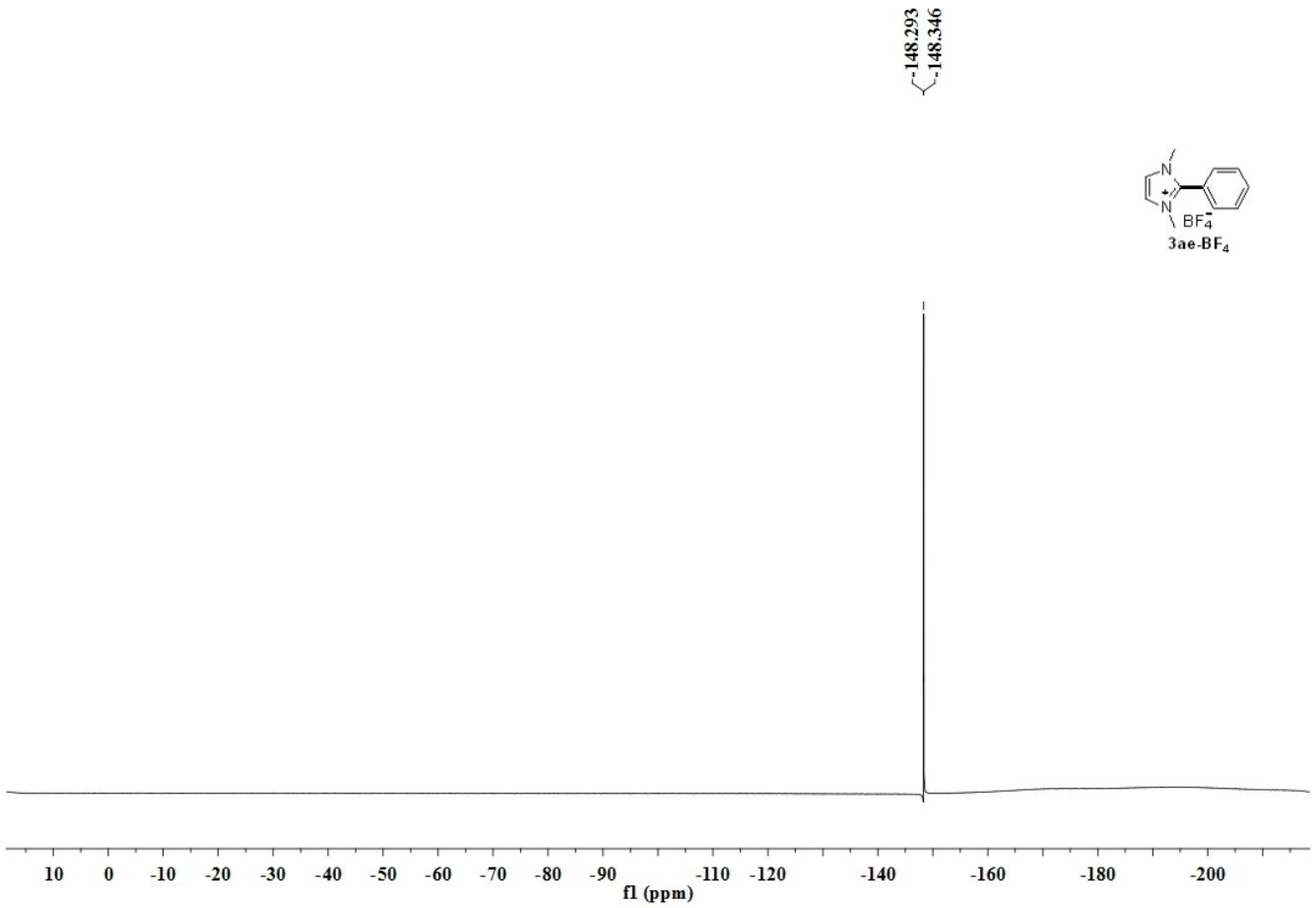
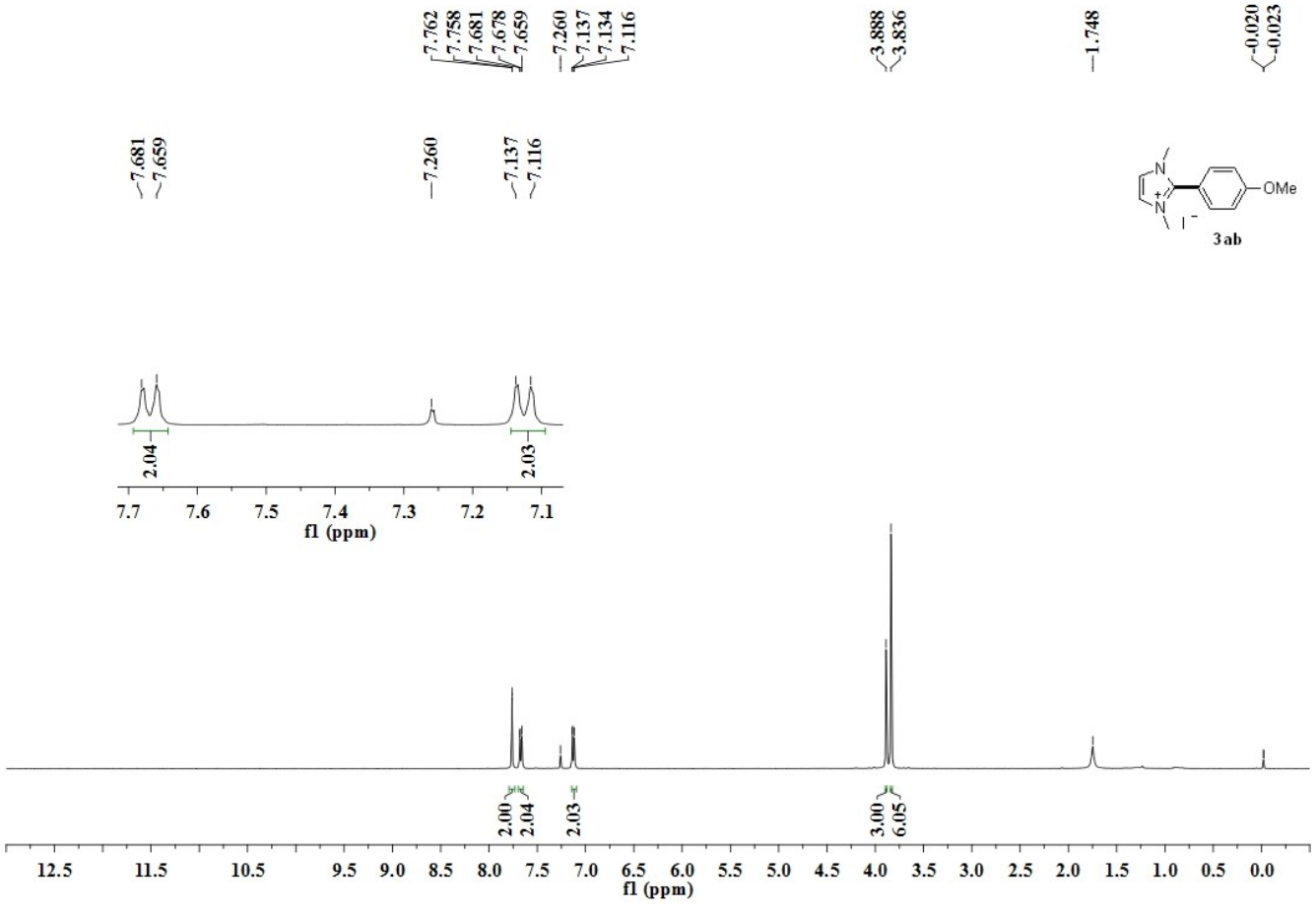
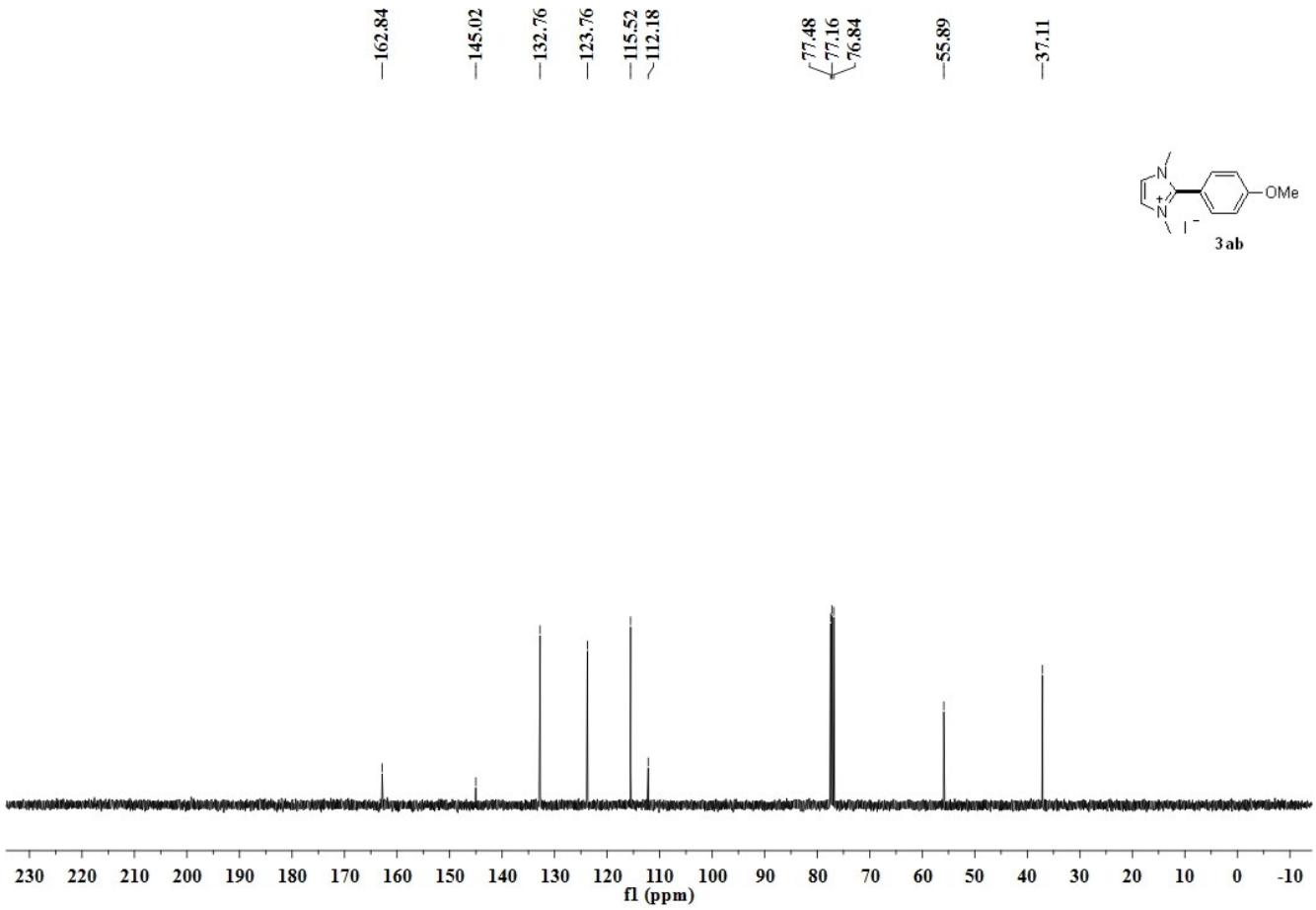
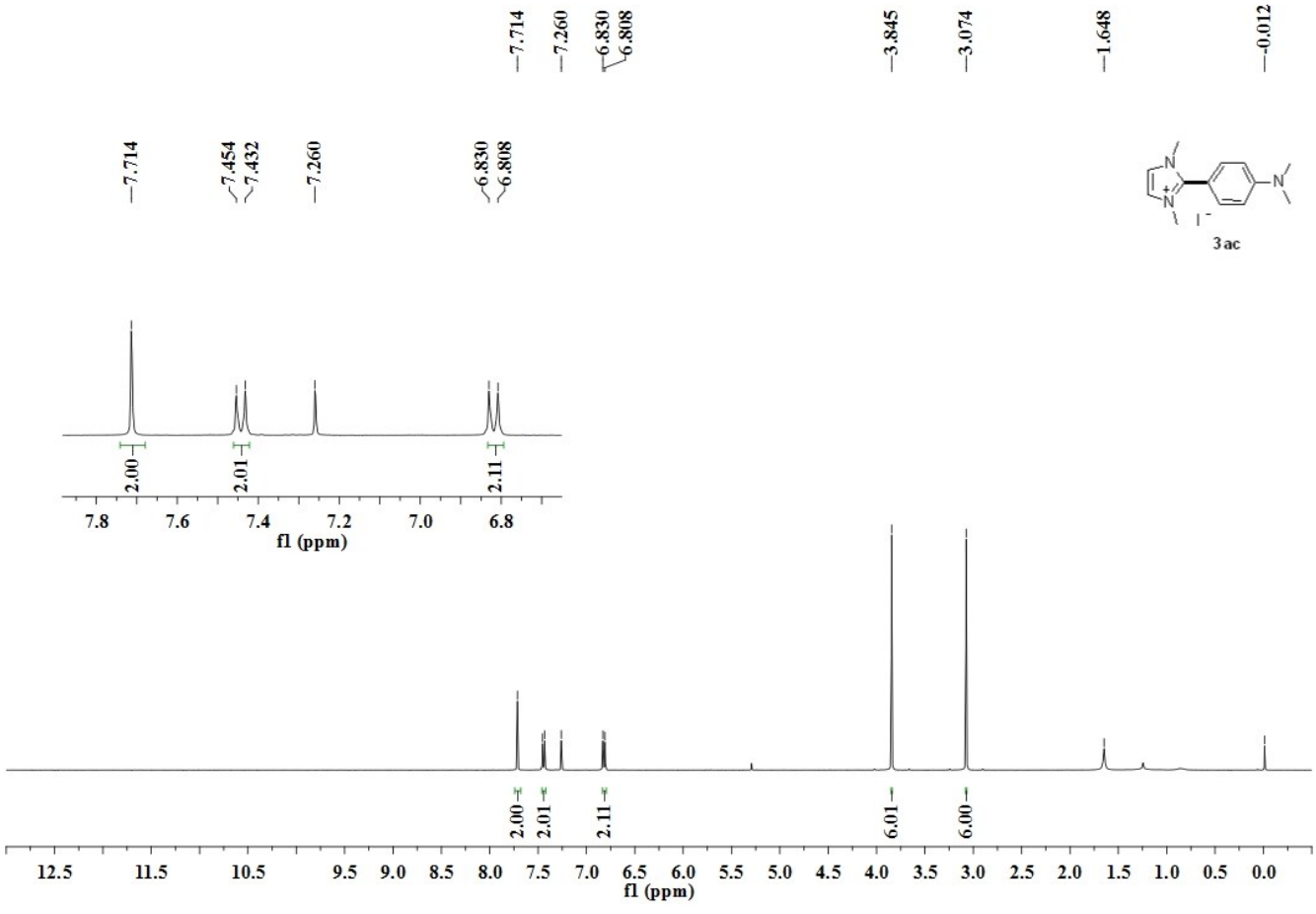
7.723
7.721
7.718
7.707
7.702
7.686
3.695
3.323
2.509
2.505
2.500
2.496
2.491
0.004
BF4
3aa-BF4
2.00
5.07
6.00
fl (ppm)

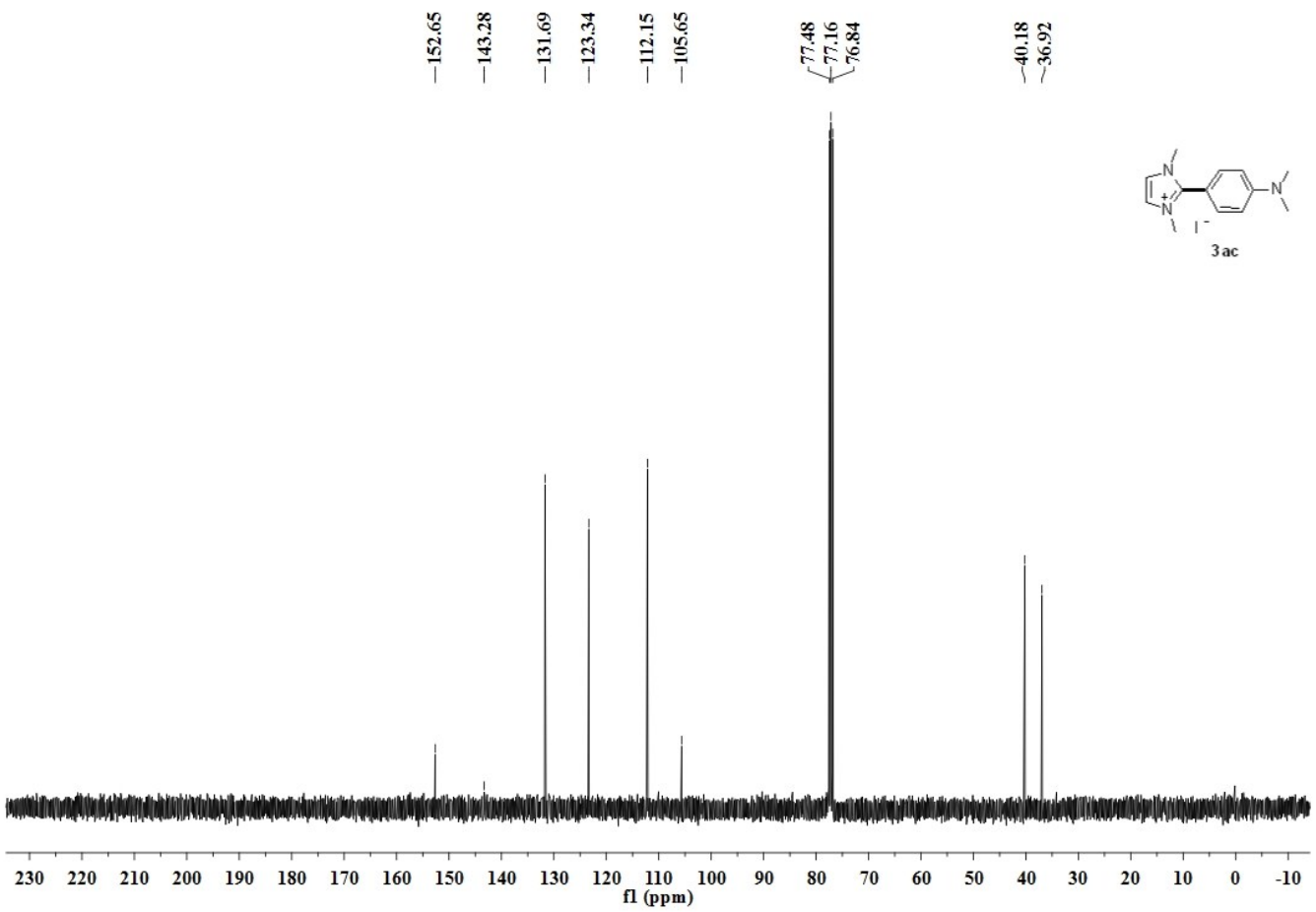

144.11
132.29
130.55
129.38
123.16
121.16
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.69
BF4
3aa-BF4
fl (ppm)

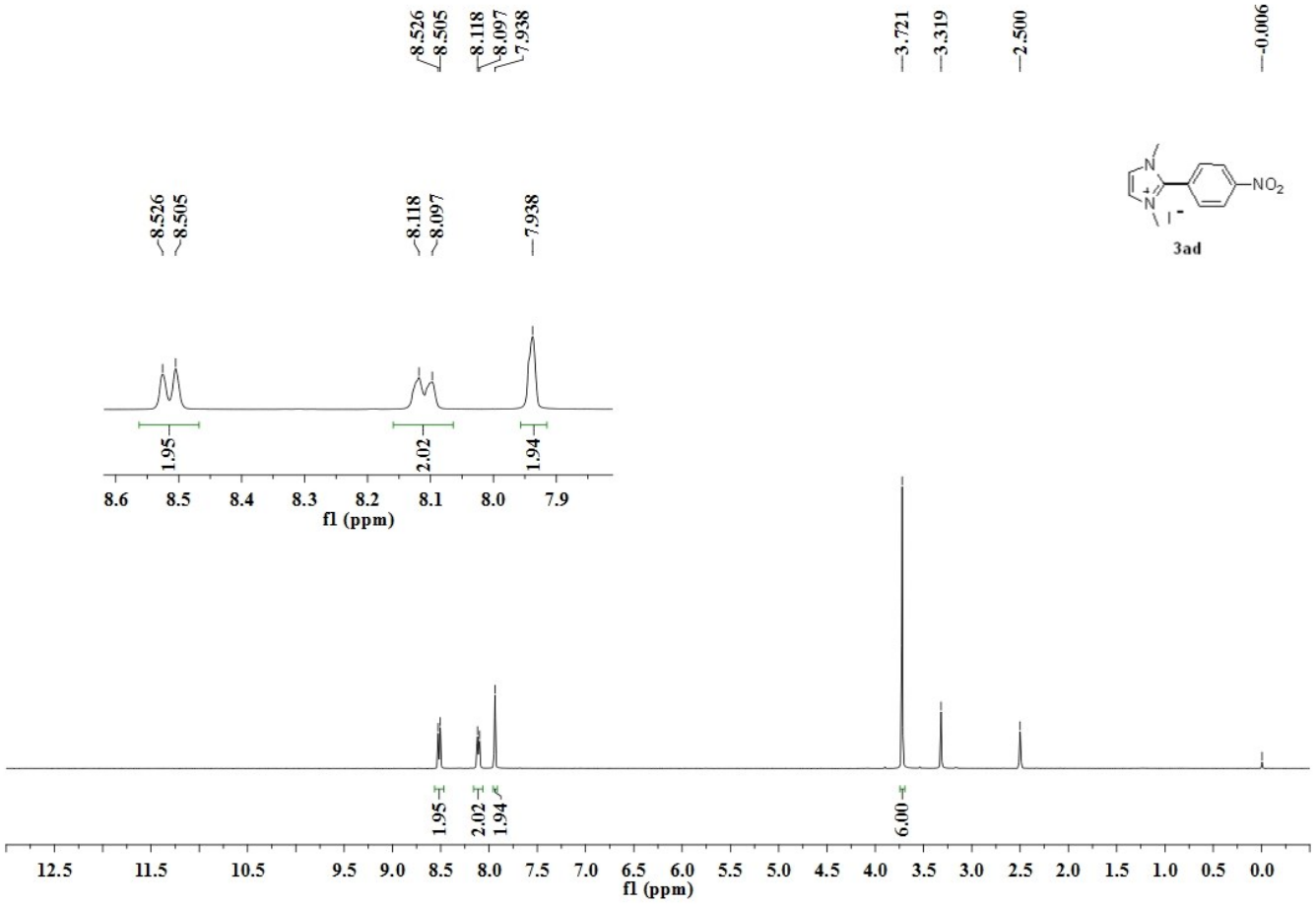

-148.293
-148.346
BF4
3ae-BF4
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -120 -140 -160 -180 -200
f1 (ppm)

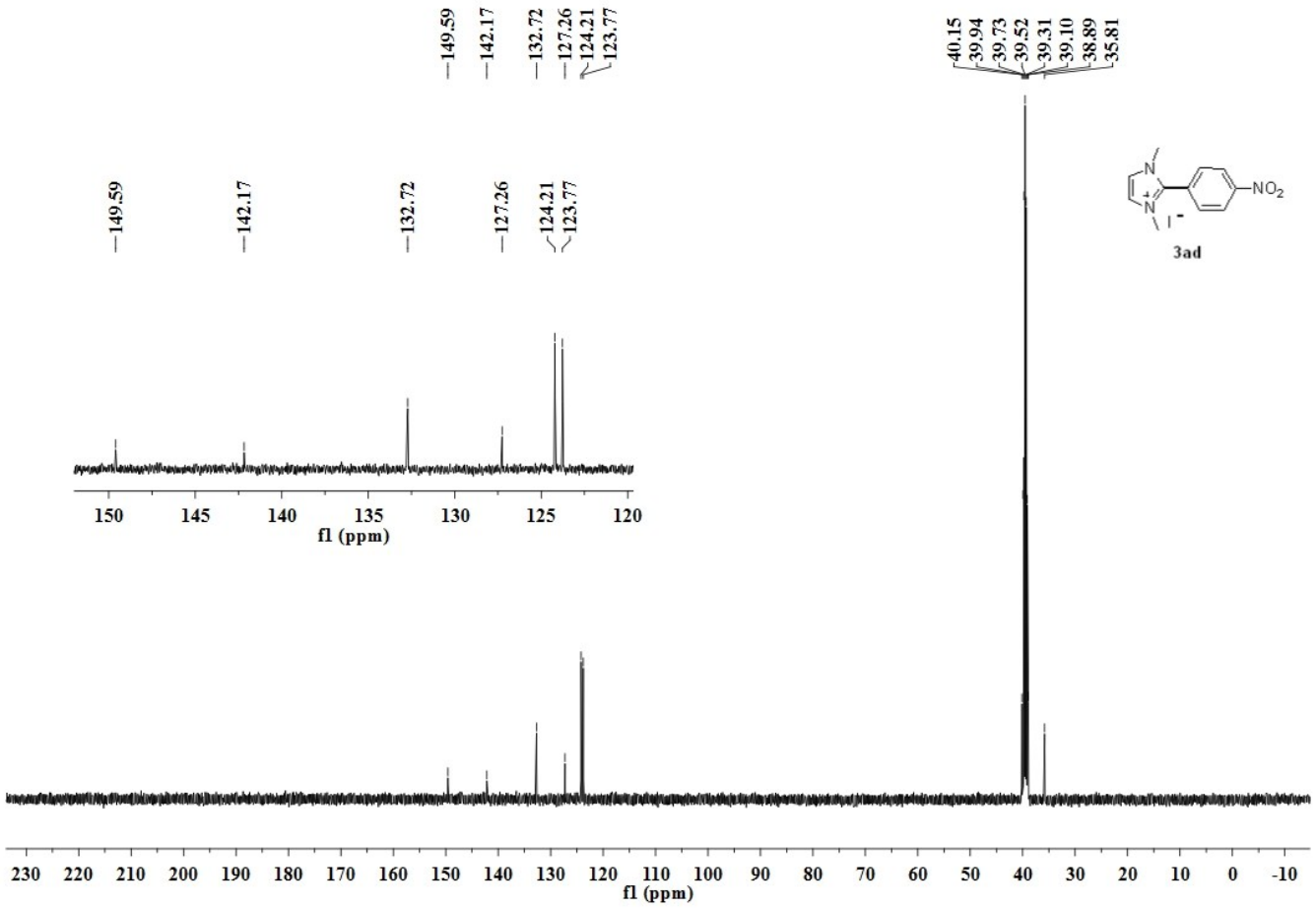

7.762
7.758
7.681
7.678
7.659
7.260
7.137
7.134
7.116
3.888
3.836
1.748
-0.020
-0.023
7.681
7.659
7.260
7.137
7.116
OMe
I
3ab
2.04
2.03
7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
2.00
2.04
2.03
3.00
6.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

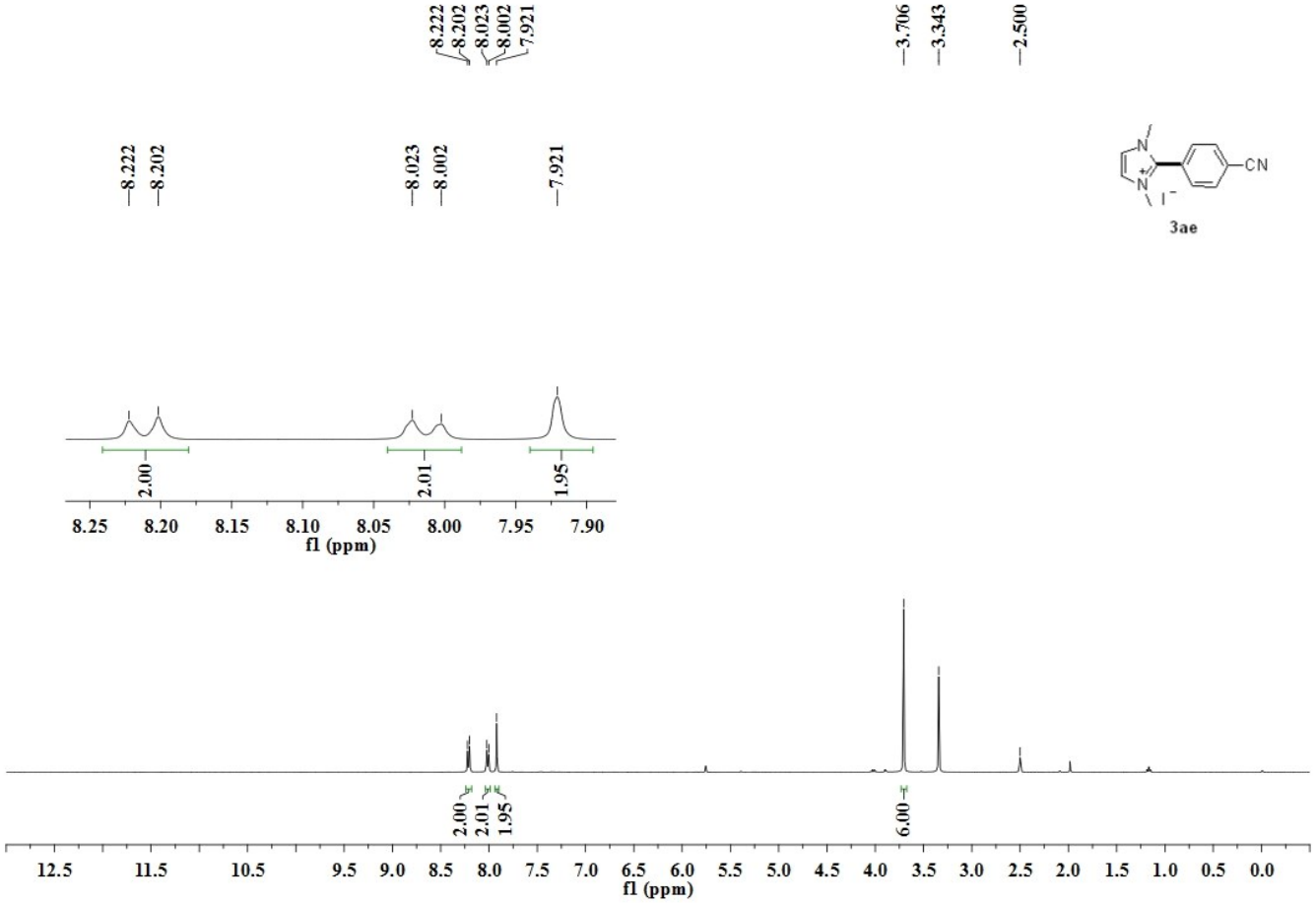

162.84
145.02
132.76
123.76
115.52
112.18
77.48
77.16
76.84
55.89
37.11
OMe
3ab
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

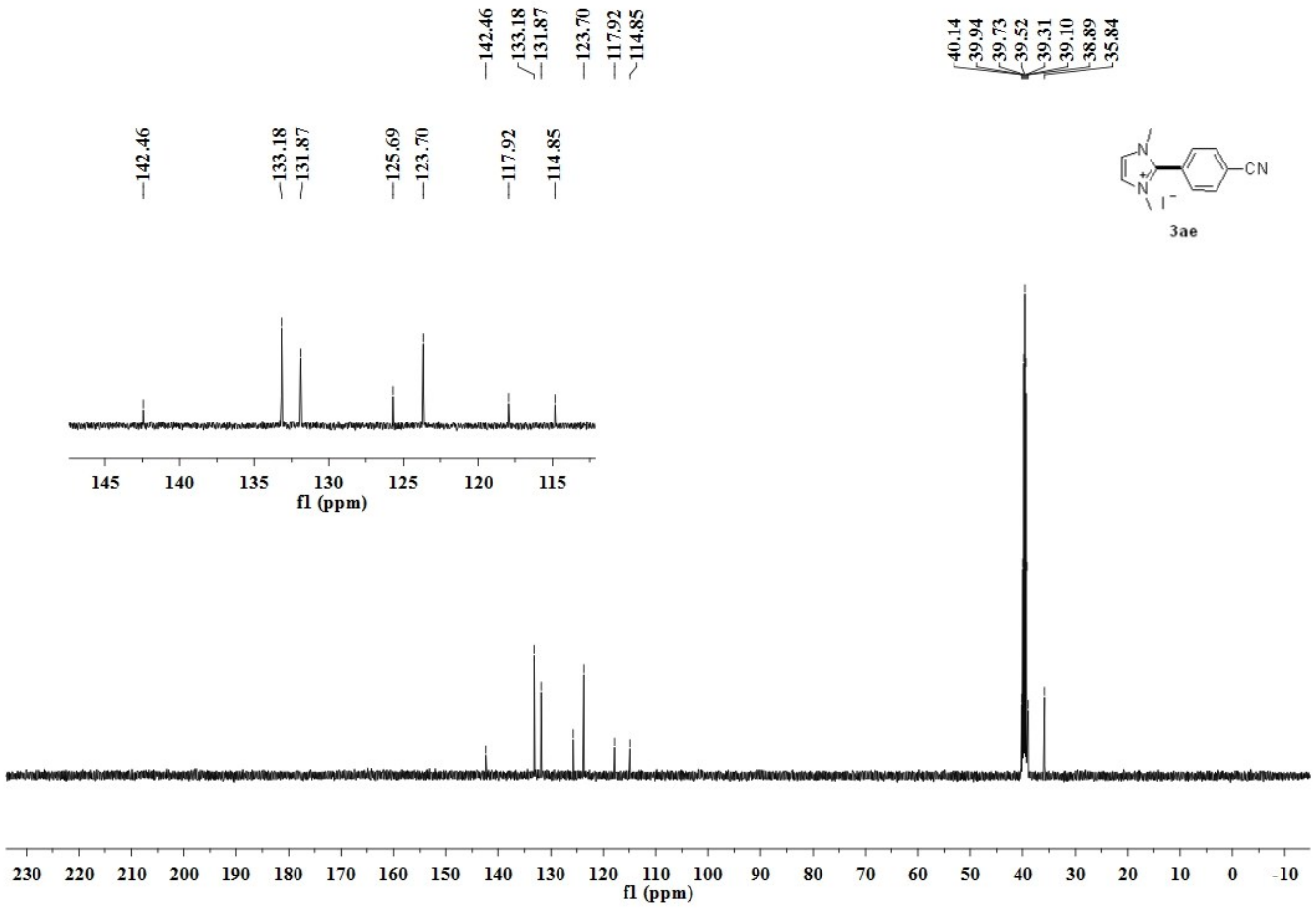

7.714
7.260
6.830
6.808
3.845
3.074
1.648
0.012
7.714
7.454
7.432
7.260
6.830
6.808
3ac
2.00
2.01
2.11
7.8 7.6 7.4 7.2 7.0 6.8
f1 (ppm)
2.00
2.01
2.11
6.01
6.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

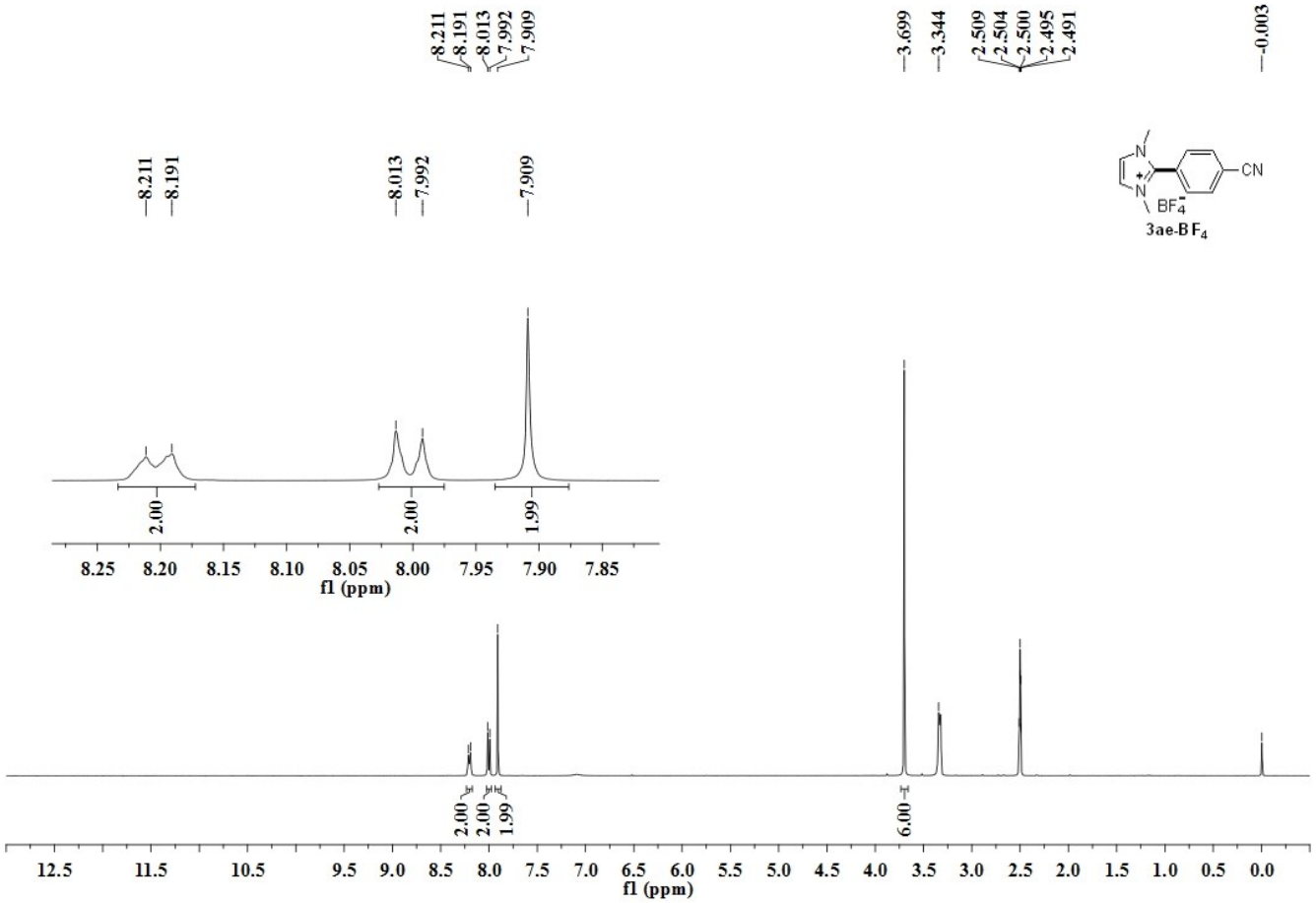

152.65
143.28
131.69
123.34
112.15
105.65
77.48
77.16
76.84
40.18
36.92
3ac
fl (ppm)

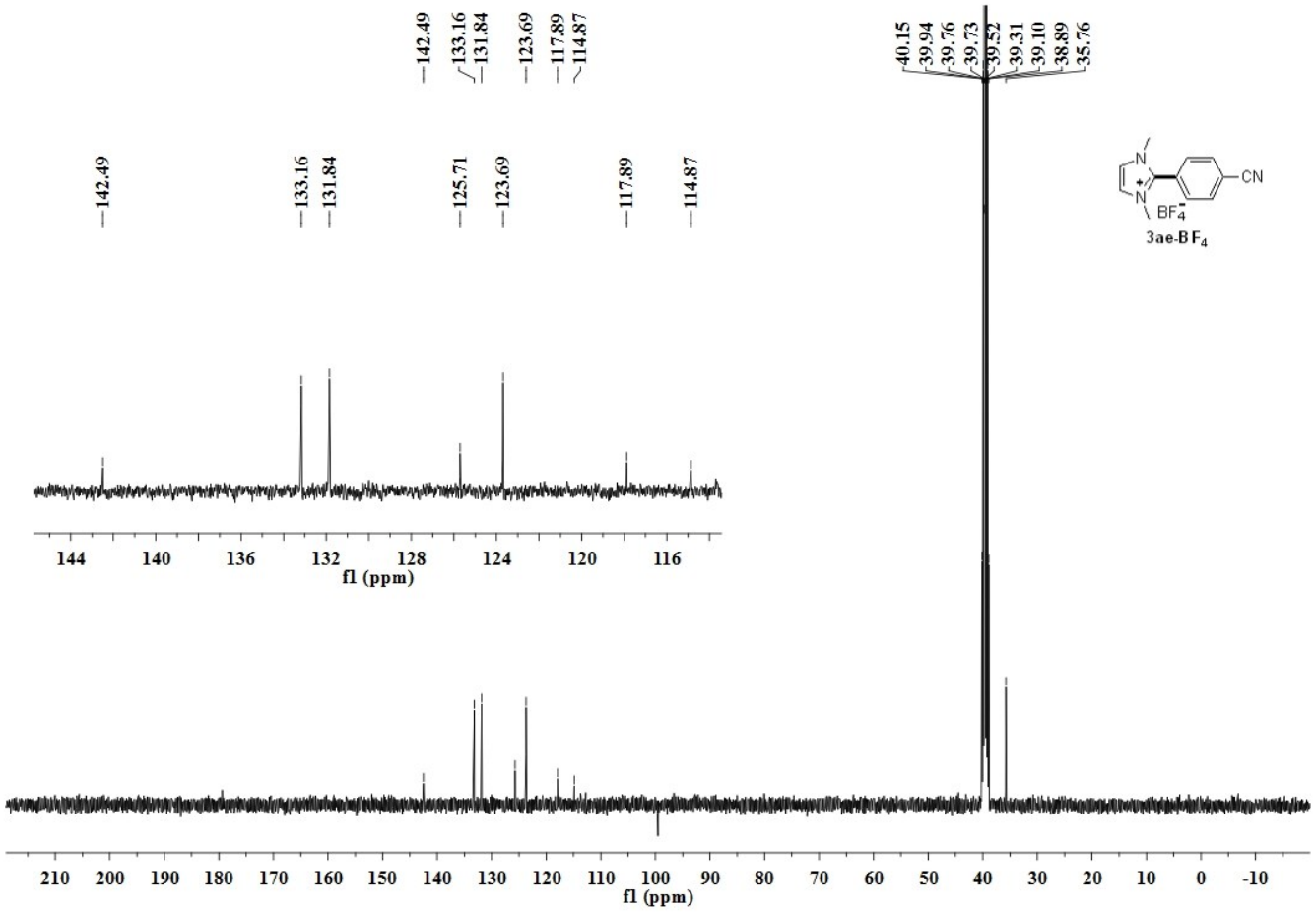

8.526
8.505
8.118
8.097
7.938
3.721
3.319
2.500
-0.006
3ad
1.95
2.02
1.94
6.00
fl (ppm)

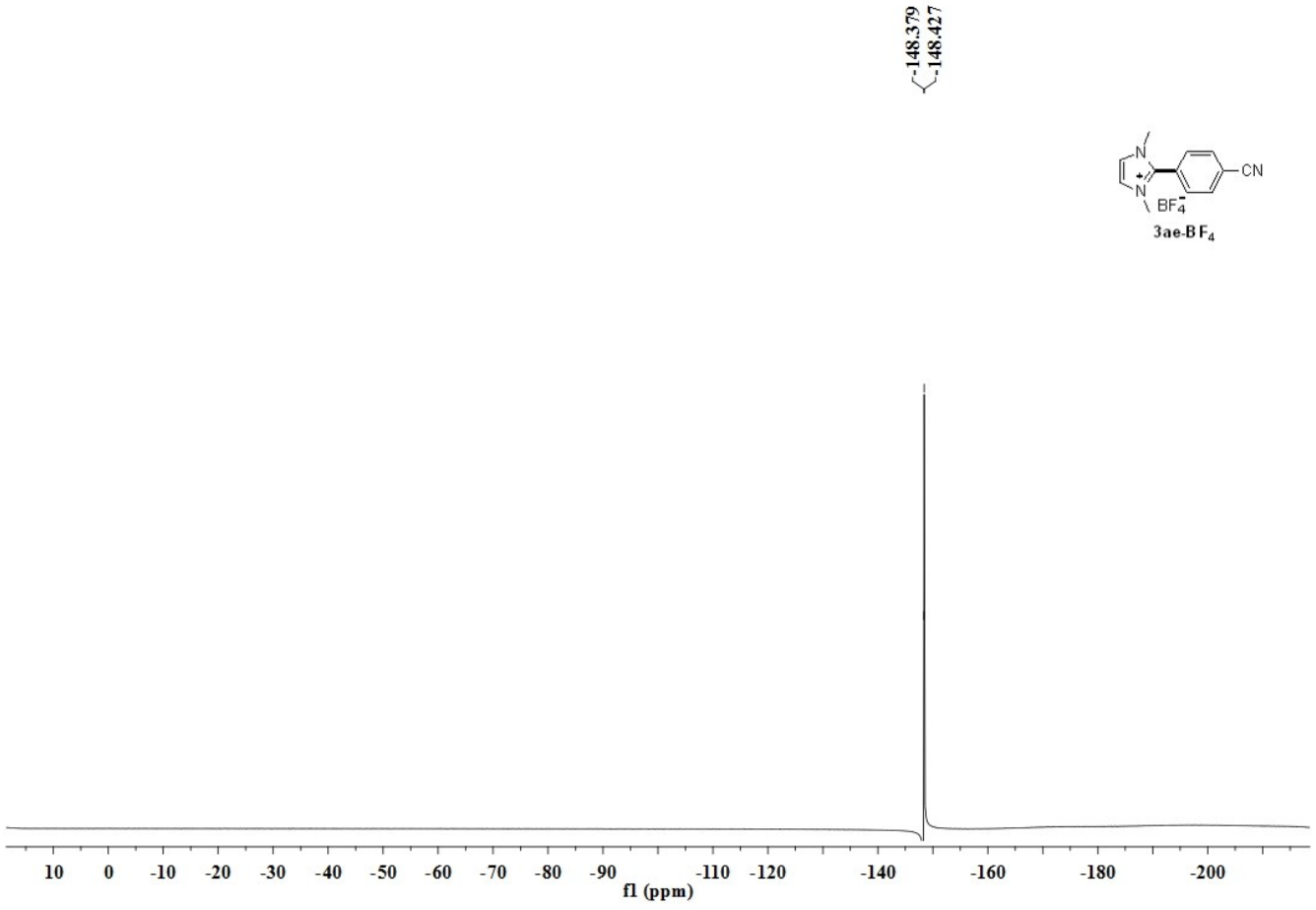

149.59
142.17
132.72
127.26
124.21
123.77
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.81
NO2
I-
3ad
fl (ppm)

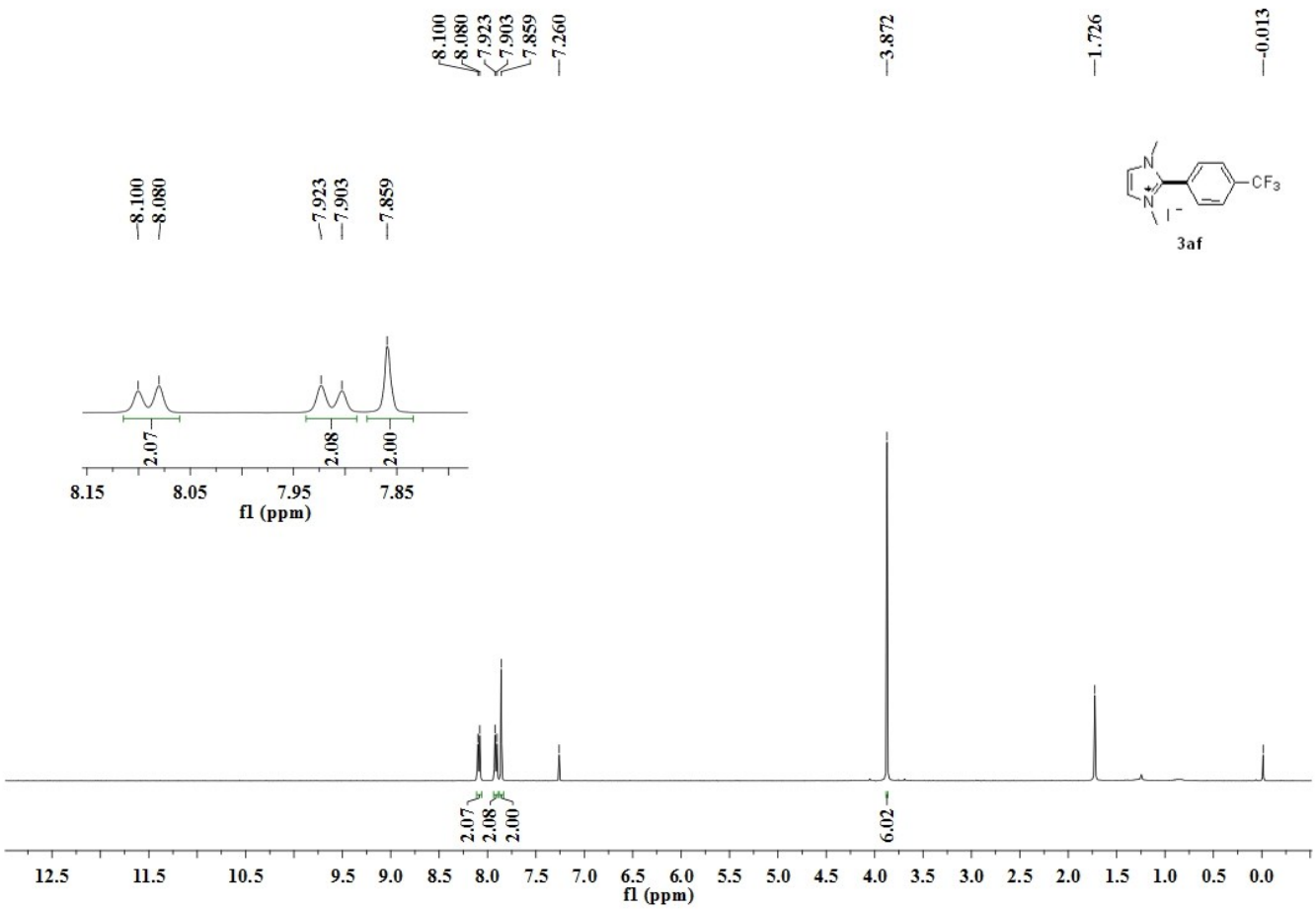

8.222
8.202
8.023
8.002
7.921
3.706
3.343
2.500
CN
I-
3ae
2.00
2.01
1.95
6.00
fl (ppm)

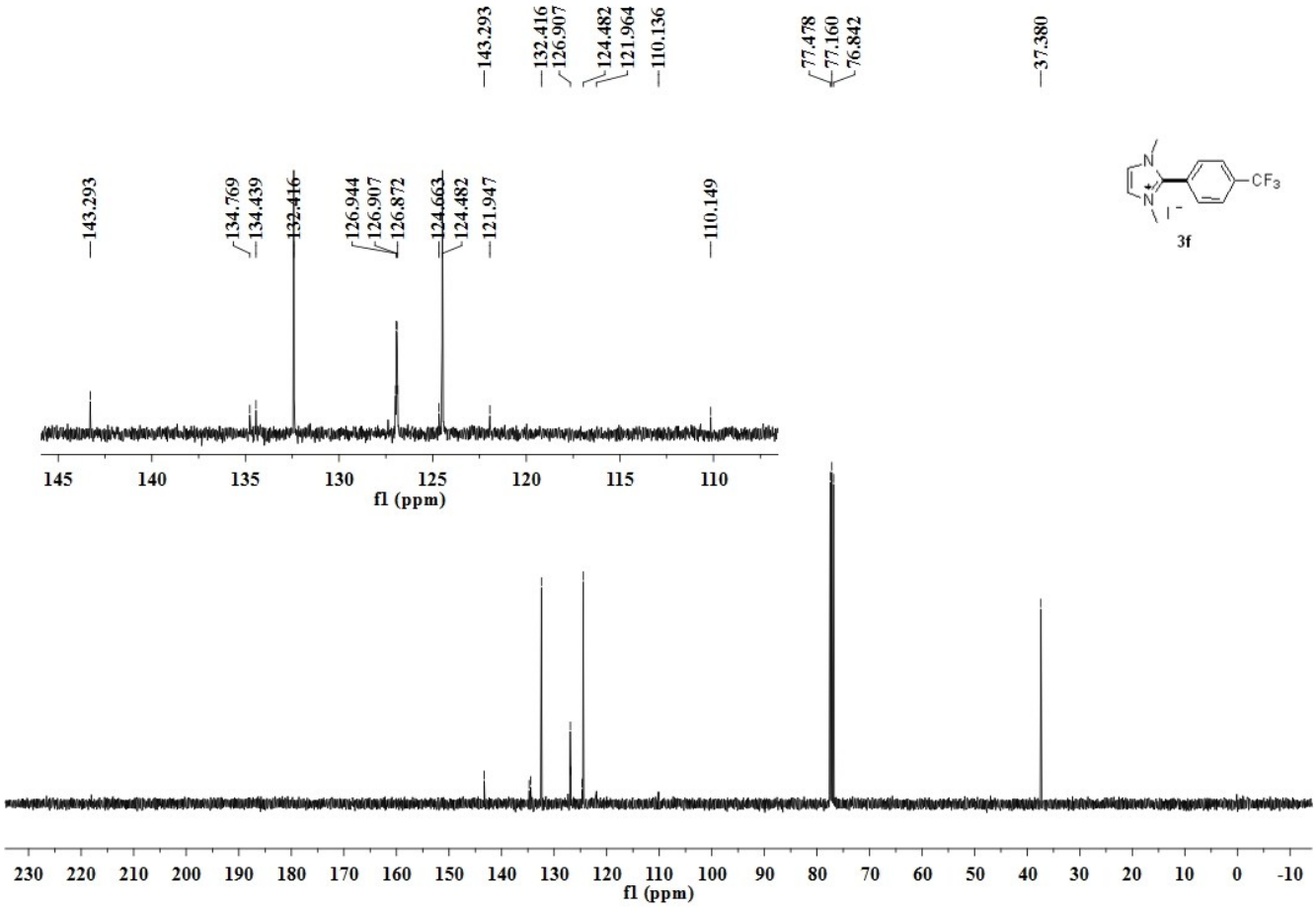

142.46
133.18
131.87
123.70
117.92
114.85
40.14
39.94
39.73
39.52
39.31
39.10
38.89
35.84
CN
I⁻
3ae
fl (ppm)

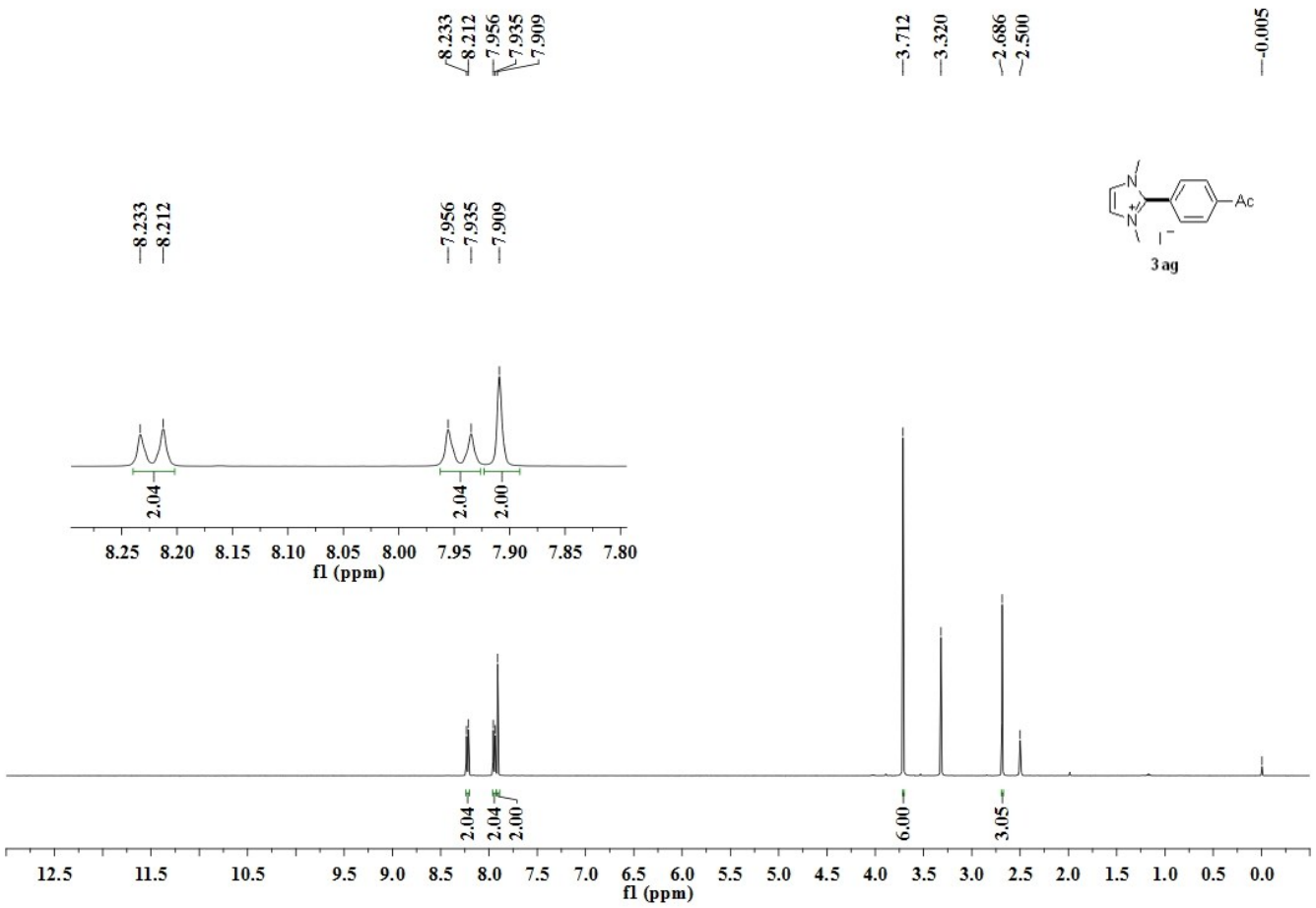

8.211
8.191
8.013
7.992
7.909
3.699
3.344
2.509
2.504
2.500
2.495
2.491
-0.003
CN
BF4⁻
3ae-BF4
2.00
2.00
1.99
6.00
fl (ppm)

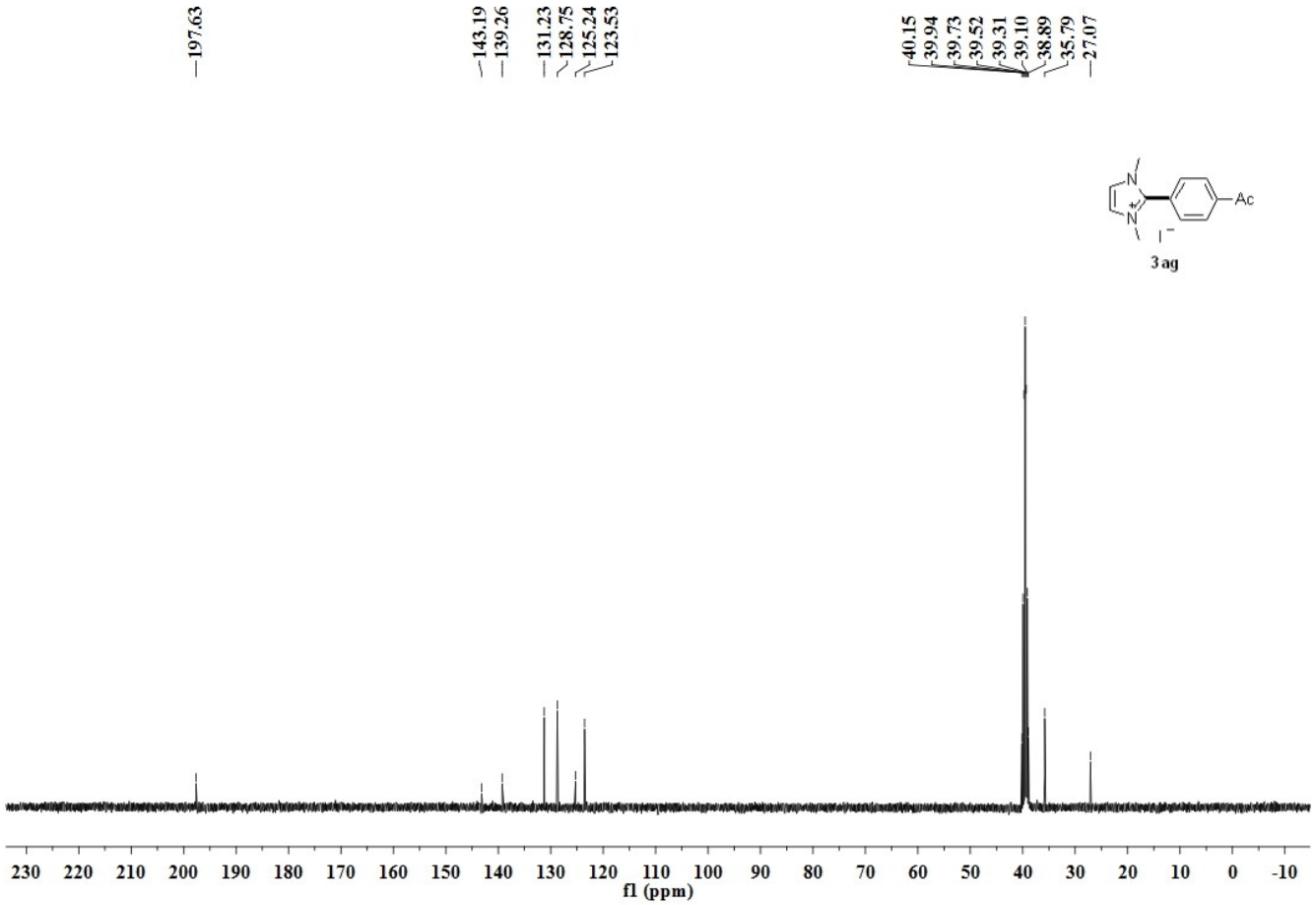

142.49
133.16
131.84
123.69
117.89
114.87
40.15
39.94
39.76
39.73
39.52
39.31
39.10
38.89
35.76
125.71
CN
BF4
3ae-BF4
144
140
136
132
128
124
120
116
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

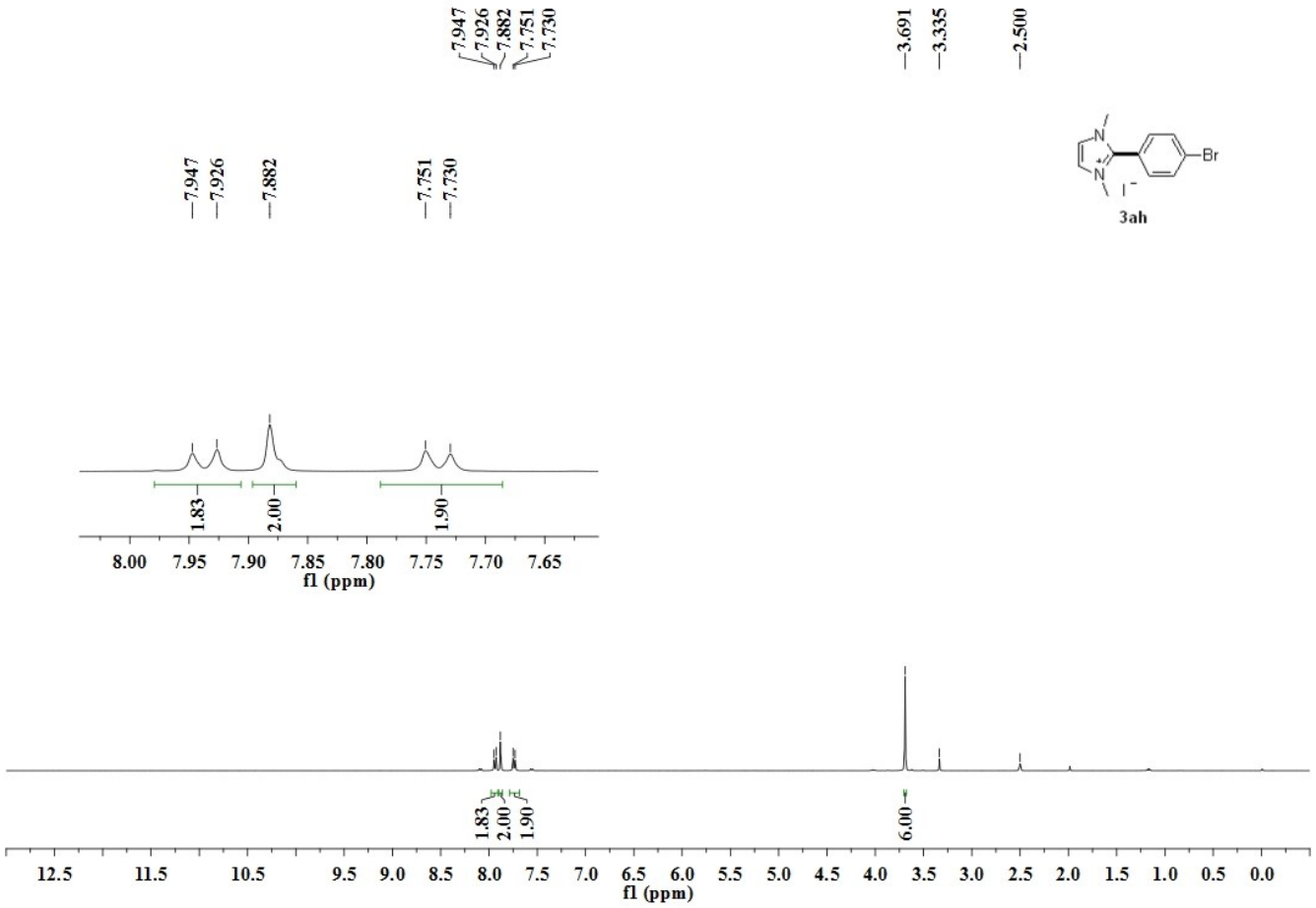

-148.379
-148.427
CN
BF4
3ae-BF4
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

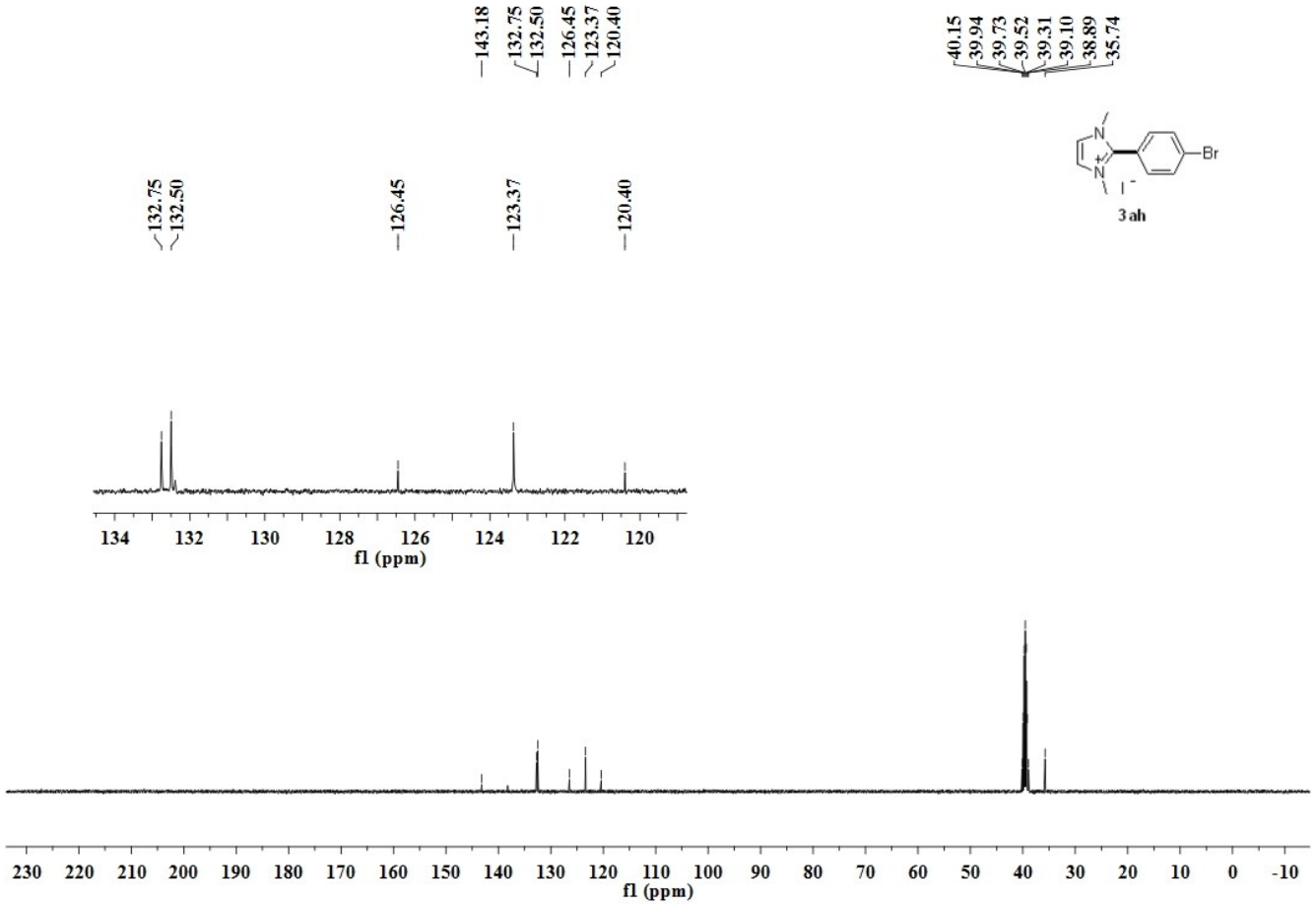

8.100
8.080
7.923
7.903
7.859
7.260
3.872
1.726
-0.013
3af
2.07
2.08
2.00
6.02
fl (ppm)

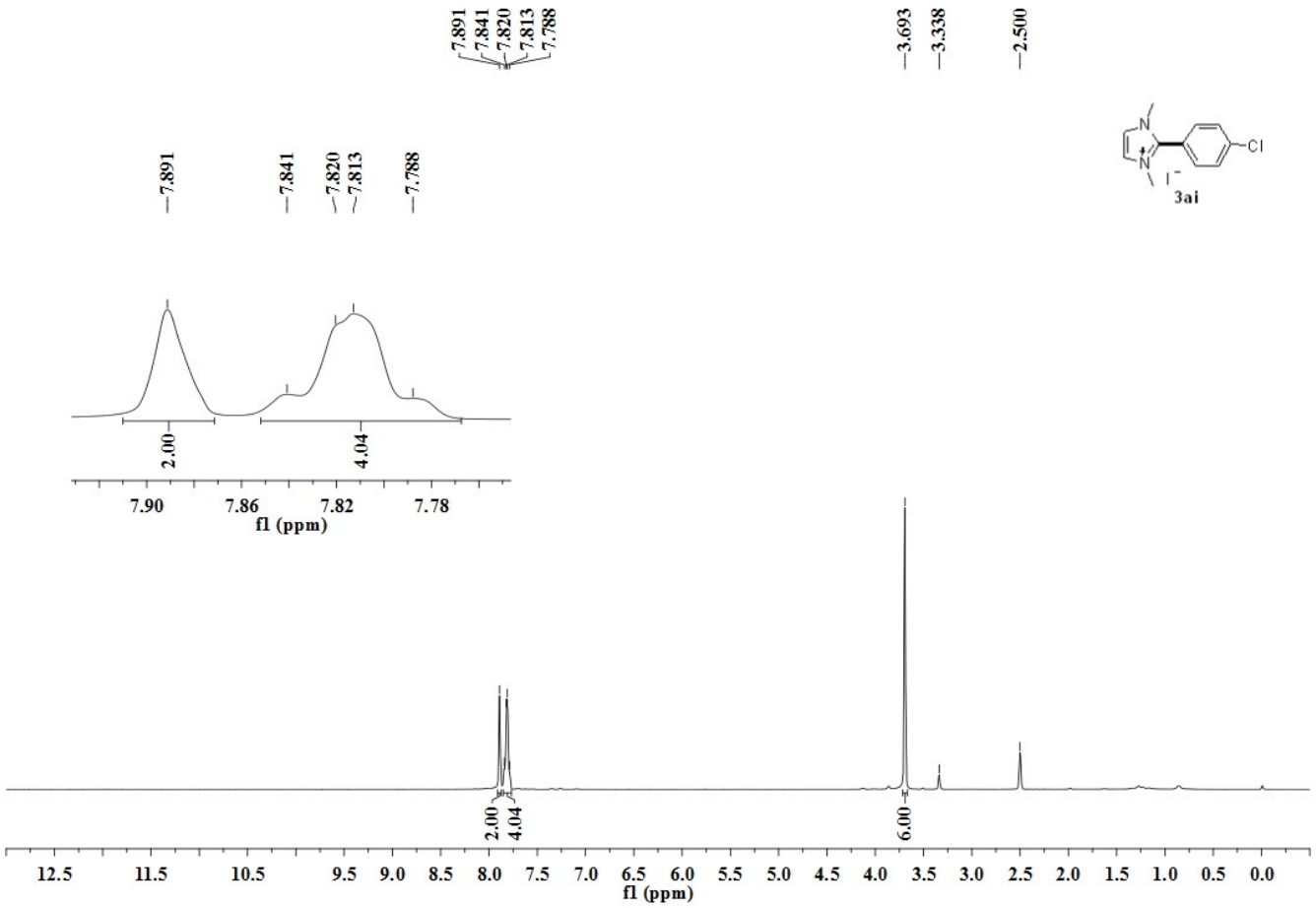

143.293
132.416
126.907
124.482
121.964
110.136
77.478
77.160
76.842
37.380
134.769
134.439
126.944
126.872
124.663
121.947
110.149
3f
fl (ppm)

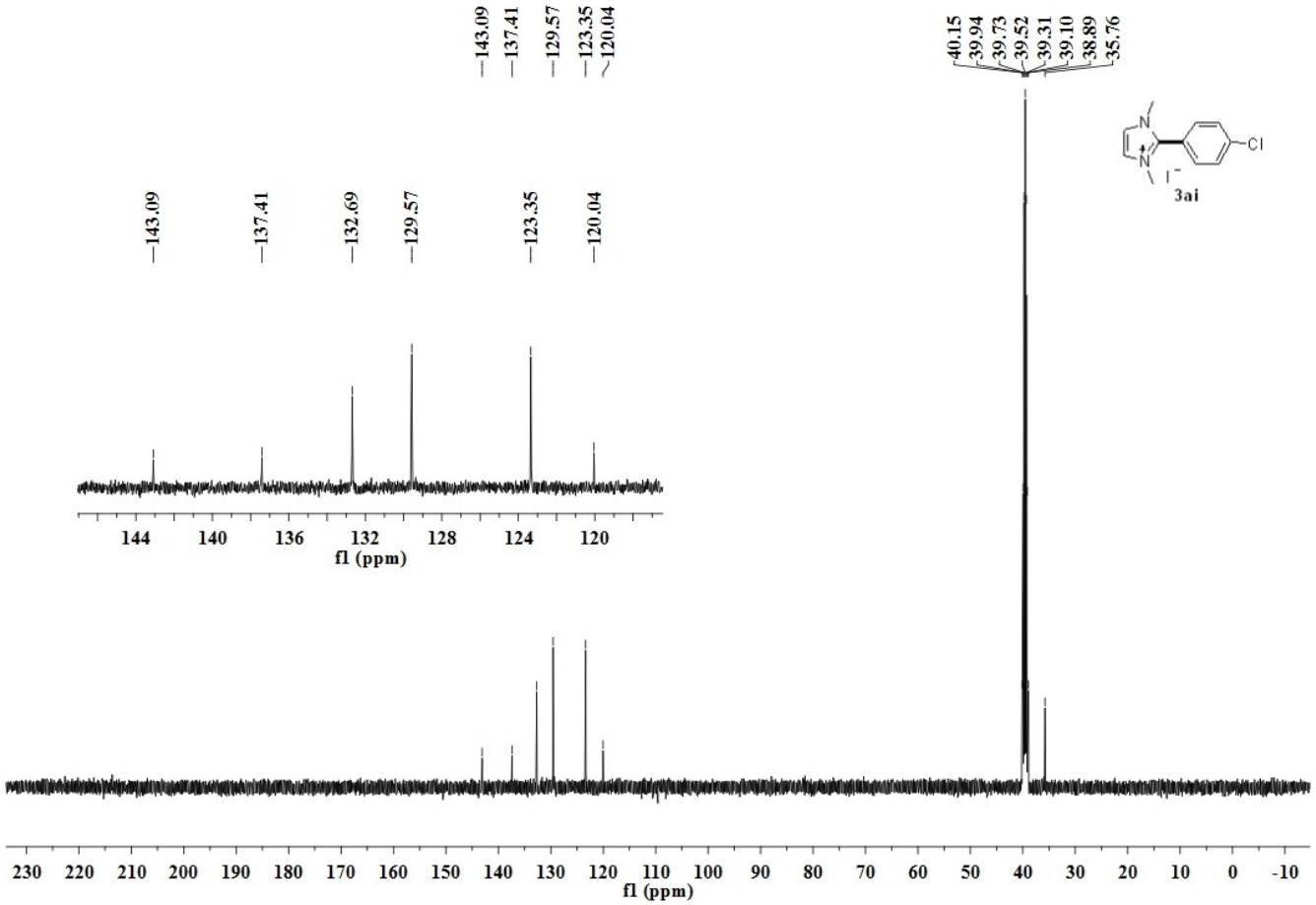

8.233
8.212
7.956
7.935
7.909
3.712
3.320
2.686
2.500
-0.005
Ac
3ag
2.04
2.04
2.00
6.00
3.05
fl (ppm)

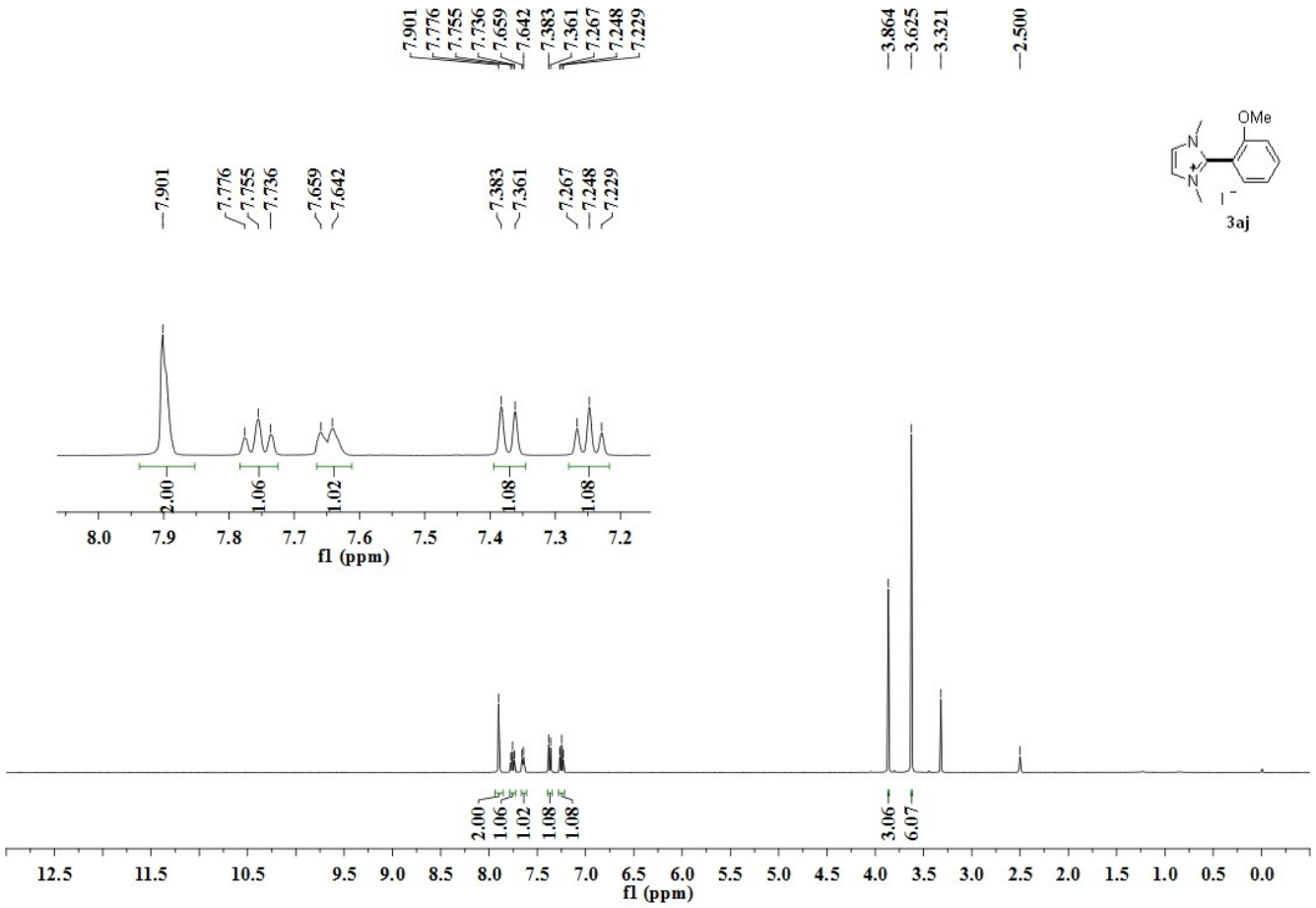

197.63
143.19
139.26
131.23
128.75
125.24
123.53
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.79
27.07
Ac
3ag
fl (ppm)

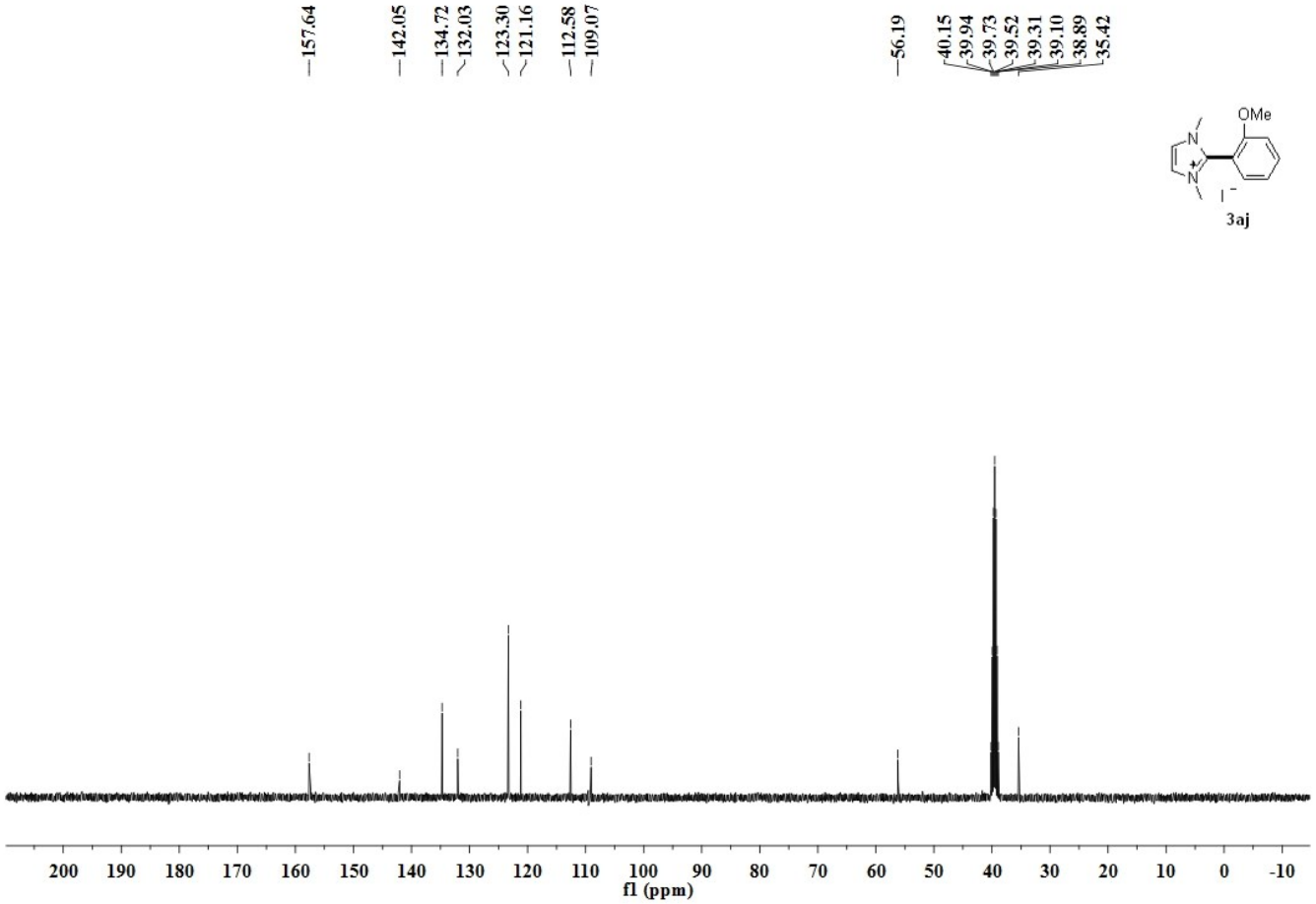

7.947
7.926
7.882
7.751
7.730
3.691
3.335
2.500
3ah
1.83
2.00
1.90
6.00
fl (ppm)

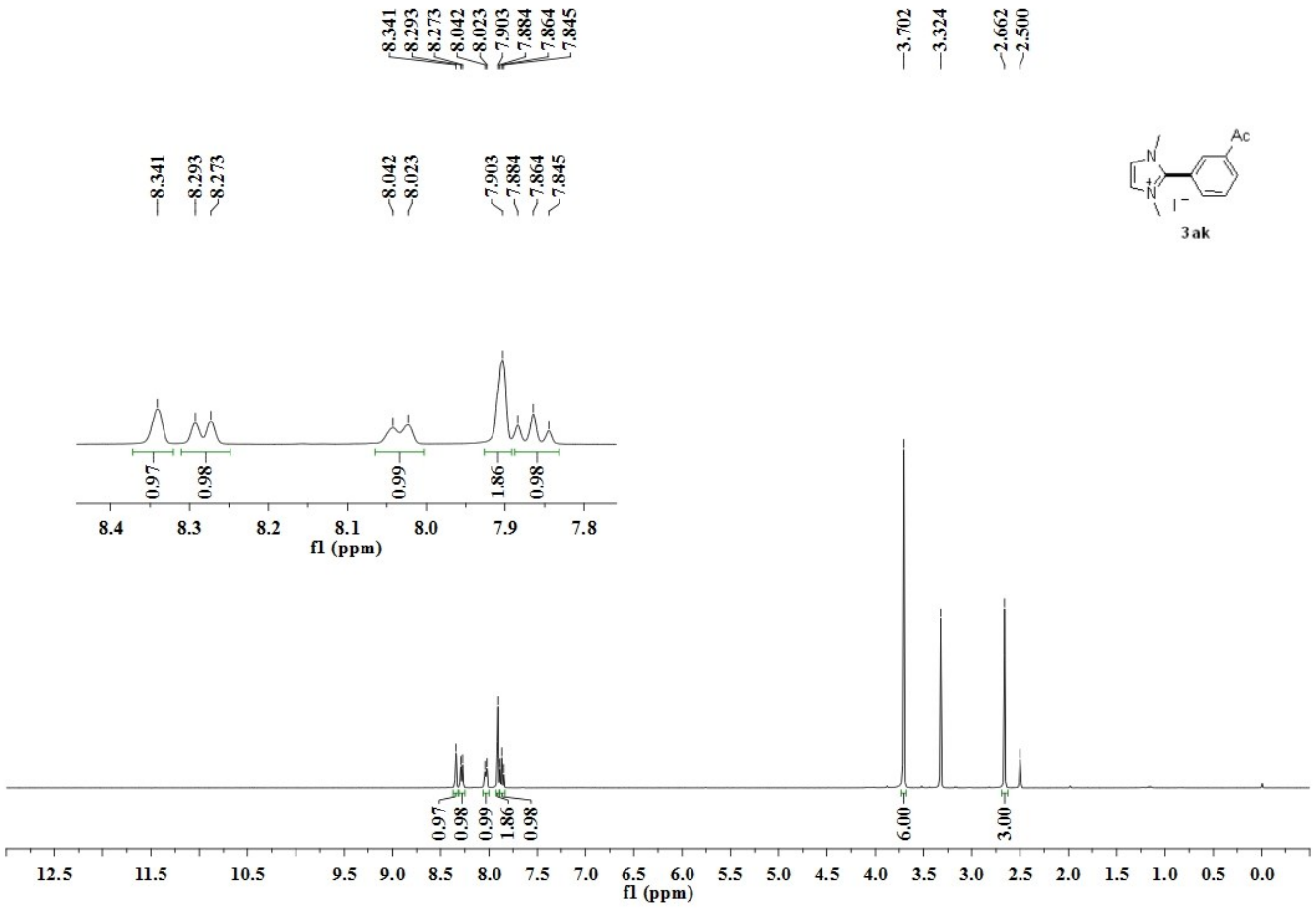

143.18
132.75
132.50
126.45
123.37
120.40
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.74
3ah
fl (ppm)

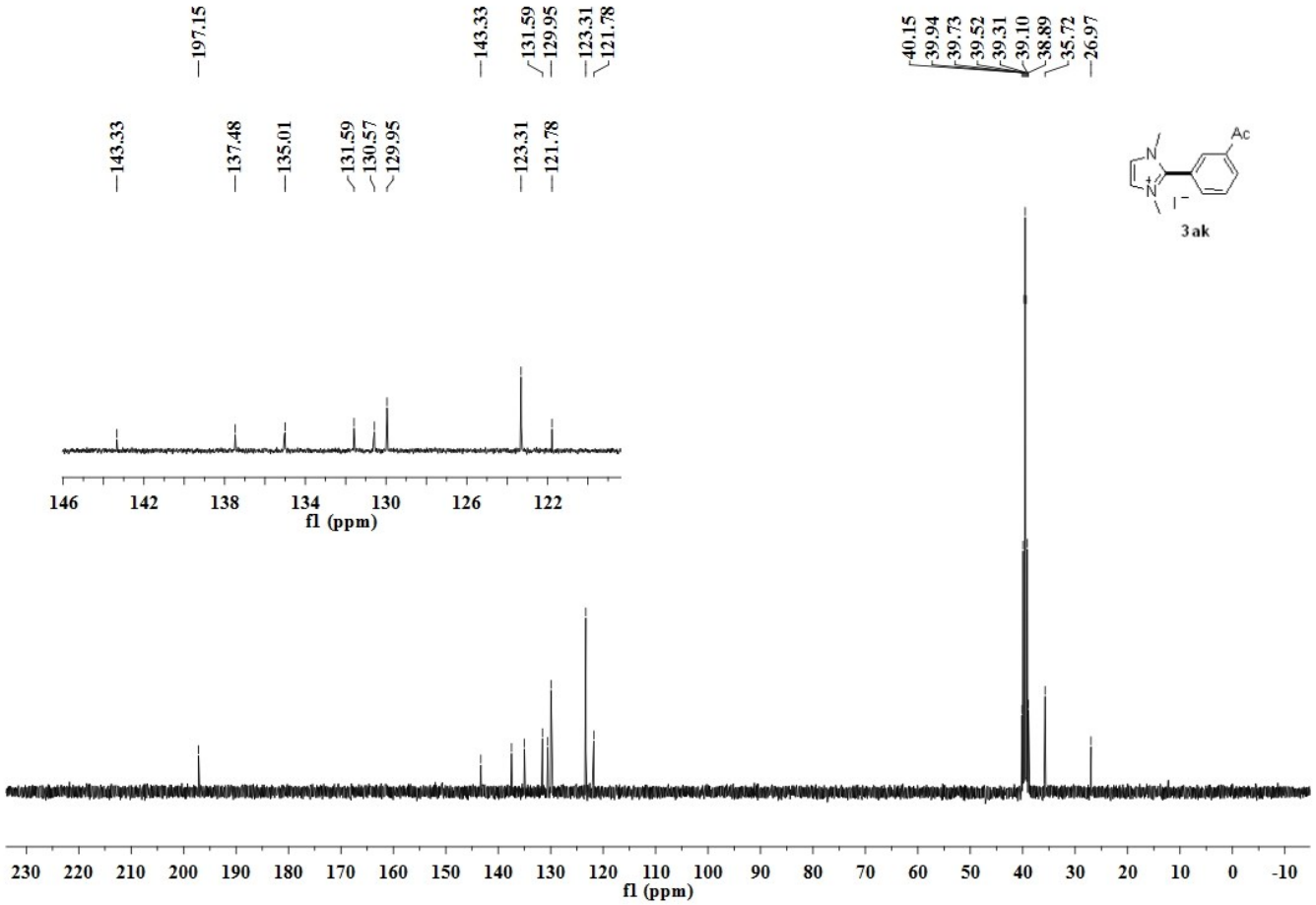

7.891
7.841
7.820
7.813
7.788
3.693
3.338
2.500
3ai
2.00
4.04
6.00
fl (ppm)

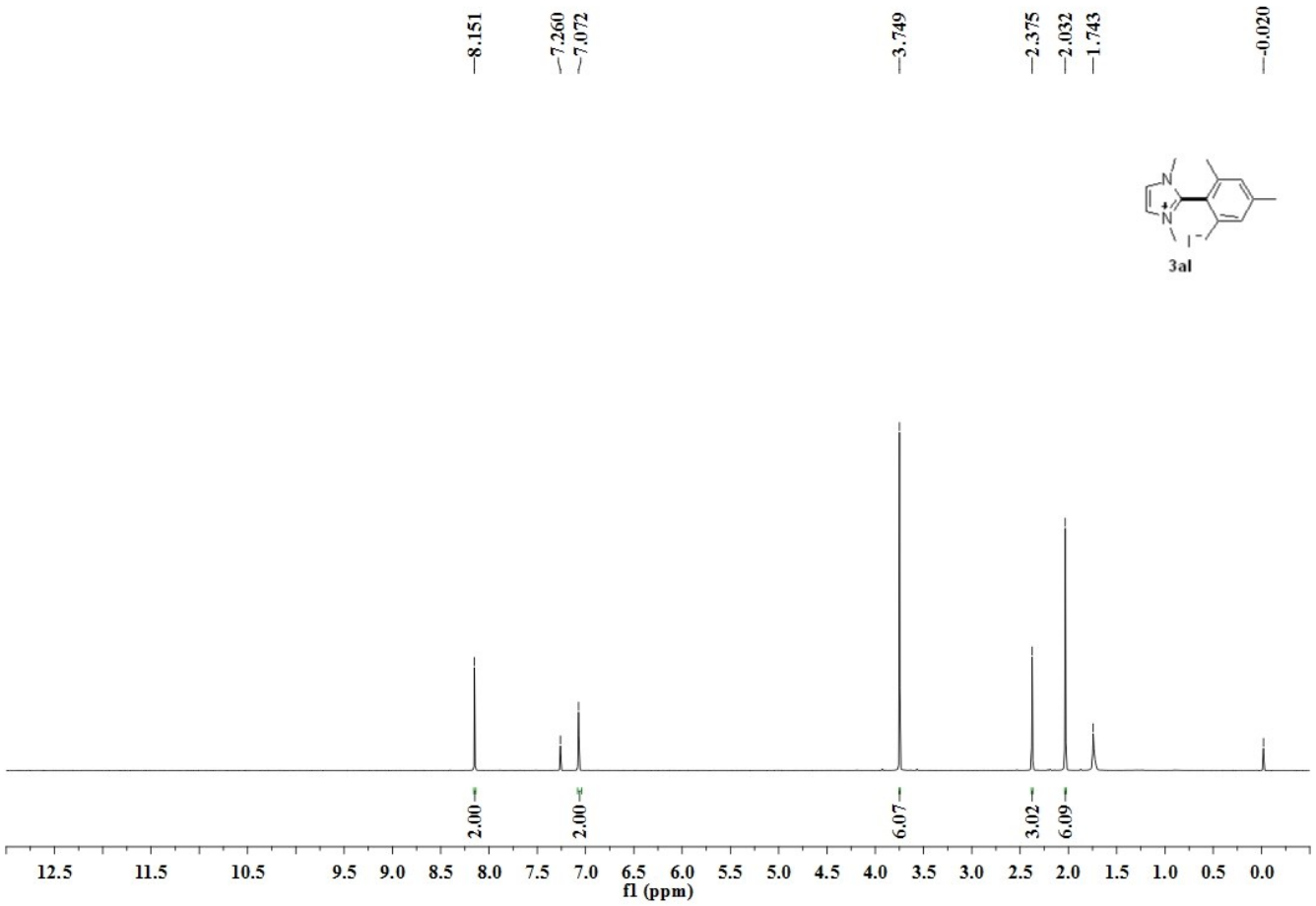

143.09
137.41
129.57
123.35
120.04
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.76
132.69
3ai
fl (ppm)

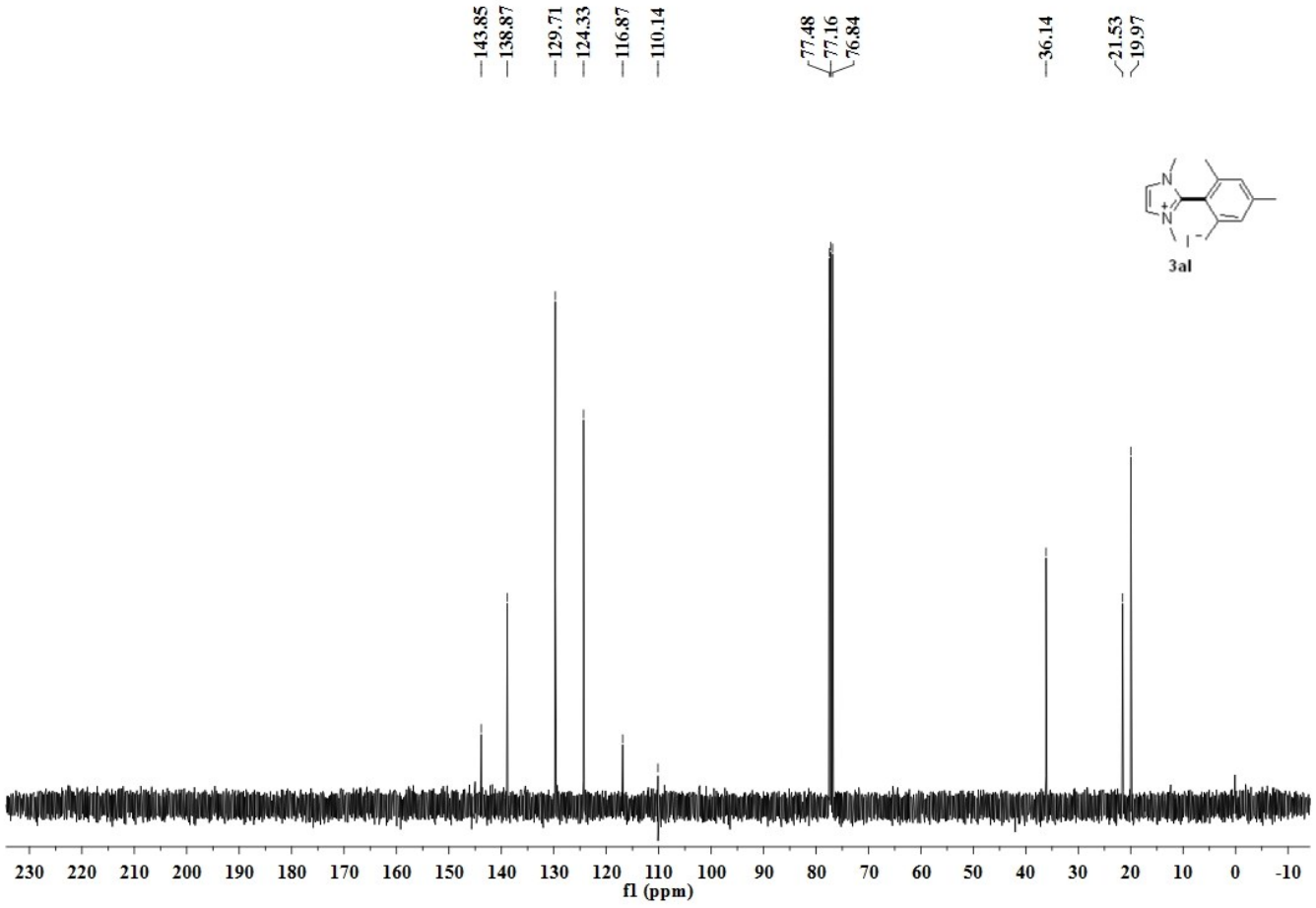

7.901
7.776
7.755
7.736
7.659
7.642
7.383
7.361
7.267
7.248
7.229
3.864
3.625
3.321
2.500
OMe
I⁻
3aj
2.00
1.06
1.02
1.08
1.08
3.06
6.07
fl (ppm)

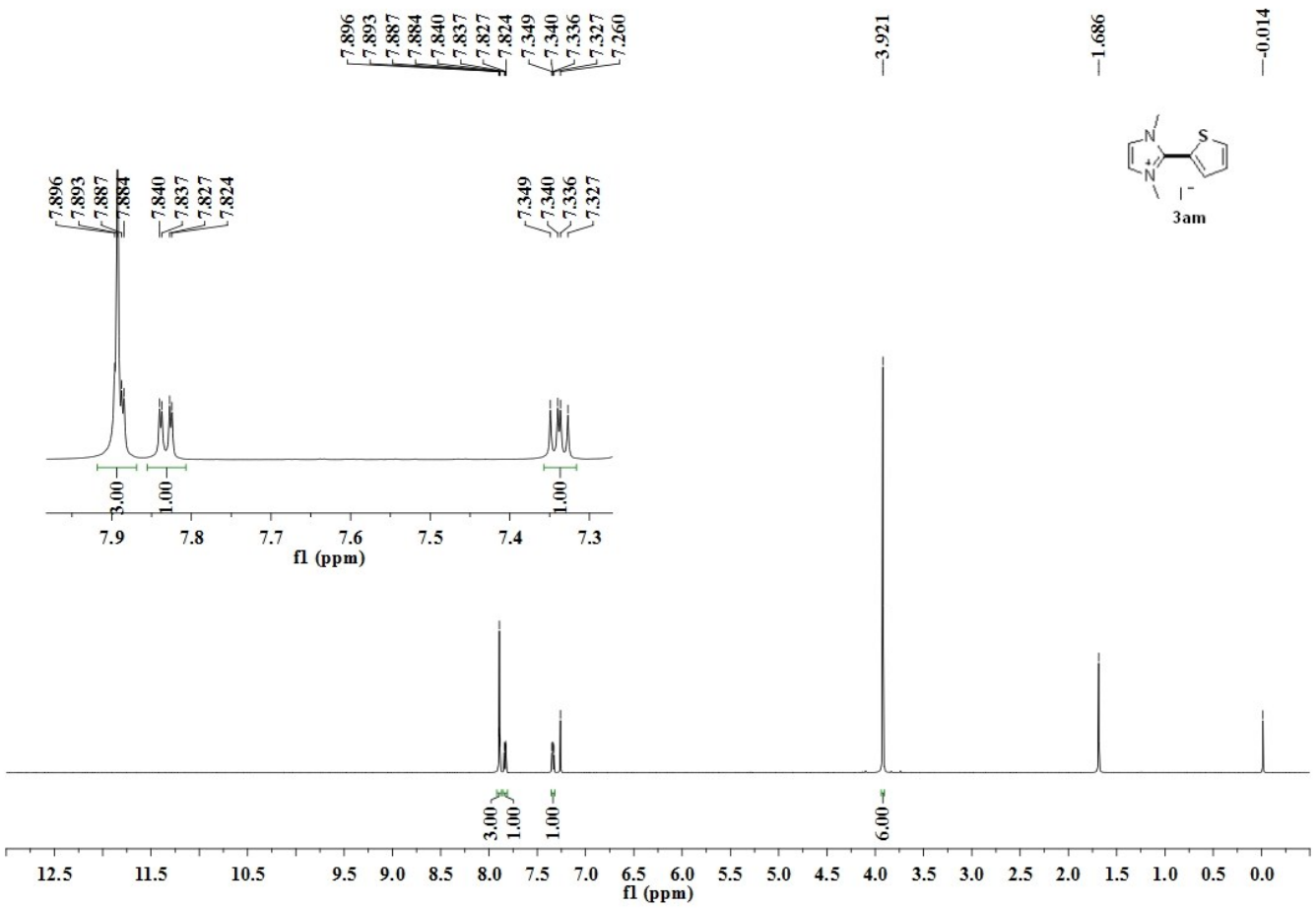

157.64
142.05
134.72
132.03
123.30
121.16
112.58
109.07
56.19
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.42
OMe
I⁻
3aj
fl (ppm)

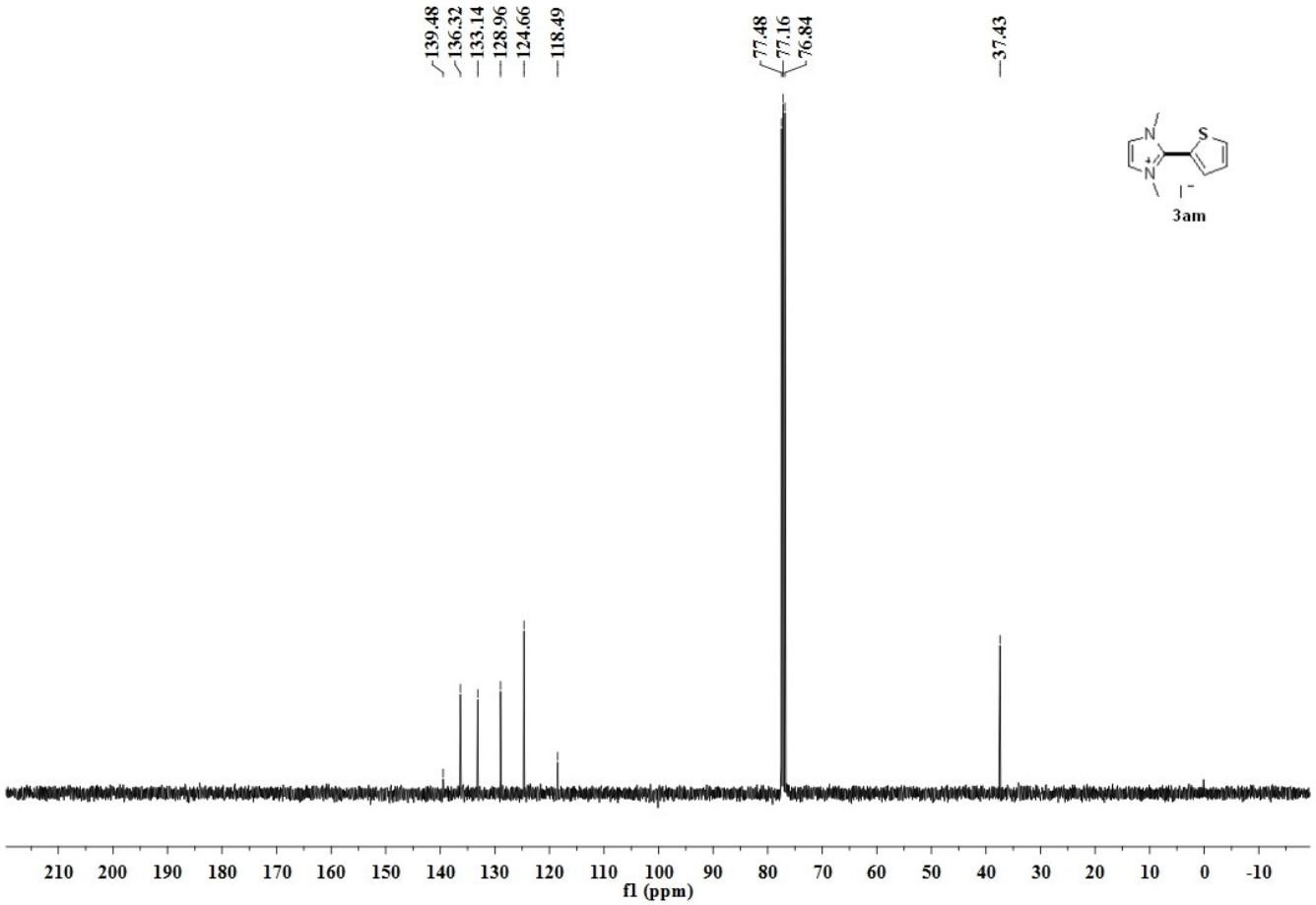

8.341
8.293
8.273
8.042
8.023
7.903
7.884
7.864
7.845
3.702
3.324
2.662
2.500
Ac
I⁻
3ak
0.97
0.98
0.99
1.86
0.98
6.00
3.00
fl (ppm)

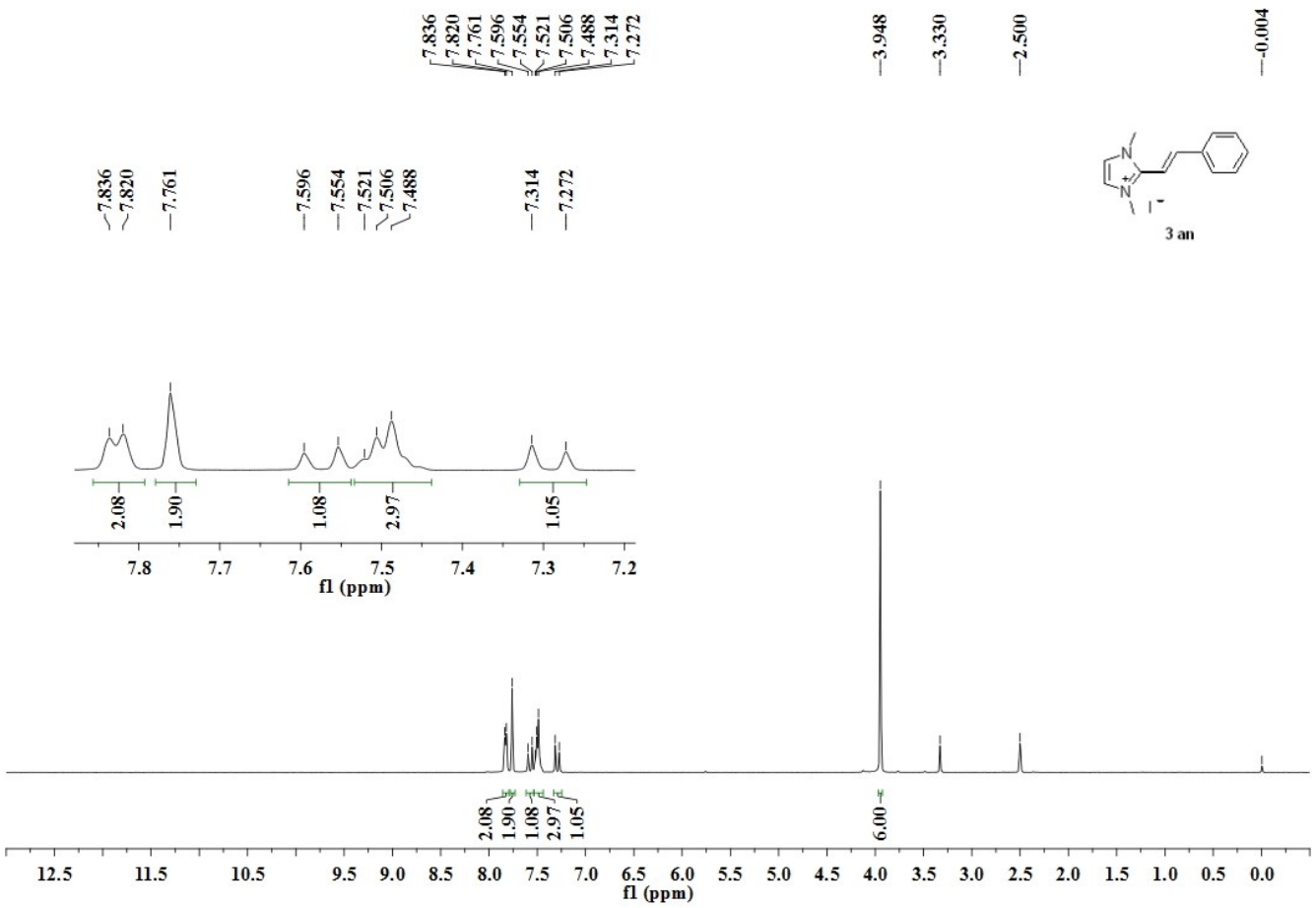

197.15
143.33
131.59
129.95
123.31
121.78
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.72
26.97
137.48
135.01
130.57
Ac
I⁻
3ak
fl (ppm)

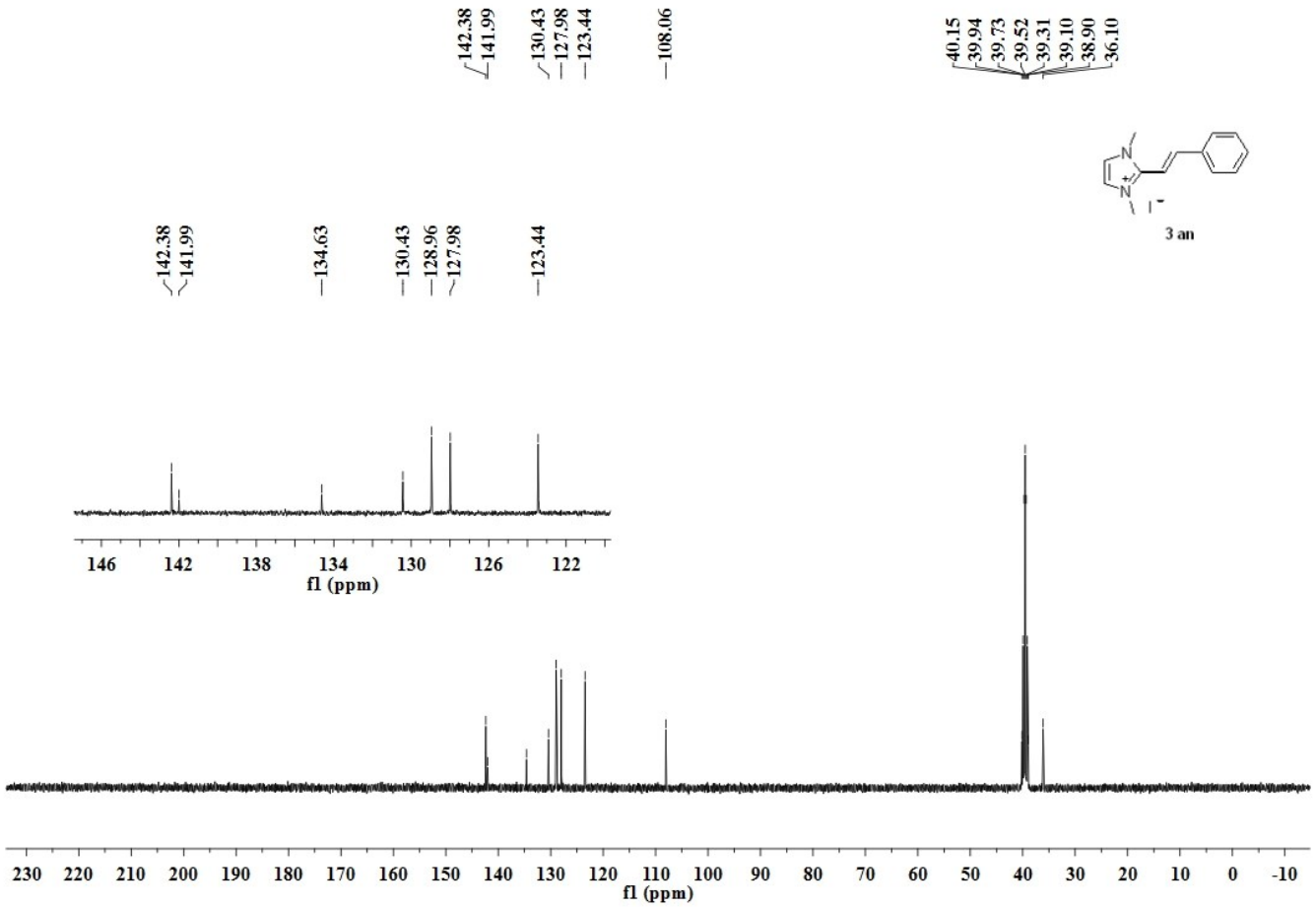

8.151
7.260
7.072
3.749
2.375
2.032
1.743
0.020
3al
2.00
2.00
6.07
3.02
6.09
fl (ppm)

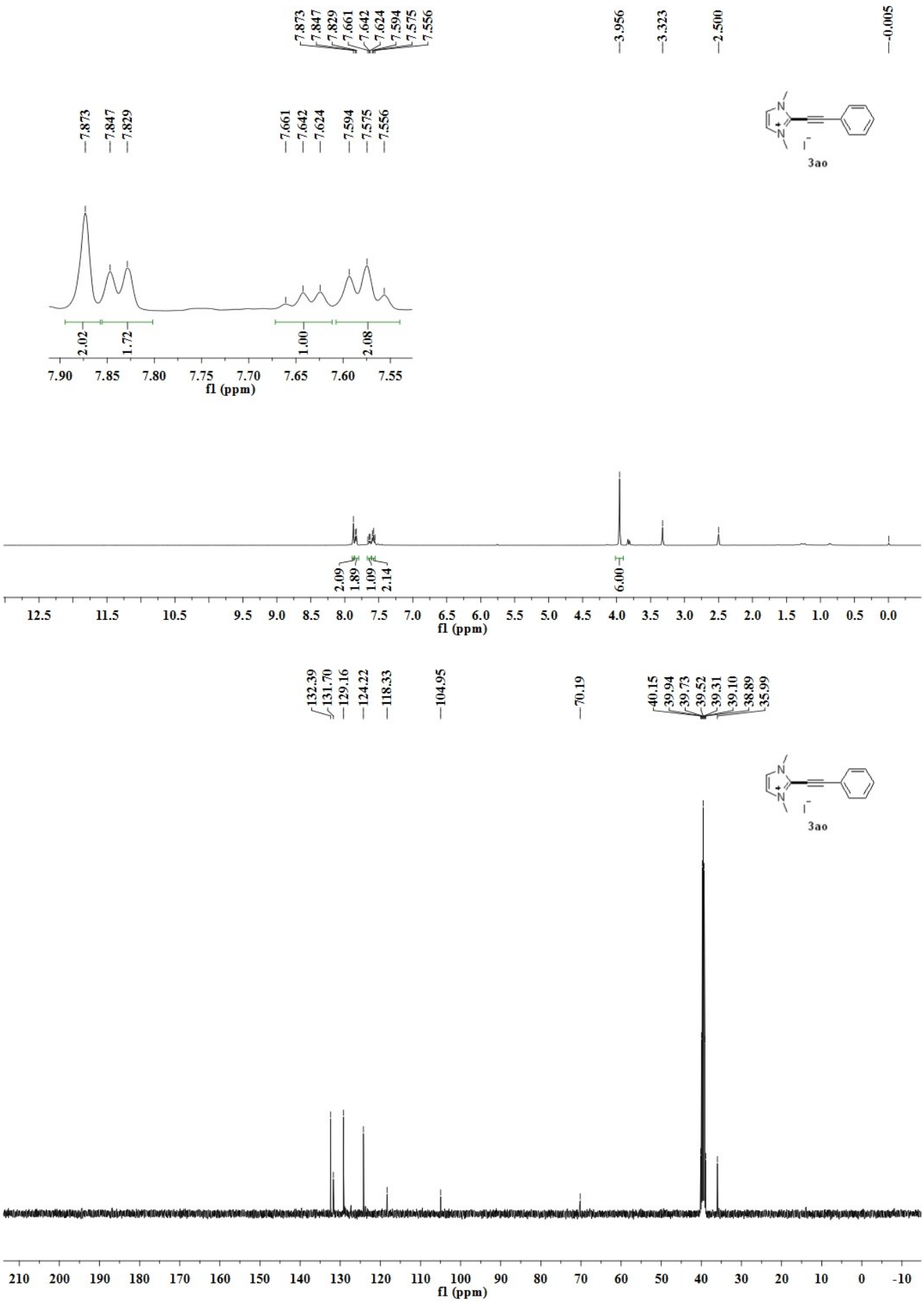

143.85
138.87
129.71
124.33
116.87
110.14
77.48
77.16
76.84
36.14
21.53
19.97
3al
fl (ppm)

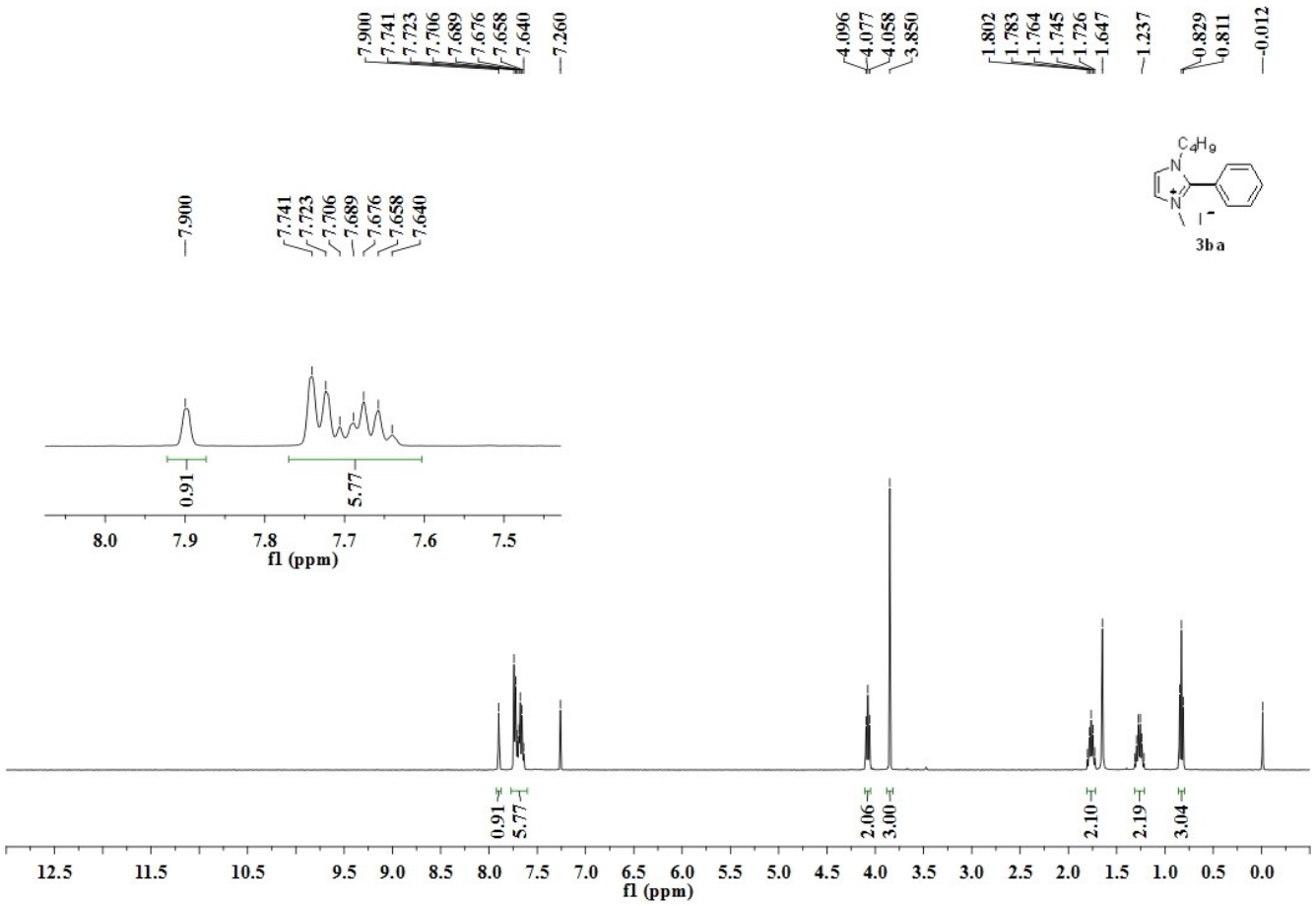

7.896
7.893
7.887
7.884
7.840
7.837
7.827
7.824
7.349
7.340
7.336
7.327
7.260
3.921
1.686
-0.014
3am
3.00
1.00
1.00
6.00
fl (ppm)

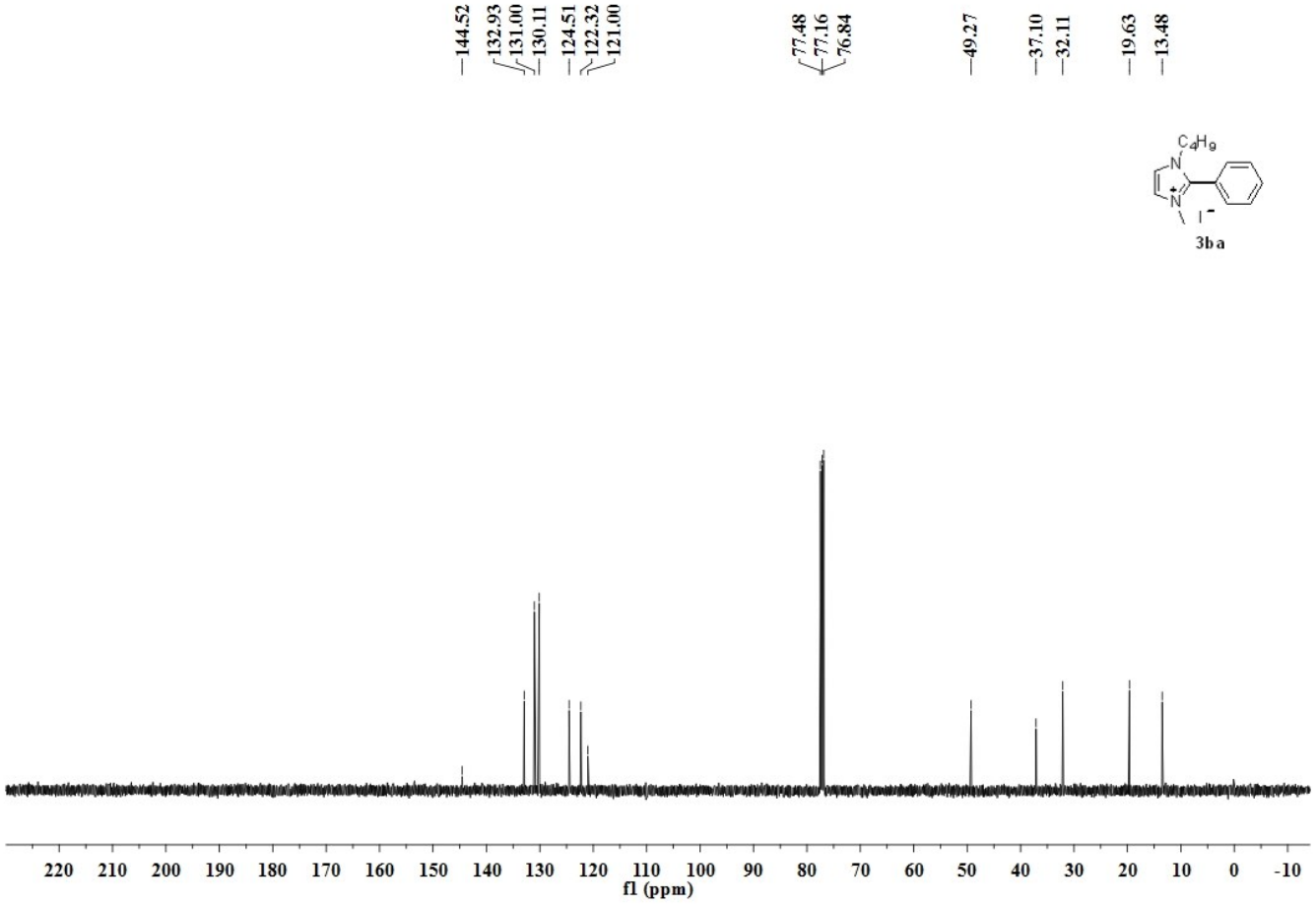

139.48
136.32
133.14
128.96
124.66
118.49
77.48
77.16
76.84
37.43
3am
fl (ppm)

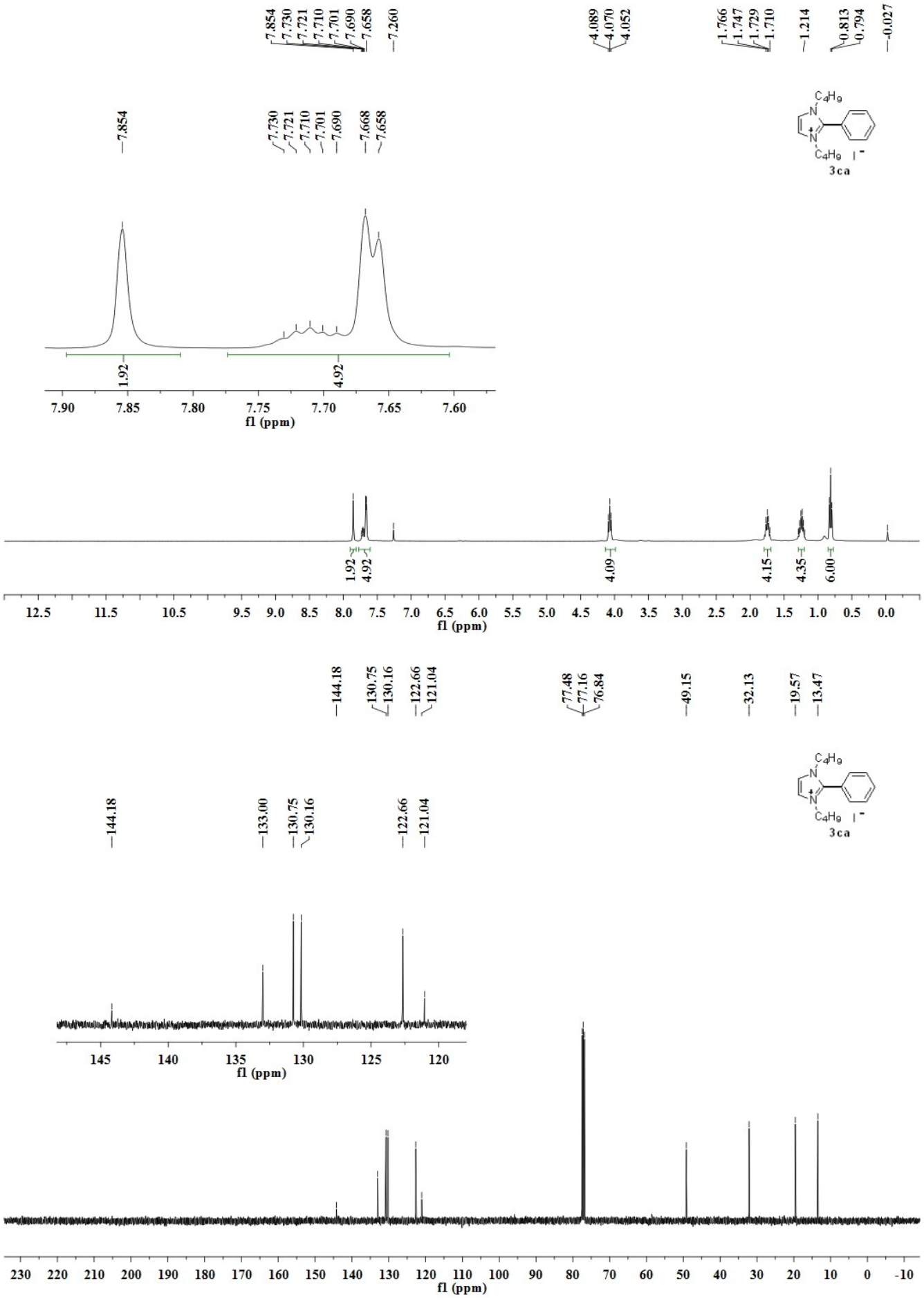

7.836
7.820
7.761
7.596
7.554
7.521
7.506
7.488
7.314
7.272
3.948
3.330
2.500
-0.004
3 an
2.08
1.90
1.08
2.97
1.05
6.00
fl (ppm)


142.38
141.99
130.43
127.98
123.44
108.06
40.15
39.94
39.73
39.52
39.31
39.10
38.90
36.10
3 an
134.63
128.96
fl (ppm)


7.873
7.847
7.829
7.661
7.642
7.624
7.594
7.575
7.556
3.956
3.323
2.500
0.005
3ao
2.02
1.72
1.00
2.08
fl (ppm)
2.09
1.89
1.09
2.14
6.00
fl (ppm)
132.39
131.70
129.16
124.22
118.33
104.95
70.19
40.15
39.94
39.73
39.52
39.31
39.10
38.89
35.99
3ao
fl (ppm)


7.900
7.741
7.723
7.706
7.689
7.676
7.658
7.640
7.260
4.096
4.077
4.058
3.850
1.802
1.783
1.764
1.745
1.726
1.647
1.237
0.829
0.811
-0.012
C4H9
3ba
0.91
5.77
2.06
3.00
2.10
2.19
3.04
fl (ppm)


144.52
132.93
131.00
130.11
124.51
122.32
121.00
77.48
77.16
76.84
49.27
37.10
32.11
19.63
13.48
C4H9
3ba
fl (ppm)


7.854
7.730
7.721
7.710
7.701
7.690
7.658
7.260
4.089
4.070
4.052
1.766
1.747
1.729
1.710
1.214
0.813
0.794
-0.027
3ca
1.92
4.92
fl (ppm)
4.09
4.15
4.35
6.00
144.18
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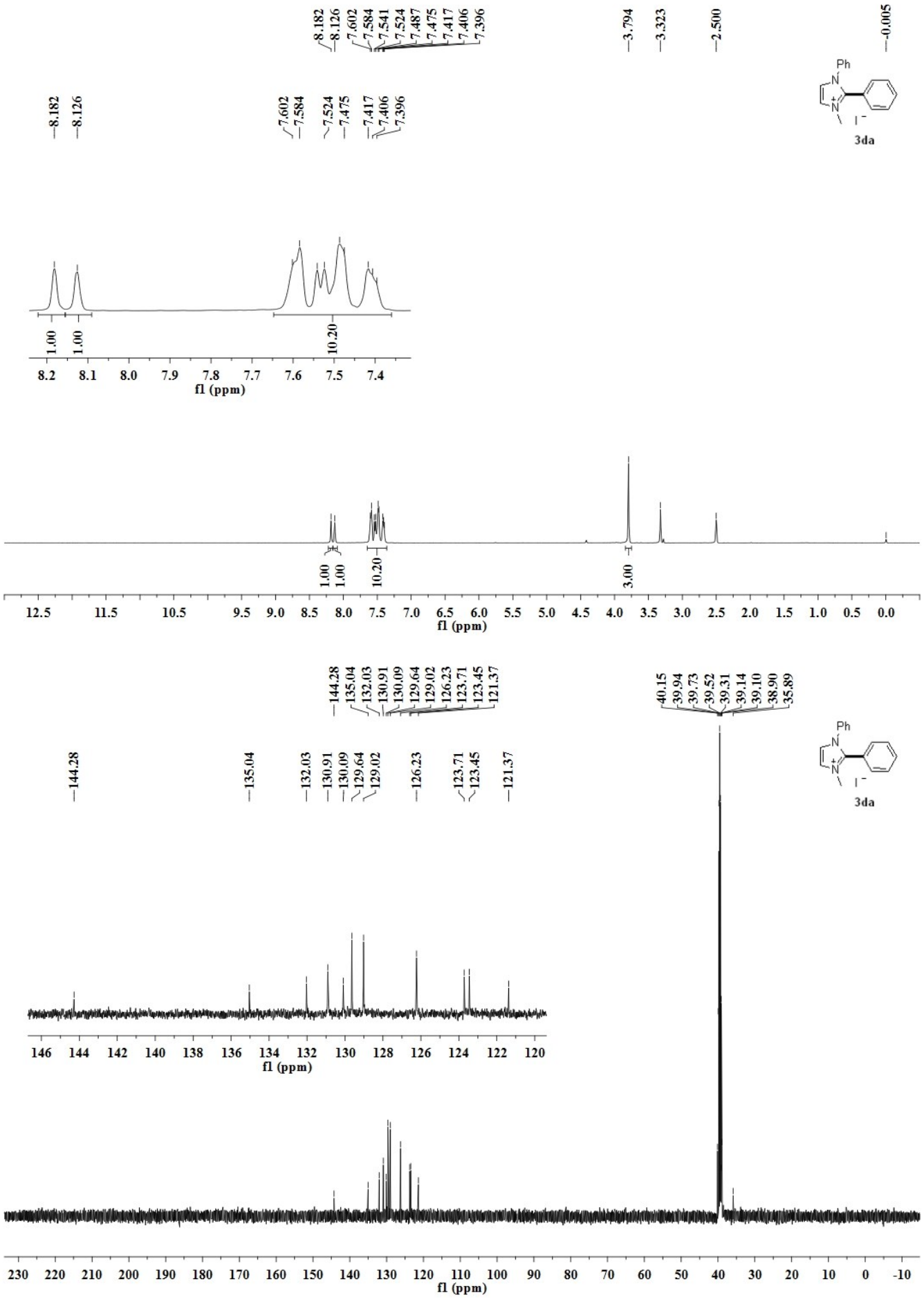
122.66
121.04
77.48
77.16
76.84
49.15
32.13
19.57
13.47
133.00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8.126
7.602
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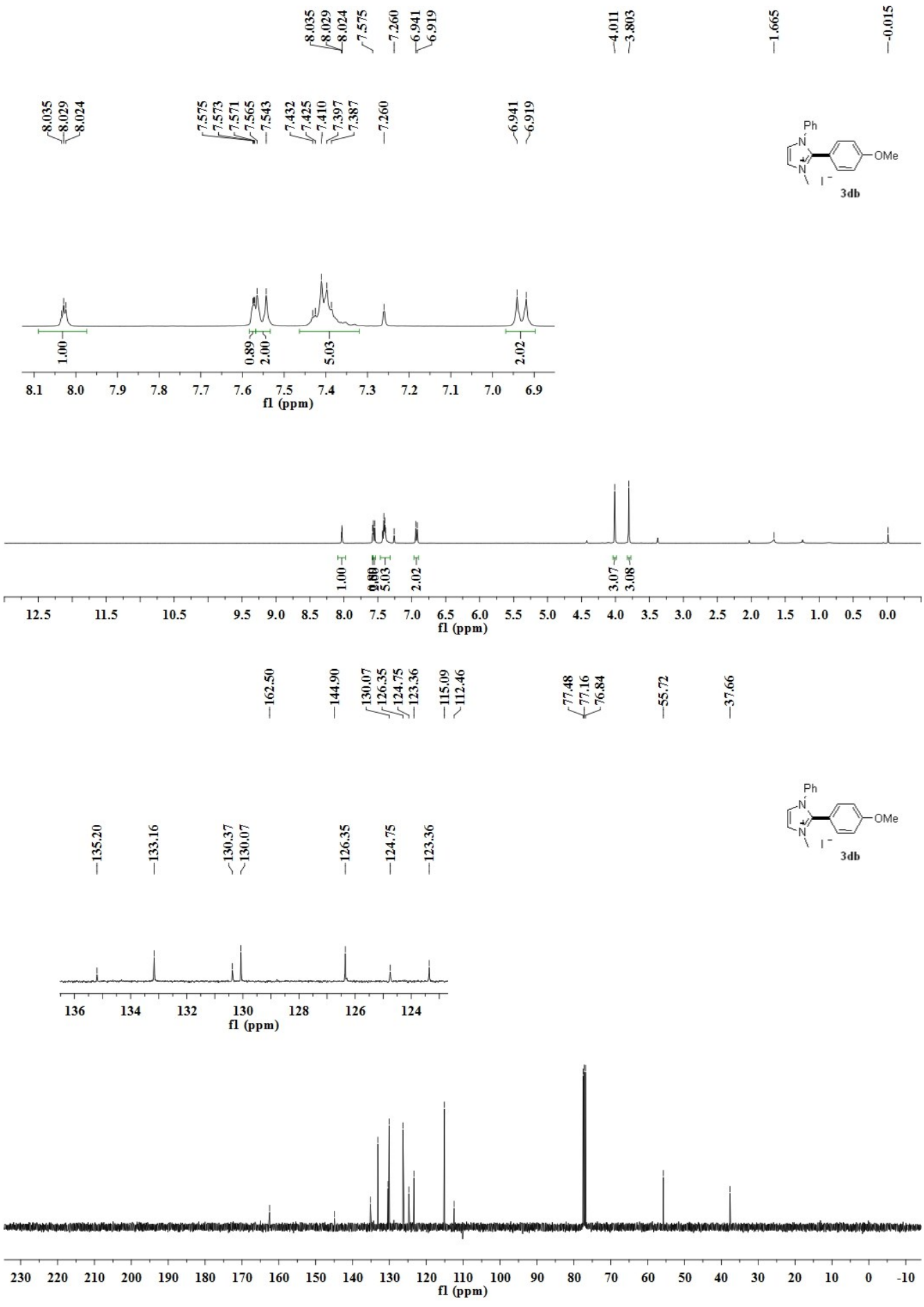
7.541
7.524
7.487
7.475
7.417
7.406
7.396
3.794
3.323
2.500
-0.005
Ph
N
N
I⁻
3da
1.00
1.00
10.20
3.00
fl (ppm)
144.28
135.04
132.03
130.91
130.09
129.64
129.02
126.23
123.71
123.45
121.37
40.15
39.94
39.73
39.52
39.31
39.14
39.10
38.90
35.89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8.029
8.024
7.575
7.260
6.941
6.919
4.011
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1.665
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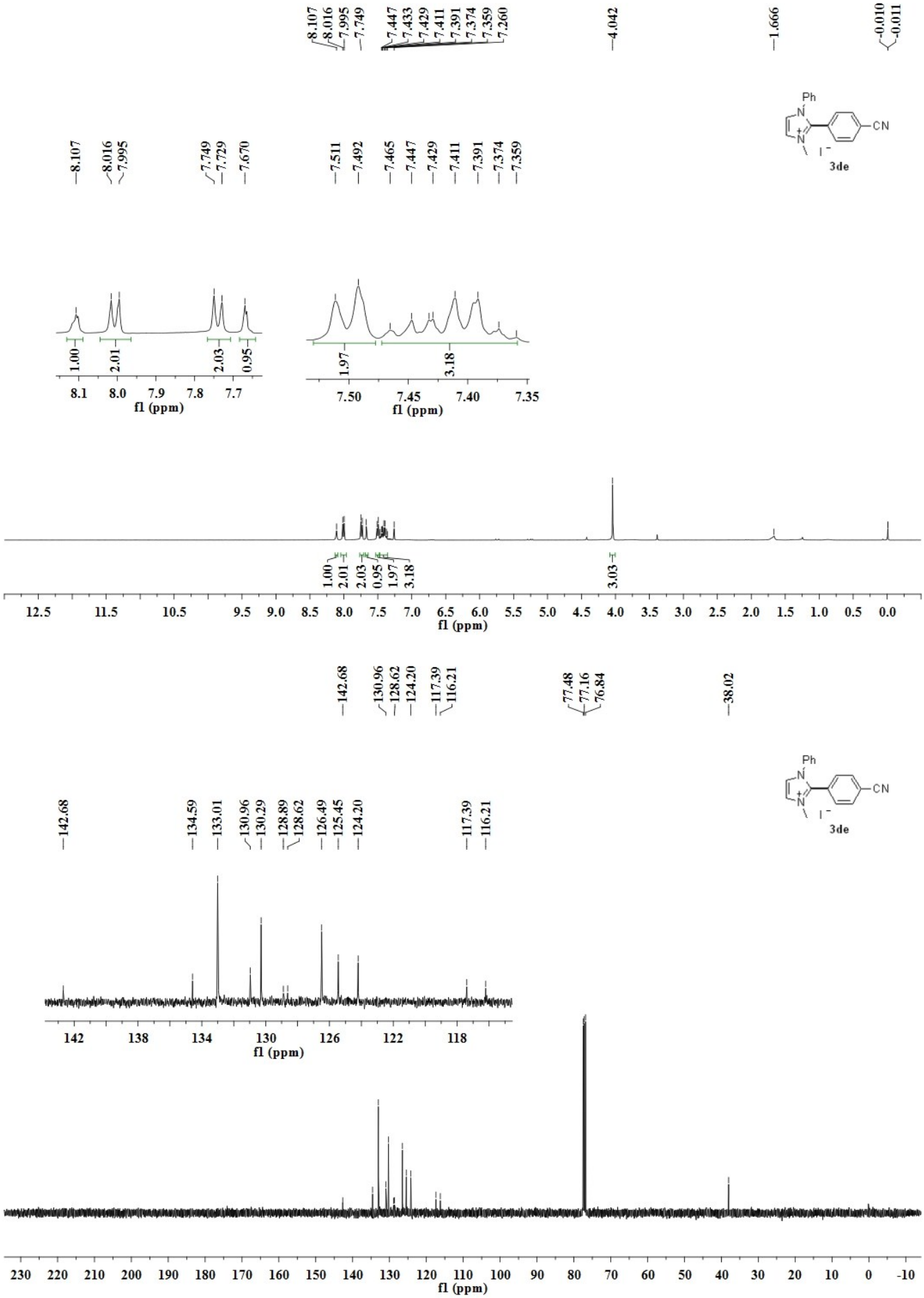
7.573
7.571
7.565
7.543
7.432
7.425
7.410
7.397
7.387
Ph
OMe
I⁻
3db
1.00
0.89
2.00
5.03
2.02
3.07
3.08
fl (ppm)
162.50
144.90
130.07
126.35
124.75
123.36
115.09
112.46
77.48
77.16
76.84
55.72
37.66
135.20
133.16
130.37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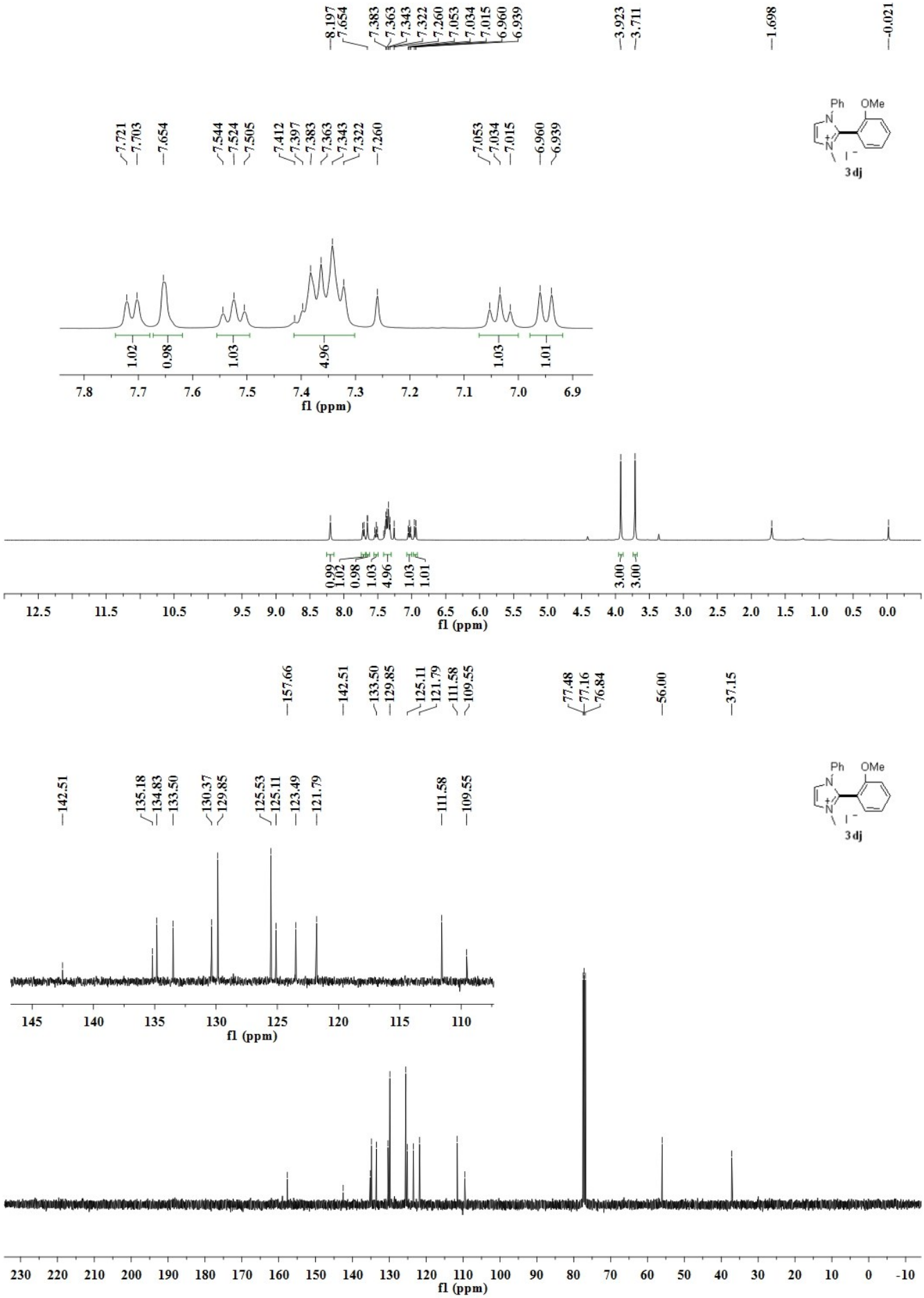
8.016
7.995
7.749
7.447
7.433
7.429
7.411
7.391
7.374
7.359
7.260
4.042
1.666
0.010
0.011
Ph
CN
I⁻
3de
7.729
7.670
7.511
7.492
7.465
7.391
1.00
2.01
2.03
0.95
1.97
3.18
3.03
fl (ppm)
142.68
130.96
128.62
124.20
117.39
116.21
77.48
77.16
76.84
38.02
134.59
133.01
130.29
128.89
128.62
126.49
125.45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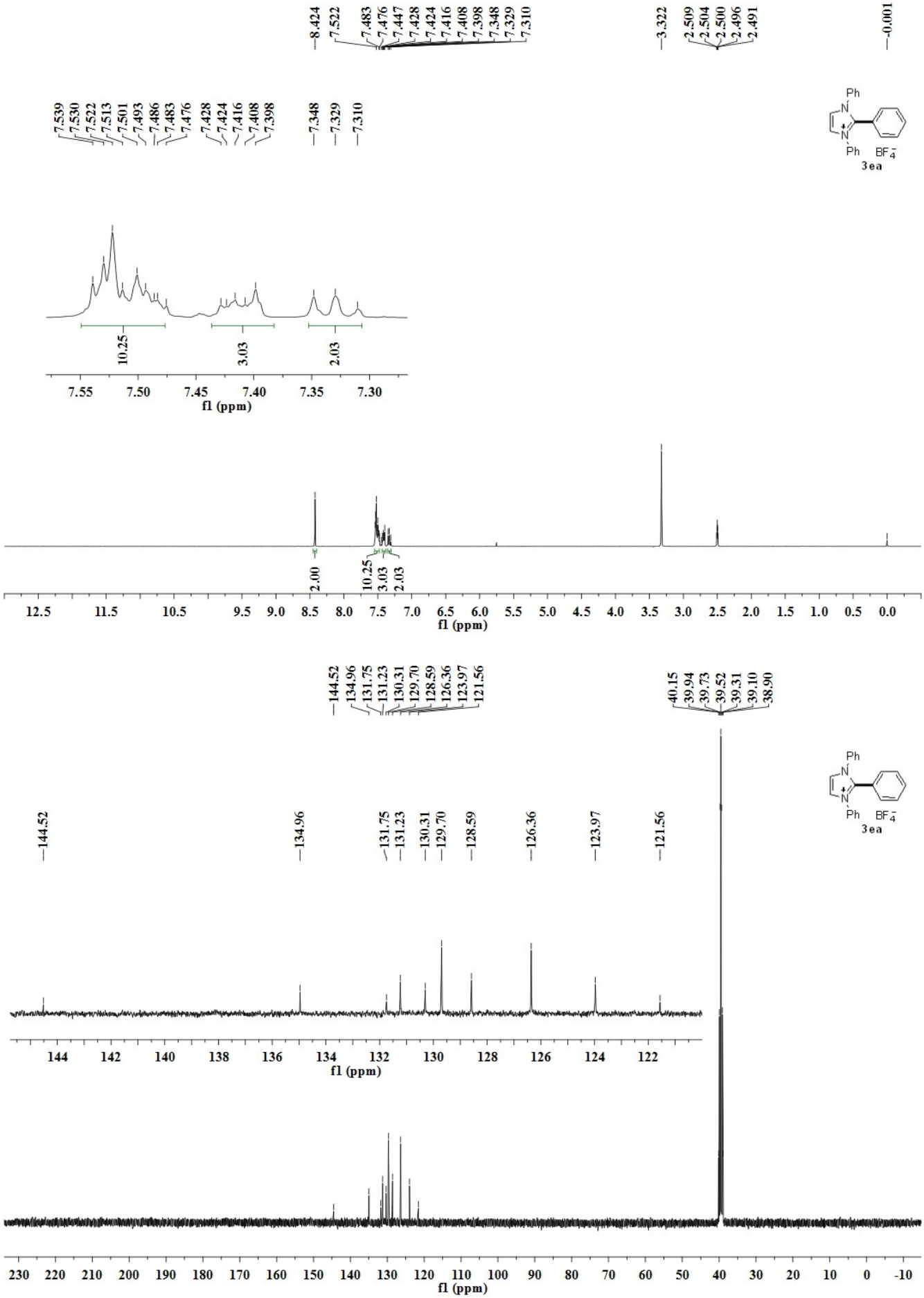
7.654
7.383
7.363
7.343
7.322
7.260
7.053
7.034
7.015
6.960
6.939
3.923
3.711
1.698
-0.021
Ph
OMe
I -
3dj
7.721
7.703
7.654
7.544
7.524
7.505
7.412
7.397
7.383
7.363
7.343
7.322
7.260
7.053
7.034
7.015
6.960
6.939
1.02
0.98
1.03
4.96
1.03
1.01
fl (ppm)
0.99
1.02
0.98
1.03
4.96
1.03
1.01
3.00
3.00
fl (ppm)
157.66
142.51
133.50
129.85
125.11
121.79
111.58
109.55
77.48
77.16
76.84
56.00
37.15
142.51
135.18
134.83
133.50
130.37
129.85
125.53
125.11
123.49
121.79
111.58
109.55
fl (ppm)
fl (ppm)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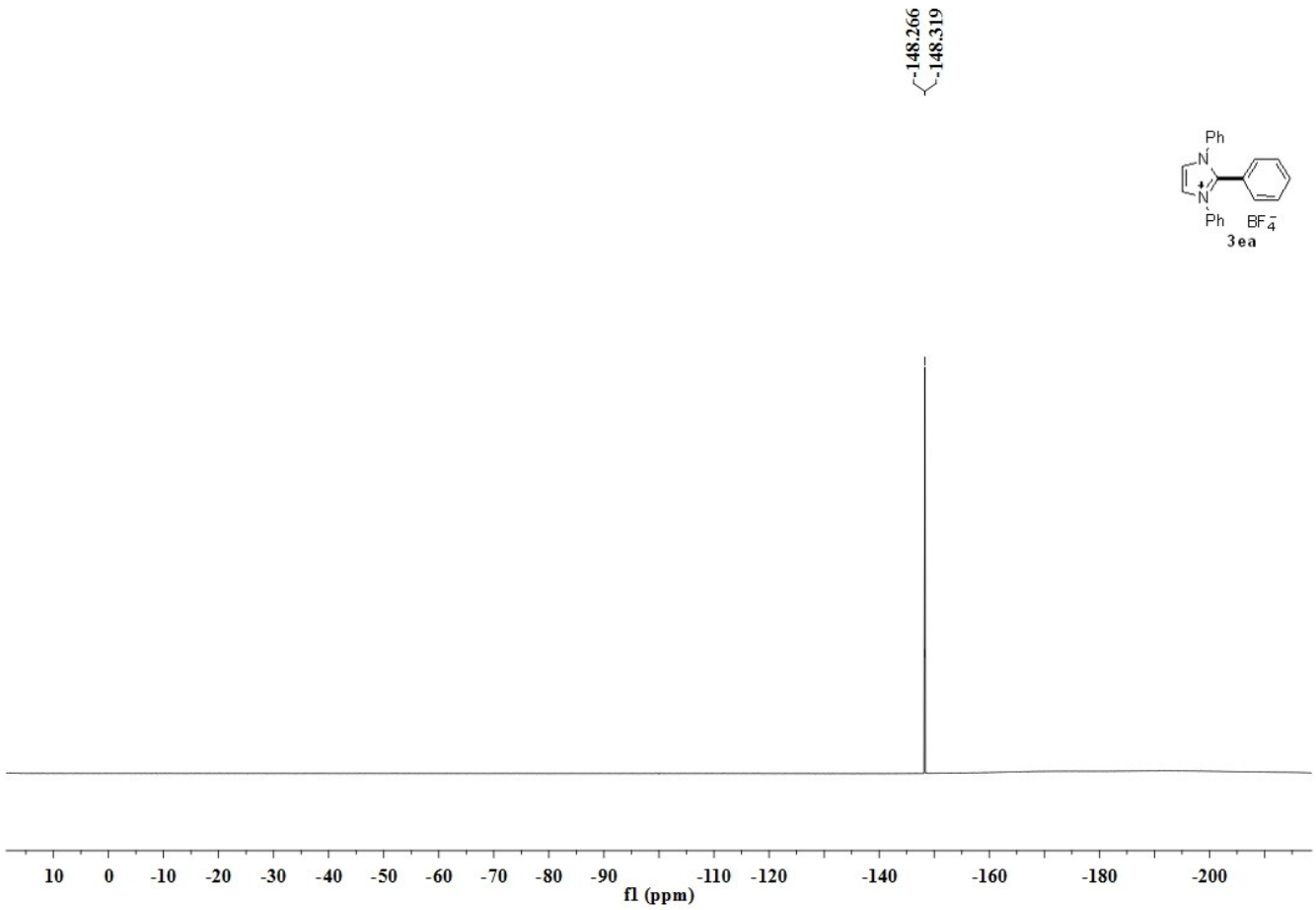
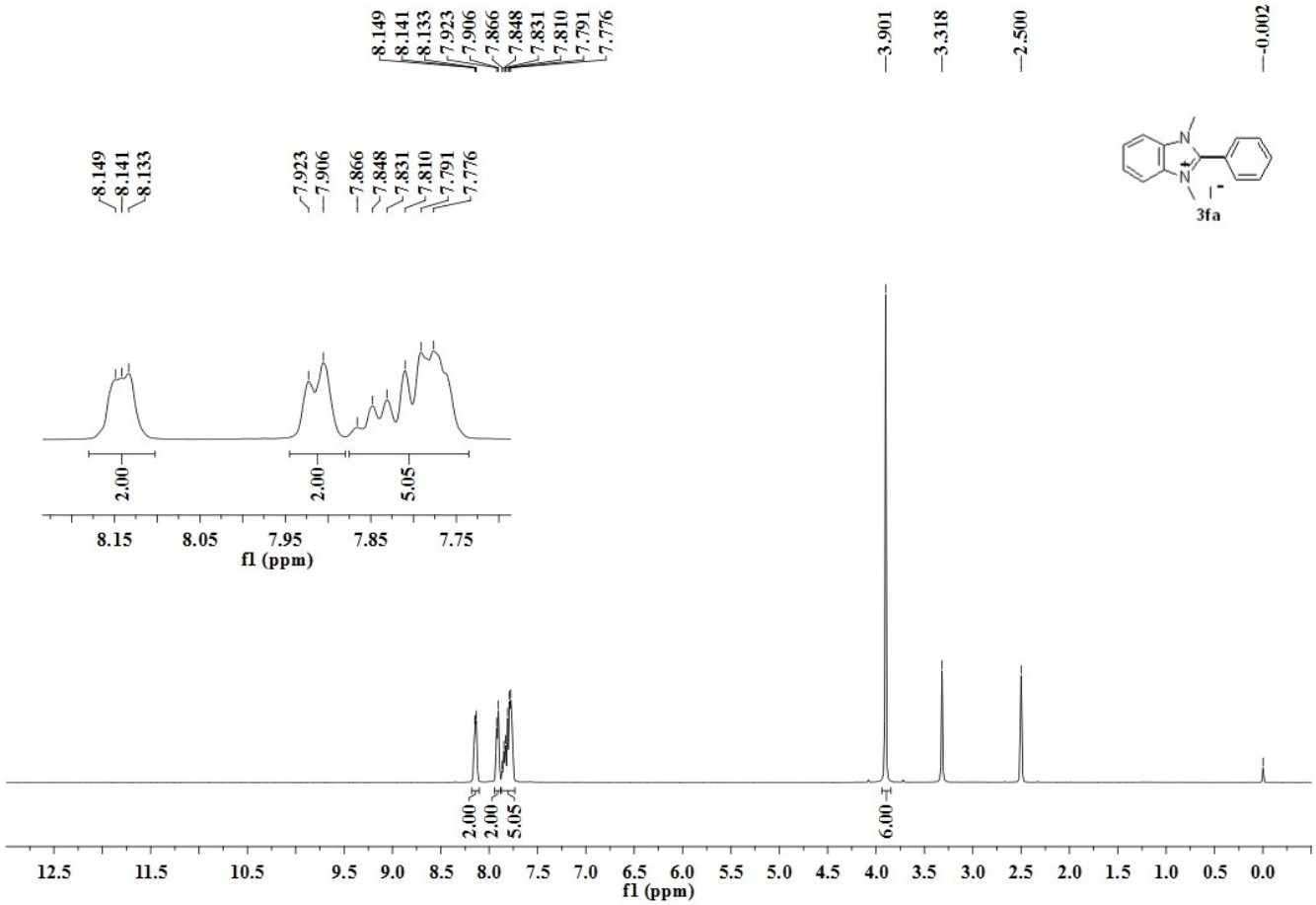
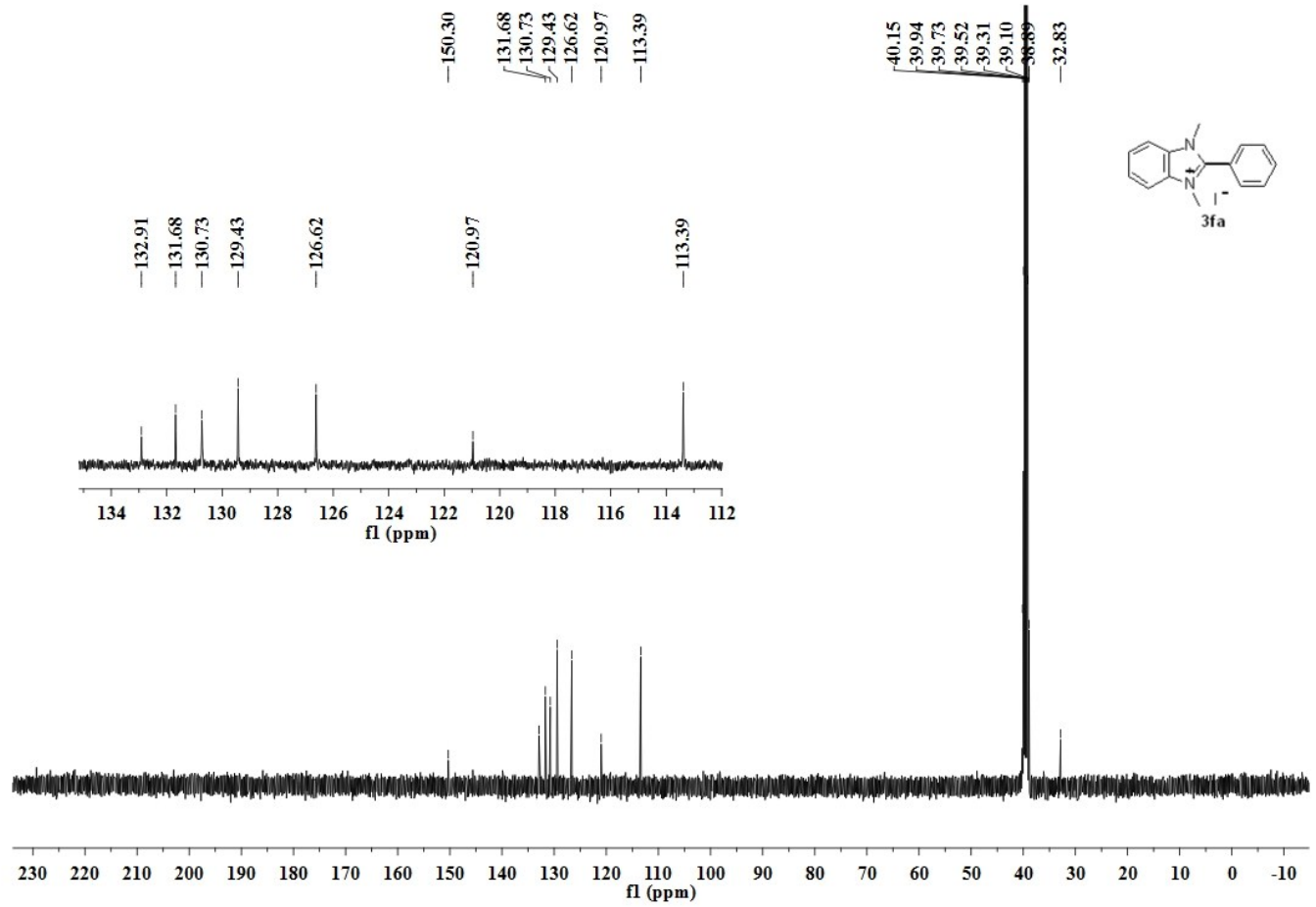
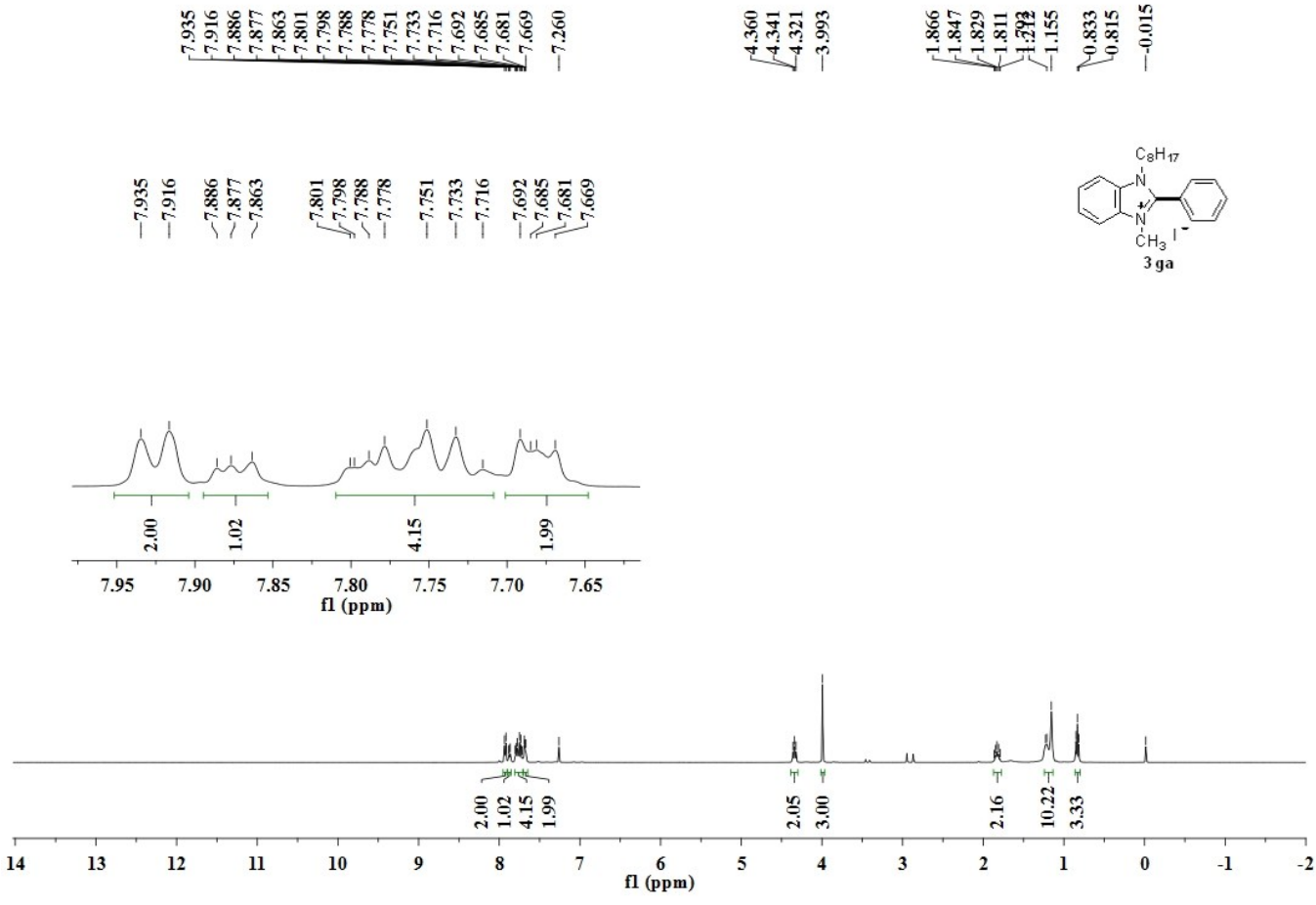
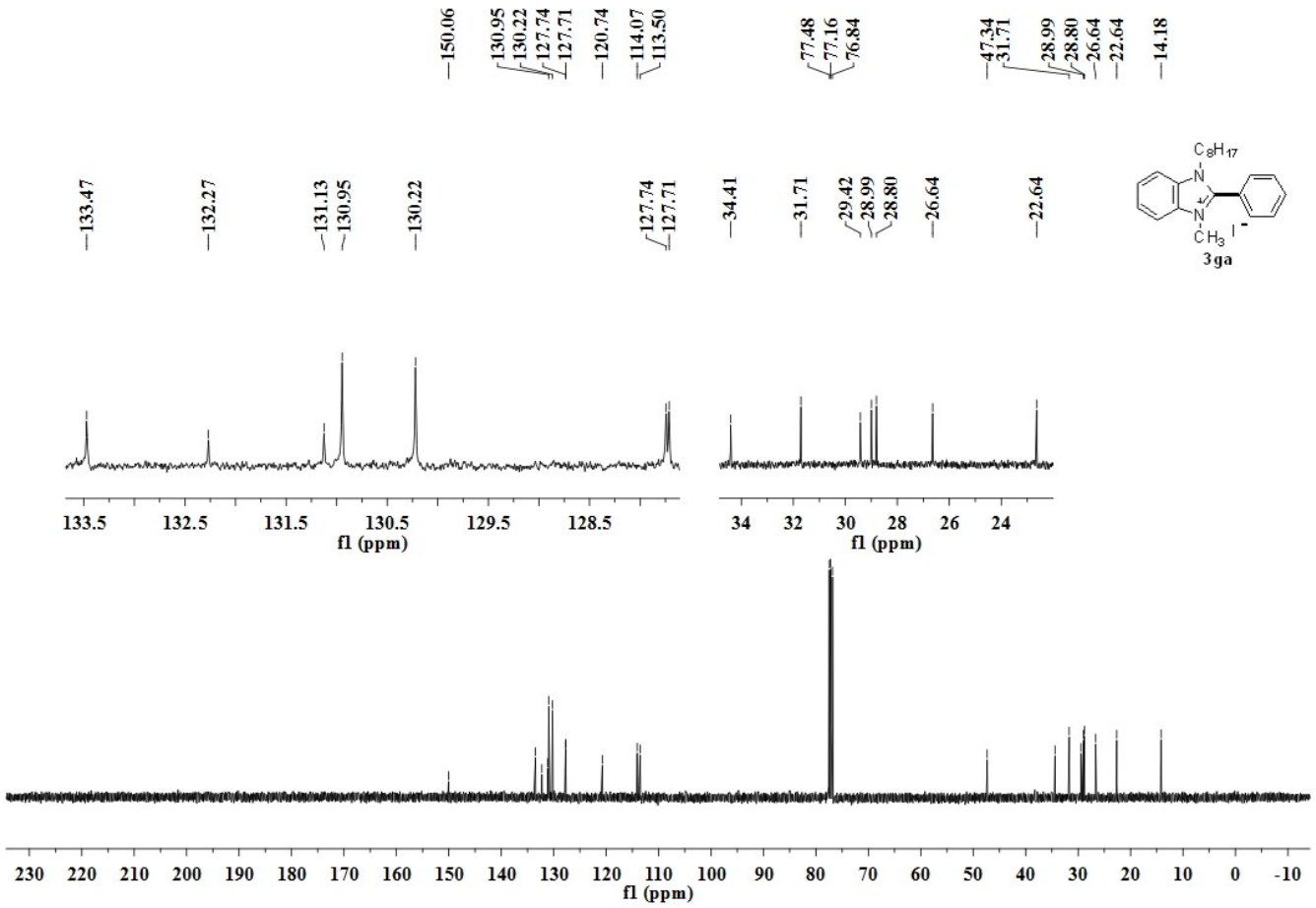
7.483
7.476
7.447
7.428
7.424
7.416
7.408
7.398
7.348
7.329
7.310
3.322
2.509
2.504
2.500
2.496
2.491
-0.001
7.539
7.530
7.522
7.513
7.501
7.493
7.486
7.483
7.476
7.428
7.424
7.416
7.408
7.398
7.348
7.329
7.310
Ph
Ph
BF4-
3ea
10.25
3.03
2.03
7.55
7.50
7.45
7.40
7.35
7.30
f1 (ppm)
2.00
10.25
3.03
2.03
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
144.52
134.96
131.75
131.23
130.31
129.70
128.59
126.36
123.97
121.56
40.15
39.94
39.73
39.52
39.31
39.10
38.90
Ph
Ph
BF4-
3ea
144.52
134.96
131.75
131.23
130.31
129.70
128.59
126.36
123.97
121.56
144
142
140
138
136
134
132
130
128
126
124
122
f1 (ppm)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-148.266
-148.319
Ph
Ph
BF4-
3ea
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -120 -140 -160 -180 -200
f1 (ppm)


8.149
8.141
8.133
7.923
7.906
7.866
7.848
7.831
7.810
7.791
7.776
3.901
3.318
2.500
0.002
I-
3fa
2.00
2.00
5.05
6.00
8.15 8.05 7.95 7.85 7.75
f1 (ppm)
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.30
131.68
130.73
129.43
126.62
120.97
113.39
40.15
39.94
39.73
39.52
39.31
39.10
38.89
32.83
3fa
132.91
131.68
130.73
129.43
126.62
120.97
113.39
134 132 130 128 126 124 122 120 118 116 114 112
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.935
7.916
7.886
7.877
7.863
7.801
7.798
7.788
7.778
7.751
7.733
7.716
7.692
7.685
7.681
7.669
7.260
4.360
4.341
4.321
3.993
1.866
1.847
1.829
1.811
1.155
0.833
0.815
-0.015
3 ga
2.00
1.02
4.15
1.99
7.95 7.90 7.85 7.80 7.75 7.70 7.65
f1 (ppm)
2.00
1.02
4.15
1.99
2.05
3.00
2.16
10.22
3.33
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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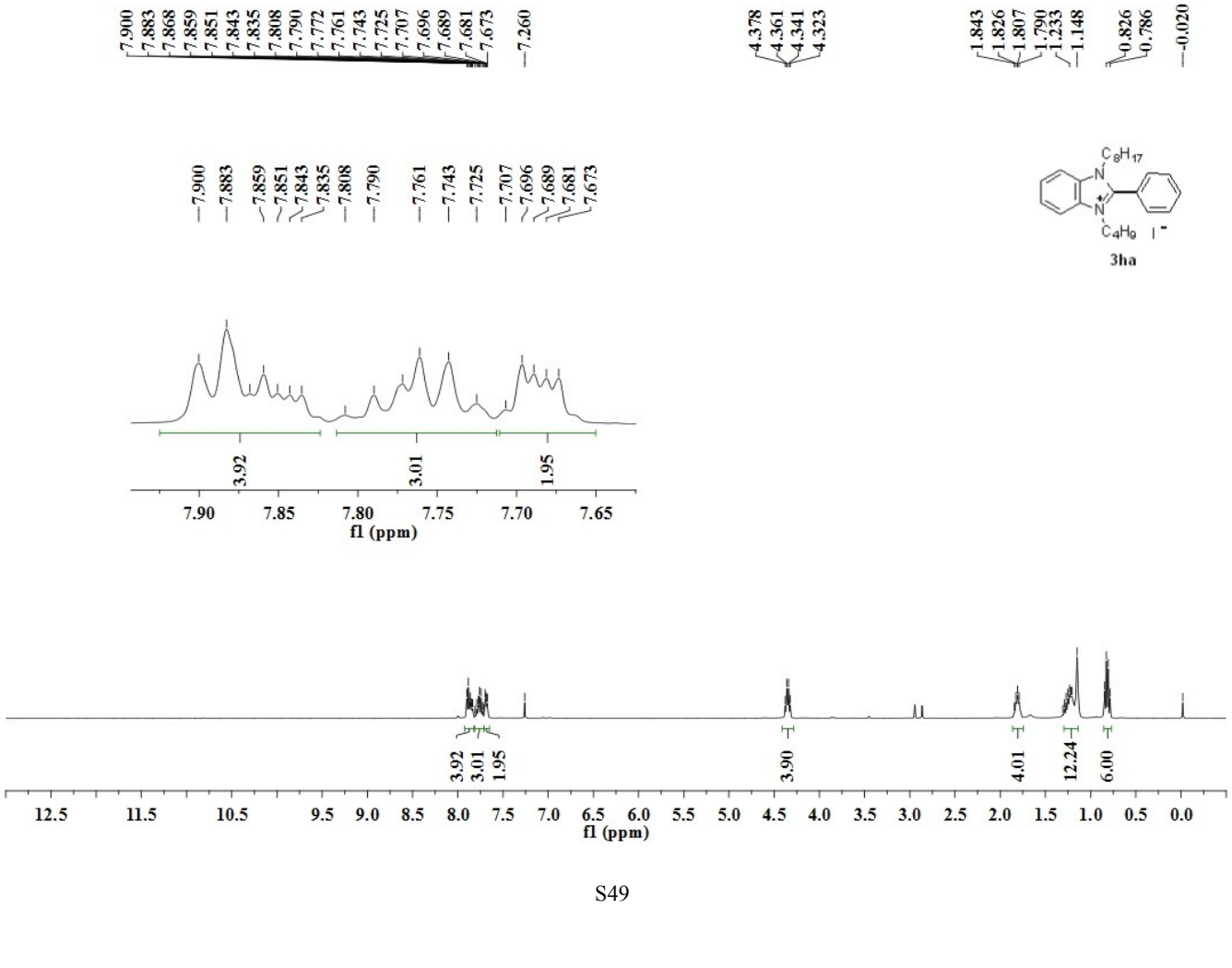
130.95
130.22
127.74
127.71
120.74
114.07
113.50
77.48
77.16
76.84
47.34
31.71
28.99
28.80
26.64
22.64
14.18
133.47
132.27
131.13
130.95
130.22
127.74
127.71
34.41
31.71
29.42
28.99
28.80
26.64
22.64
3ga
fl (ppm)
fl (ppm)
fl (ppm)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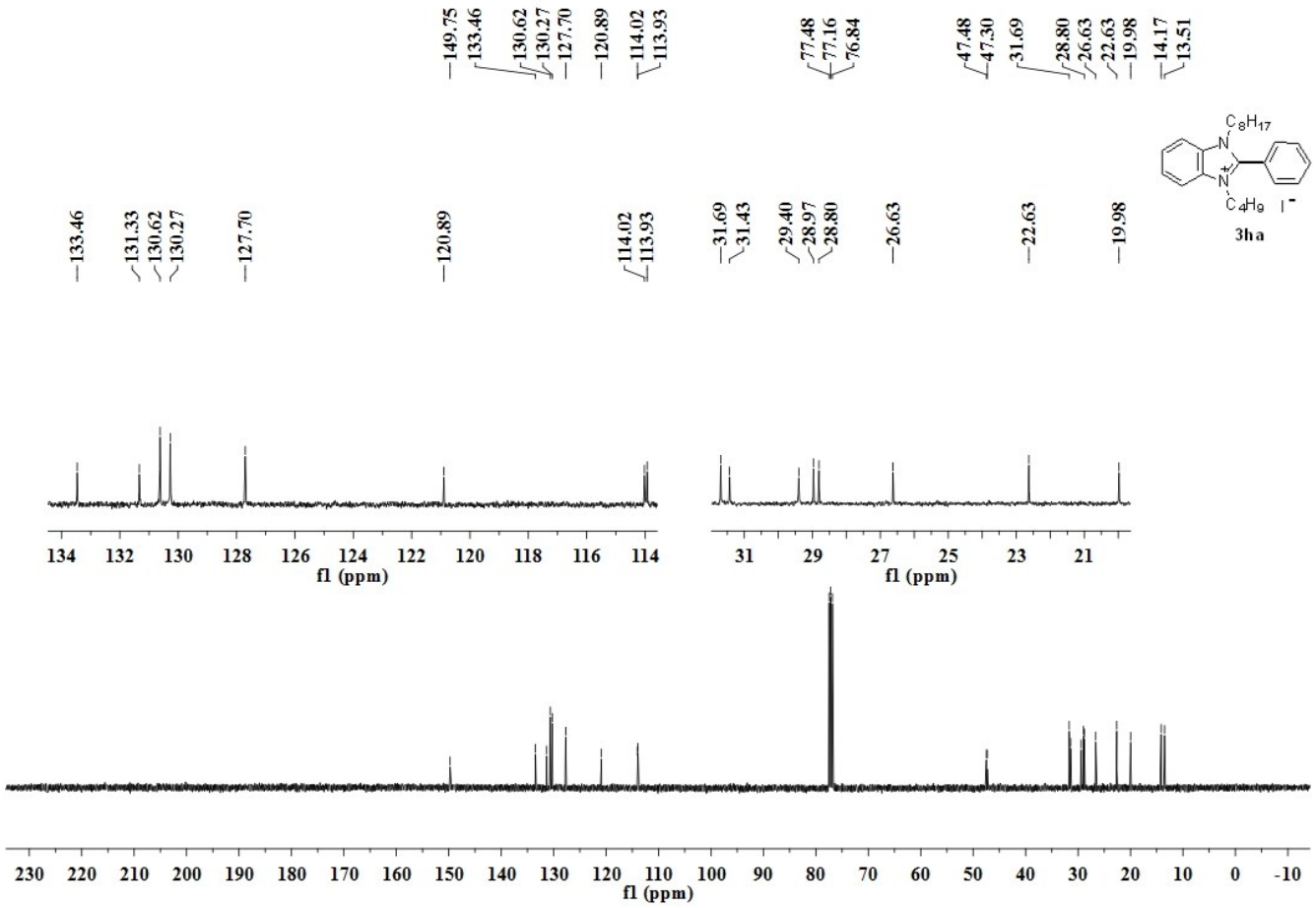
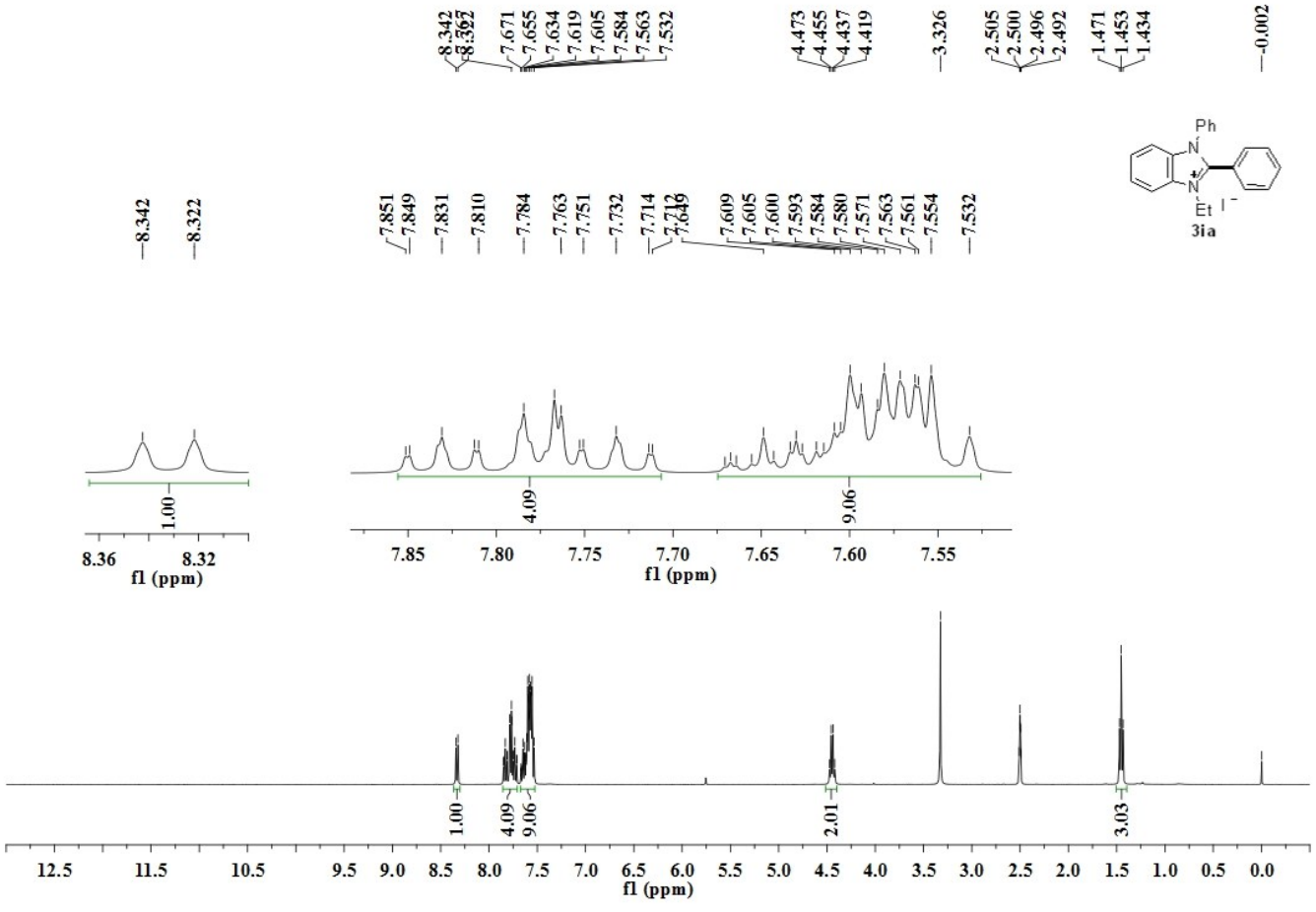
7.868
7.859
7.851
7.843
7.835
7.808
7.790
7.772
7.761
7.743
7.725
7.707
7.696
7.689
7.681
7.673
7.260
4.378
4.361
4.341
4.323
1.843
1.826
1.807
1.790
1.233
1.148
0.826
0.786
-0.020
3ha
3.92
3.01
1.95
3.90
4.01
12.24
6.00
fl (ppm)
fl (ppm)
fl (ppm)


149.75
133.46
130.62
130.27
127.70
120.89
114.02
113.93
77.48
77.16
76.84
47.48
47.30
31.69
28.80
26.63
22.63
19.98
14.17
13.51
3ha
fl (ppm)
fl (ppm)
fl (ppm)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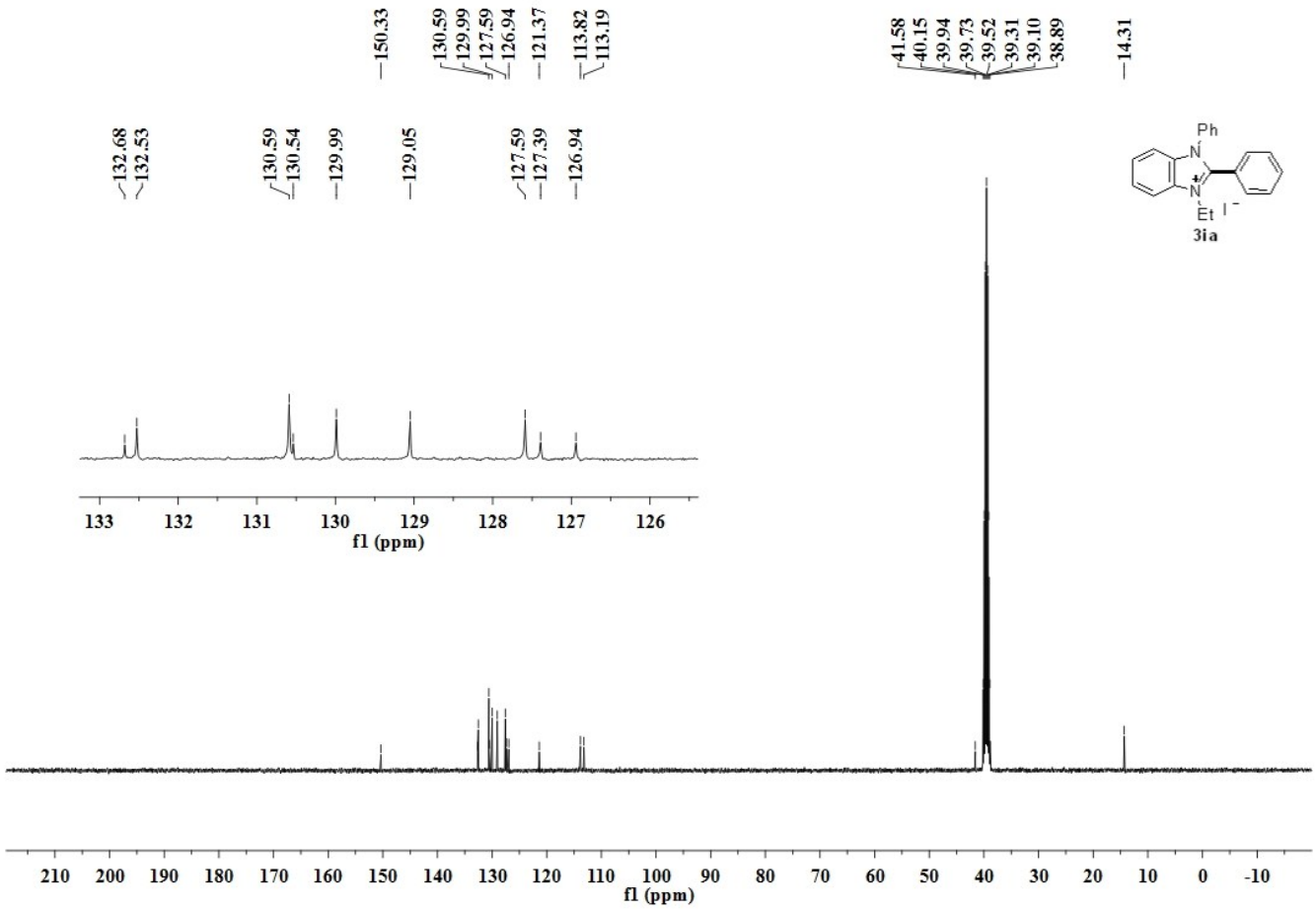
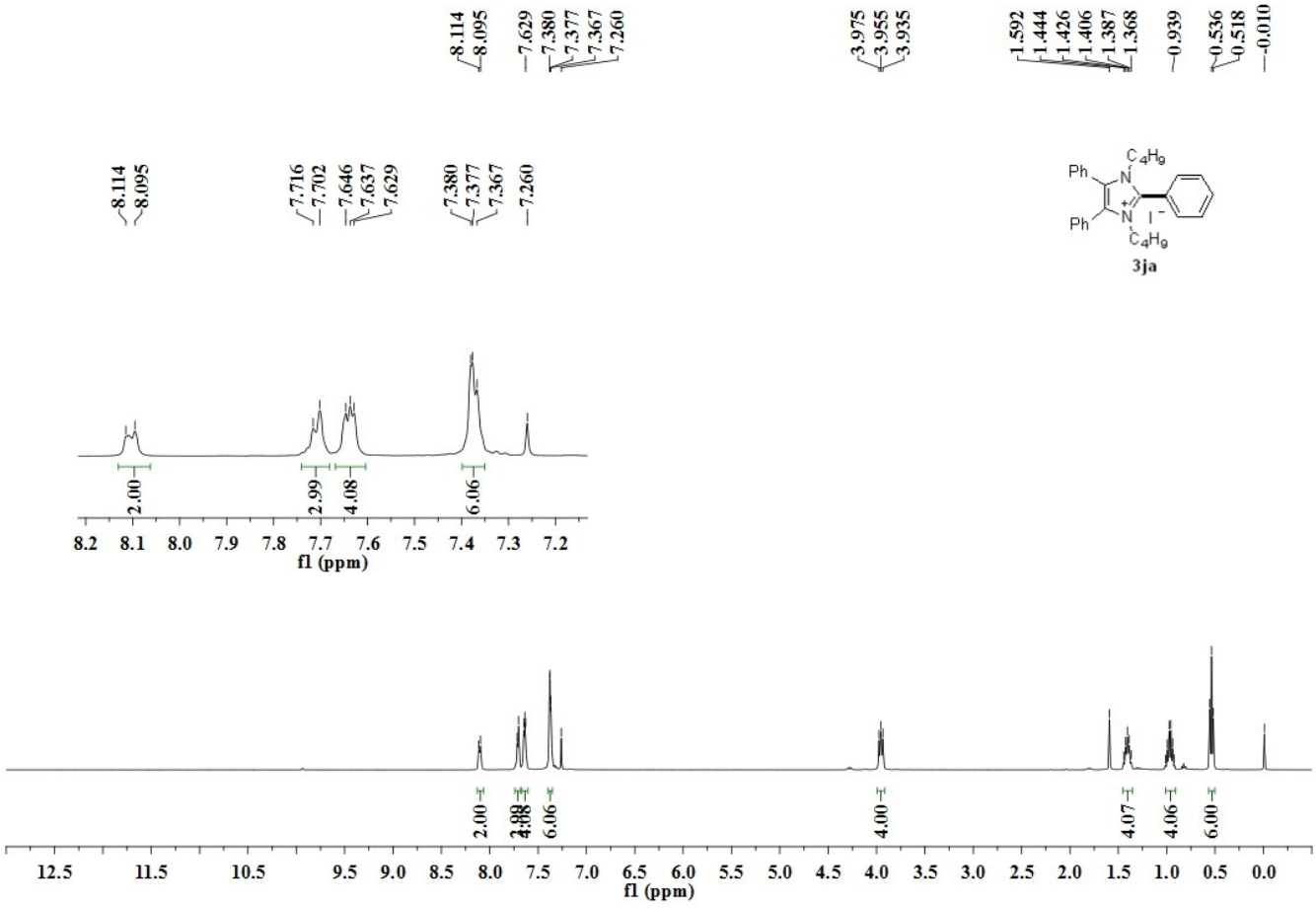
8.322
7.671
7.655
7.634
7.619
7.605
7.584
7.563
7.532
4.473
4.455
4.437
4.419
3.326
2.505
2.500
2.496
2.492
1.471
1.453
1.434
0.002
3ia
1.00
4.09
9.06
2.01
3.03
fl (ppm)
fl (ppm)
fl (ppm)


150.33
130.59
129.99
127.59
126.94
121.37
113.82
113.19
41.58
40.15
39.94
39.73
39.52
39.31
39.10
38.89
14.31
132.68
132.53
130.59
130.54
129.99
129.05
127.59
127.39
126.94
Ph
N
N
Et
I⁻
3ia
fl (ppm)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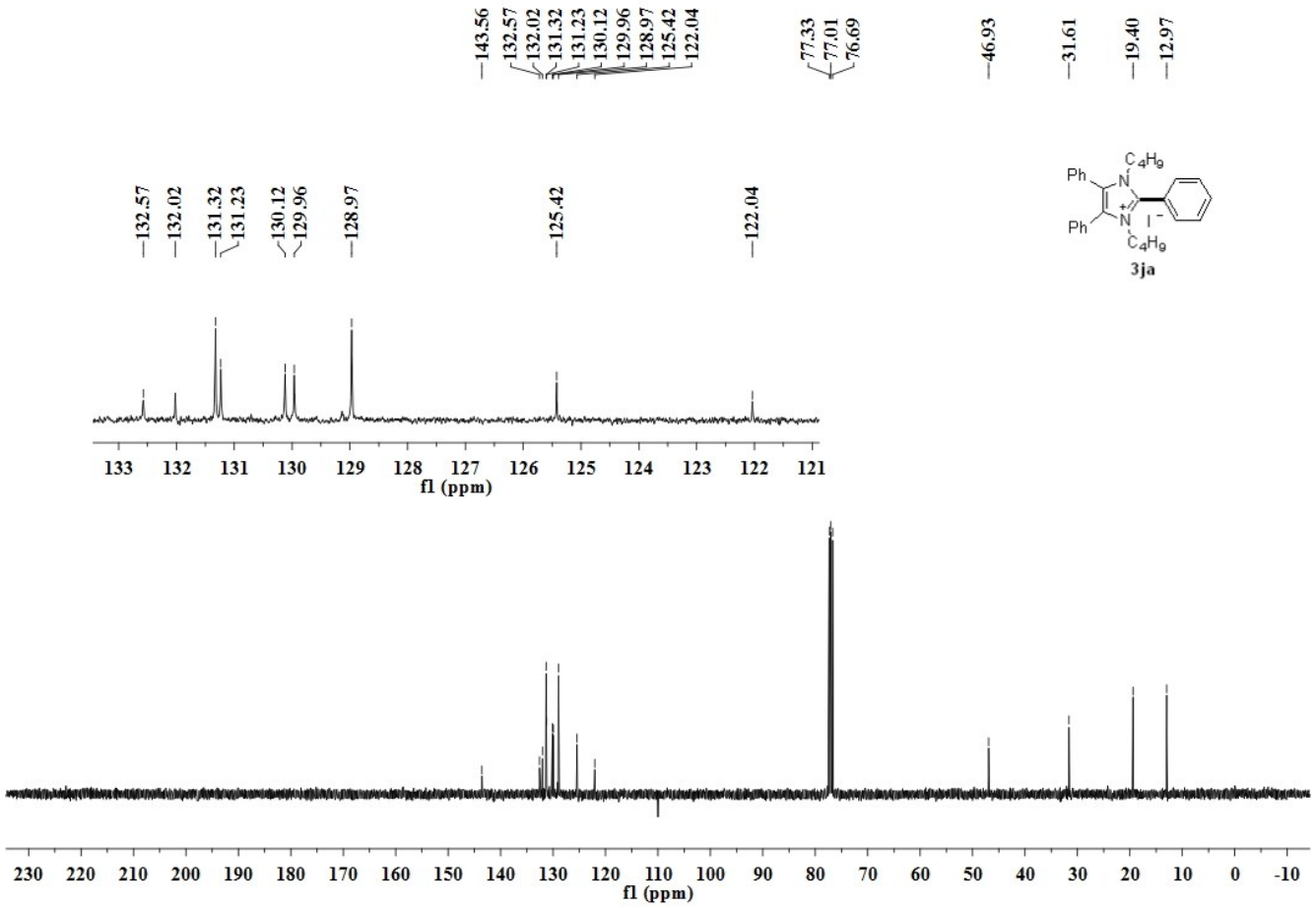
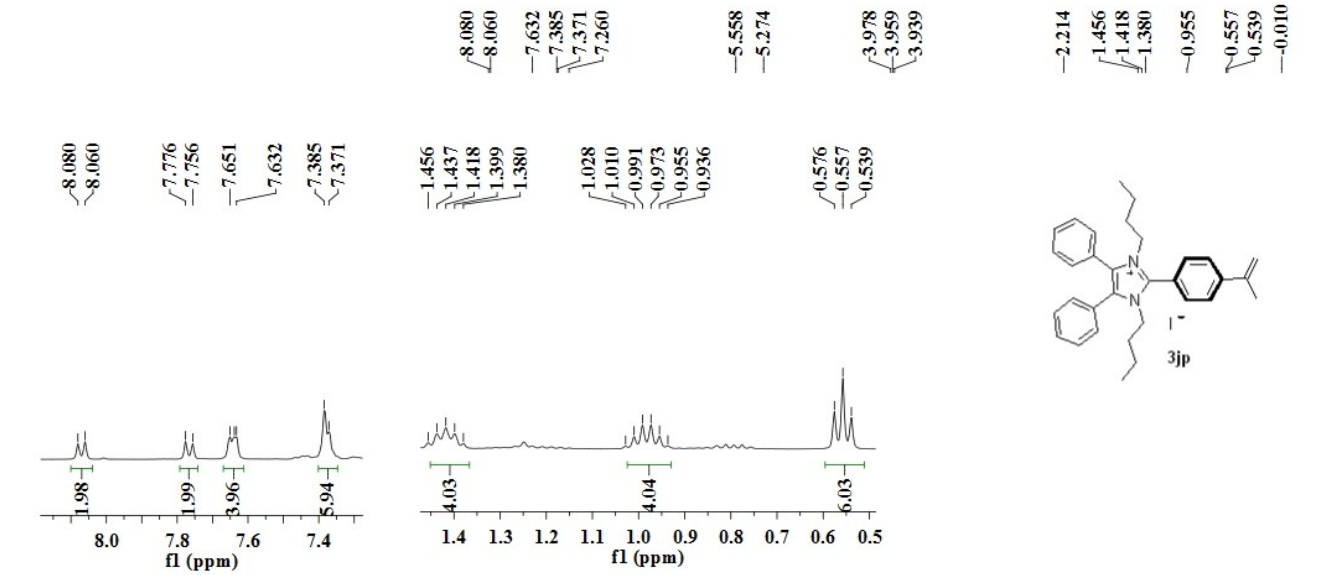
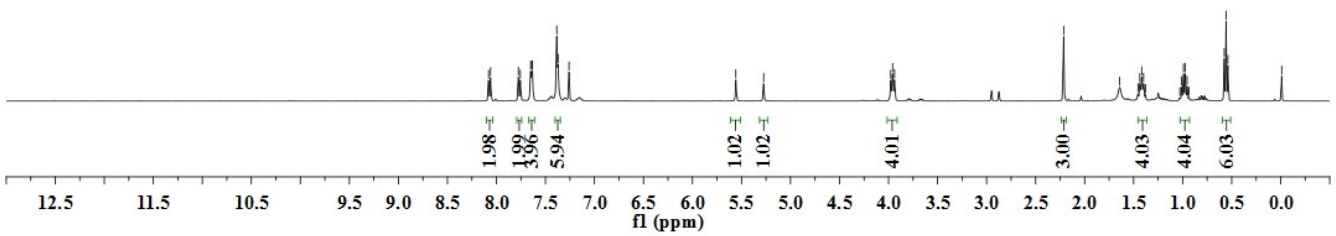
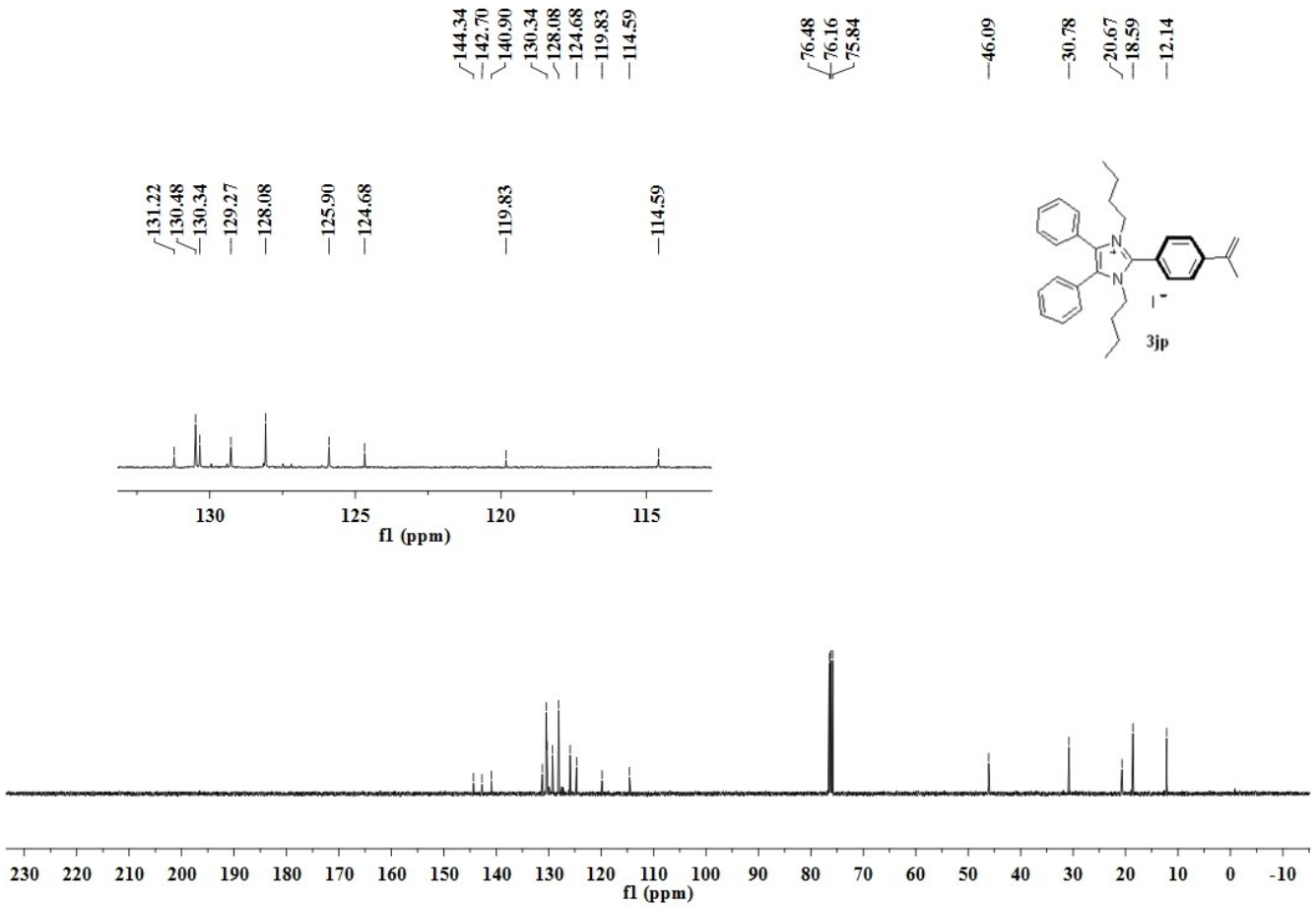
7.629
7.380
7.377
7.367
7.260
3.975
3.955
3.935
1.592
1.444
1.426
1.406
1.387
1.368
0.939
0.536
0.518
0.010
8.114
8.095
7.716
7.702
7.646
7.637
7.629
7.380
7.377
7.367
7.260
C4H9
Ph
N
N
Ph
I⁻
C4H9
3ja
2.00
2.99
4.08
6.06
4.00
4.07
4.06
6.00
fl (ppm)


143.56
132.57
132.02
131.32
131.23
130.12
129.96
128.97
125.42
122.04
77.33
77.01
76.69
46.93
31.61
19.40
12.97
3ja
fl (ppm)


8.080
8.060
7.776
7.756
7.651
7.632
7.385
7.371
7.260
5.558
5.274
3.978
3.959
3.939
2.214
1.456
1.437
1.418
1.399
1.380
1.028
1.010
0.991
0.973
0.955
0.936
0.576
0.557
0.539
0.955
0.557
0.539
-0.010
3jp
1.98
1.99
3.96
5.94
4.03
4.04
6.03
fl (ppm)


1.98
1.99
3.96
5.94
1.02
1.02
4.01
3.00
4.03
4.04
6.03
fl (ppm)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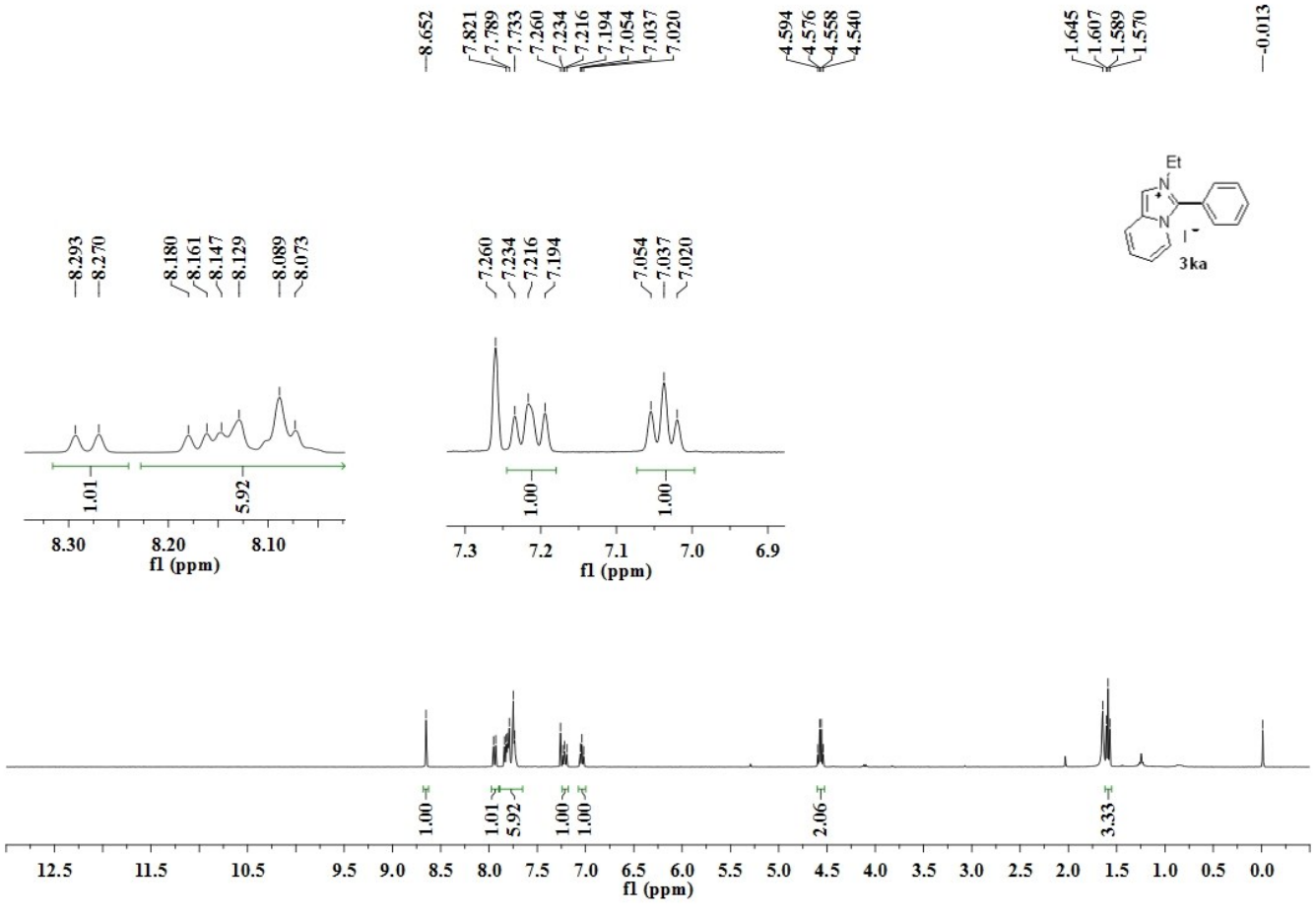
142.70
140.90
130.34
128.08
124.68
119.83
114.59
76.48
76.16
75.84
46.09
30.78
20.67
18.59
12.14
131.22
130.48
130.34
129.27
128.08
125.90
124.68
119.83
114.59
3jp
130
125
120
115
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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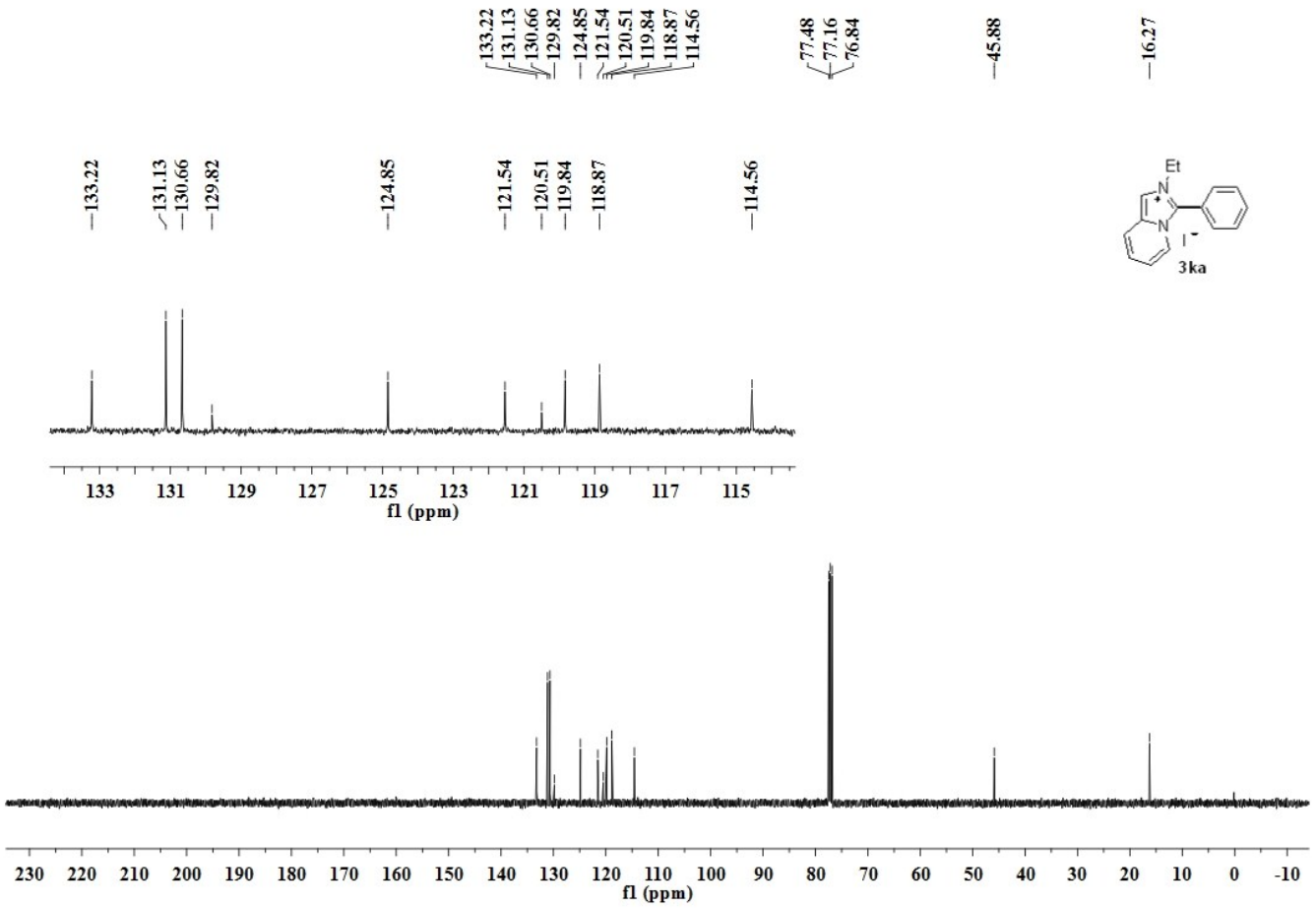
7.234
7.216
7.194
7.054
7.037
7.020
4.594
4.576
4.558
4.540
1.645
1.607
1.589
1.570
-0.013
Et
3ka
8.293
8.270
8.180
8.161
8.147
8.129
8.089
8.073
7.260
7.234
7.216
7.194
7.054
7.037
7.020
1.01
5.92
1.00
1.00
8.30
8.20
8.10
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
1.00
1.01
5.92
1.00
1.00
2.06
3.33
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


133.22
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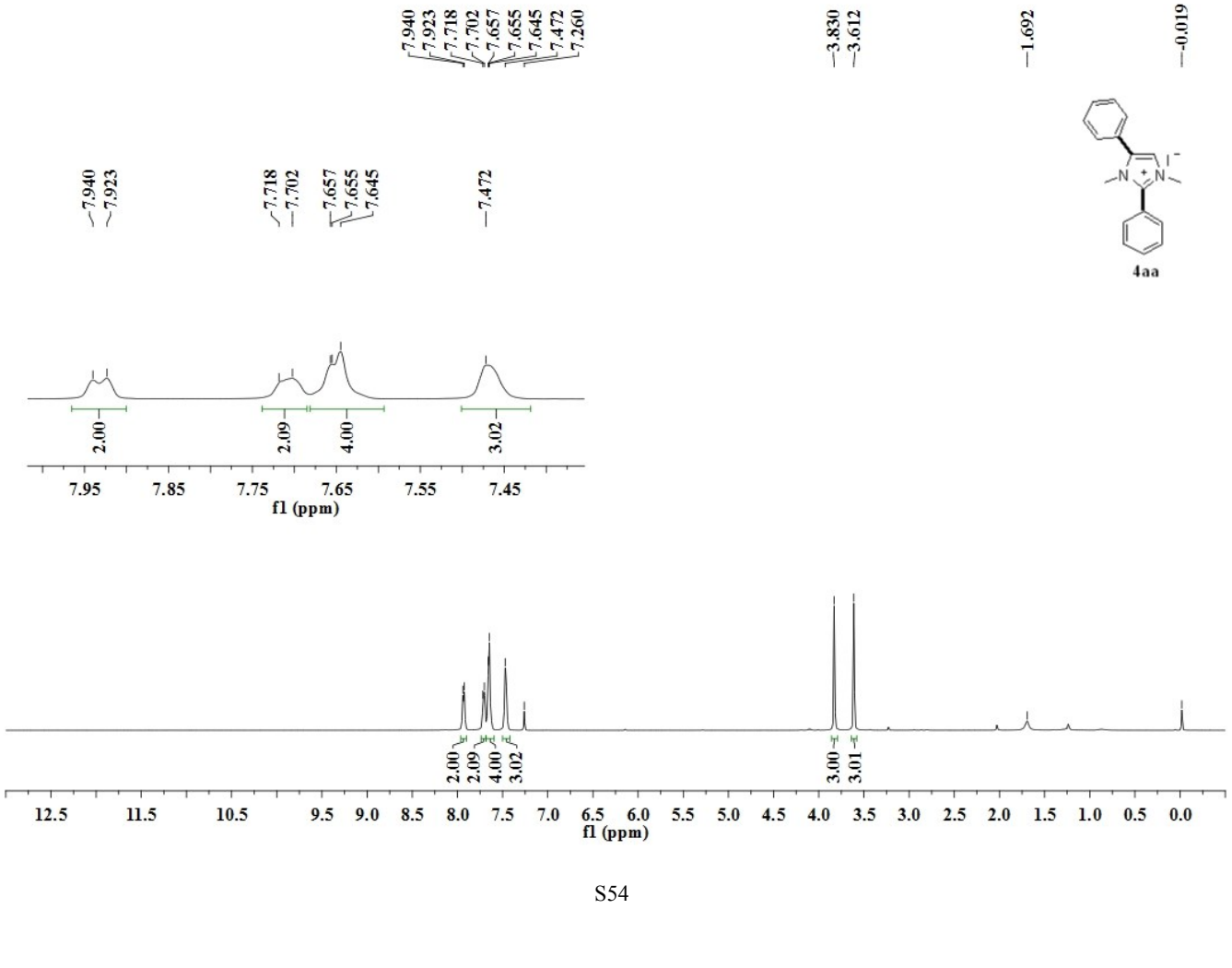
130.66
129.82
124.85
121.54
120.51
119.84
118.87
114.56
77.48
77.16
76.84
45.88
16.27
Et
3ka
f1 (ppm)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7.702
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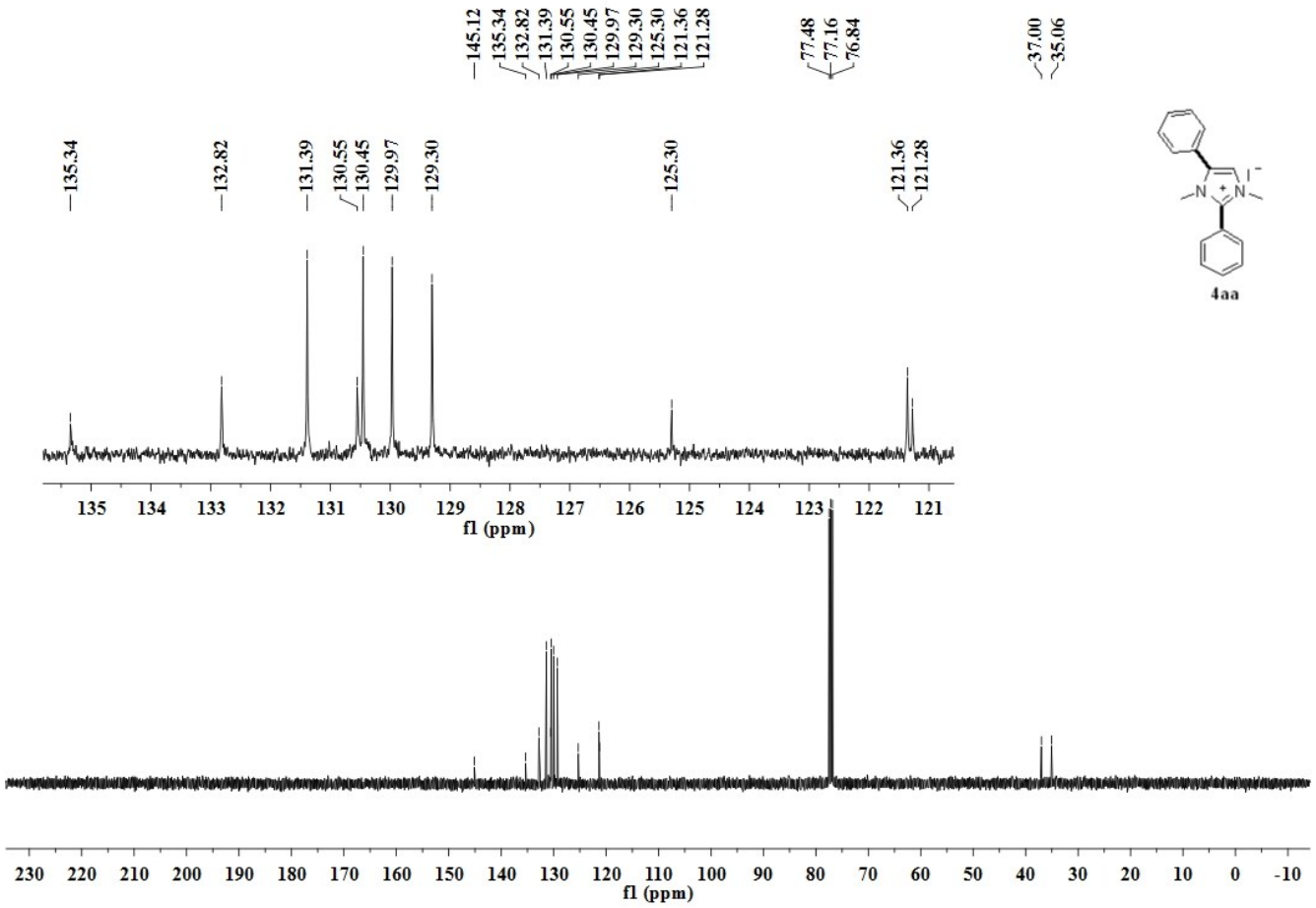
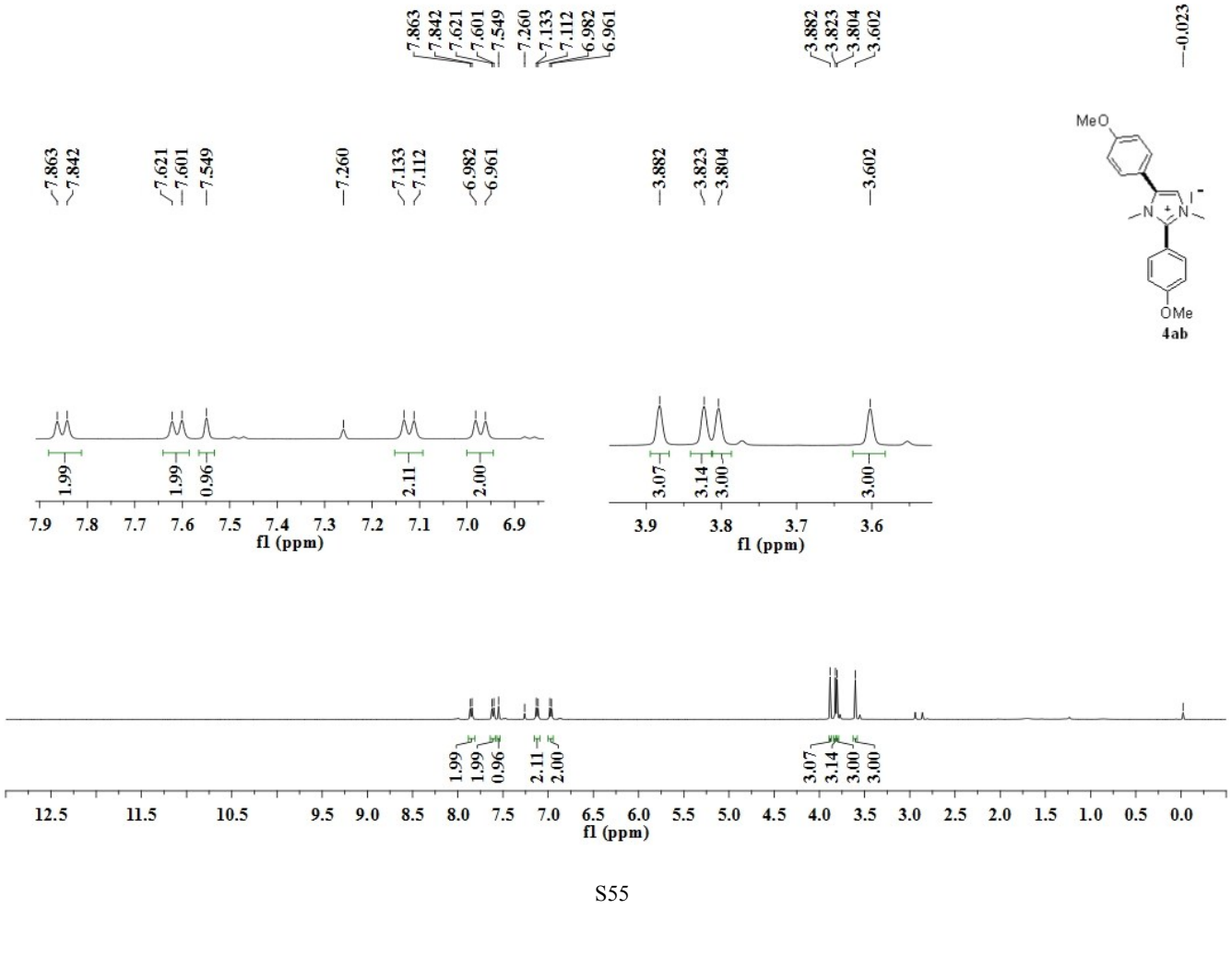
7.655
7.645
7.472
7.260
3.830
3.612
1.692
0.019
4aa
2.00
2.09
4.00
3.02
3.00
3.01
f1 (ppm)


145.12
135.34
132.82
131.39
130.55
130.45
129.97
129.30
125.30
121.36
121.28
77.48
77.16
76.84
37.00
35.06
4aa
fl (ppm)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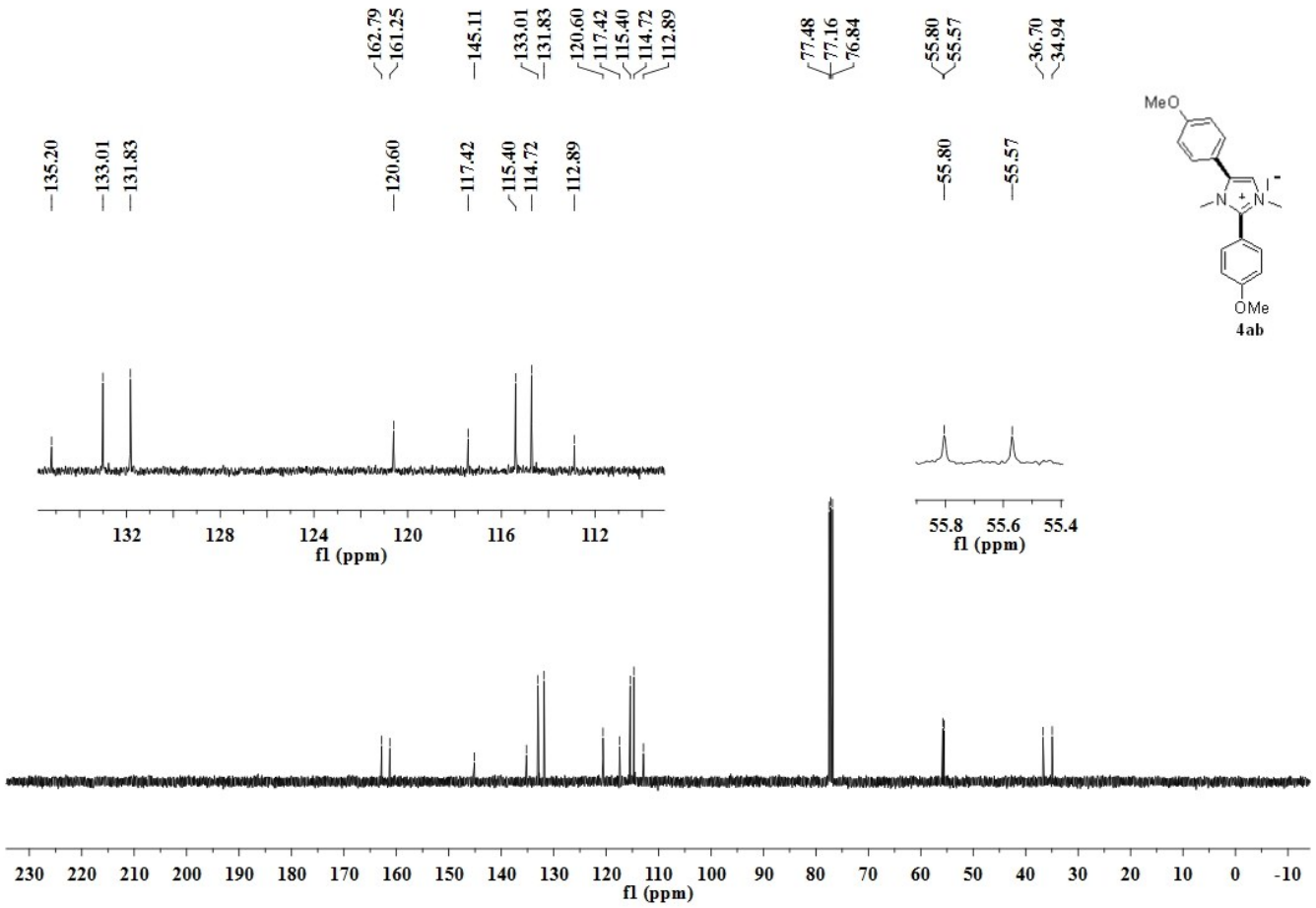
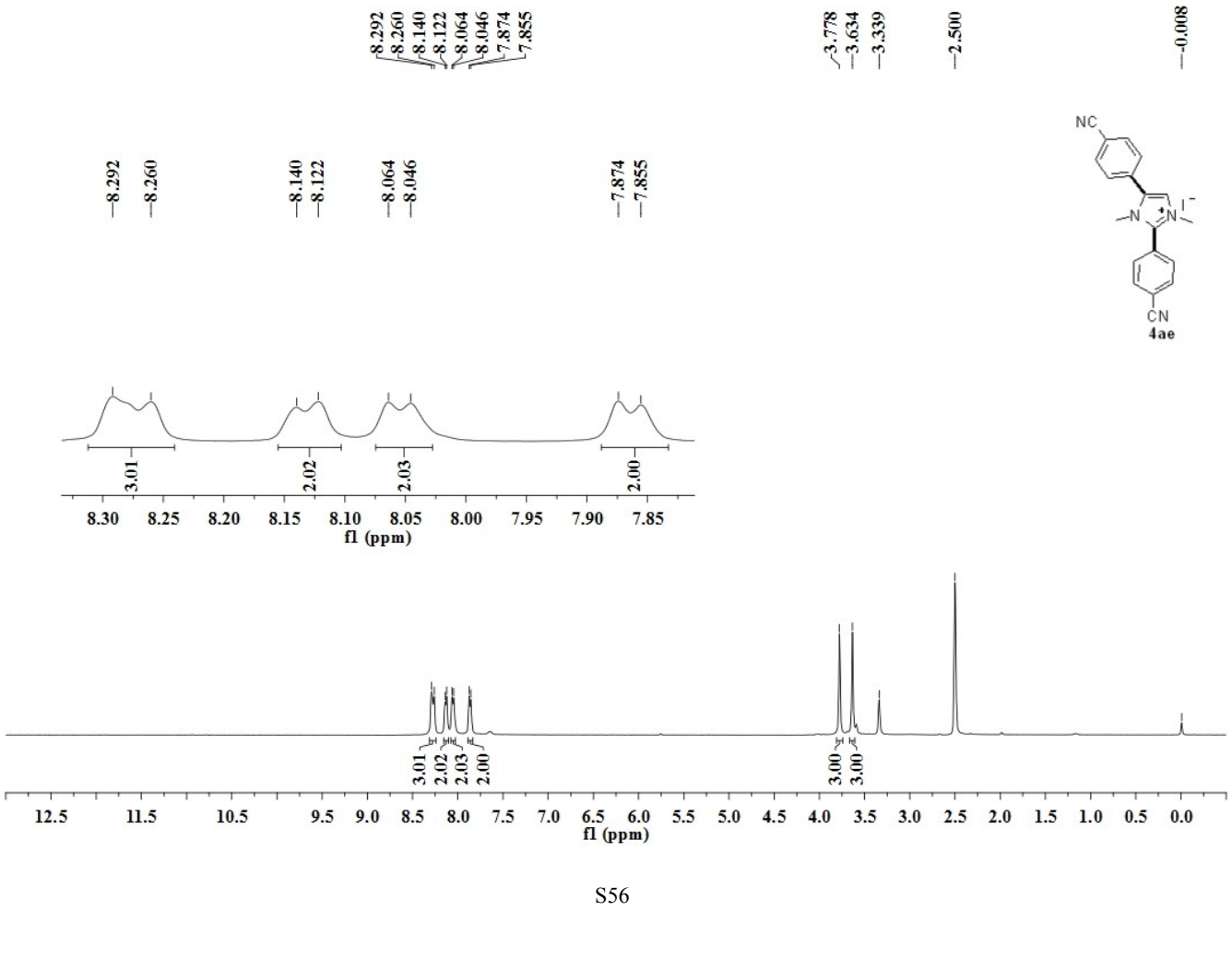
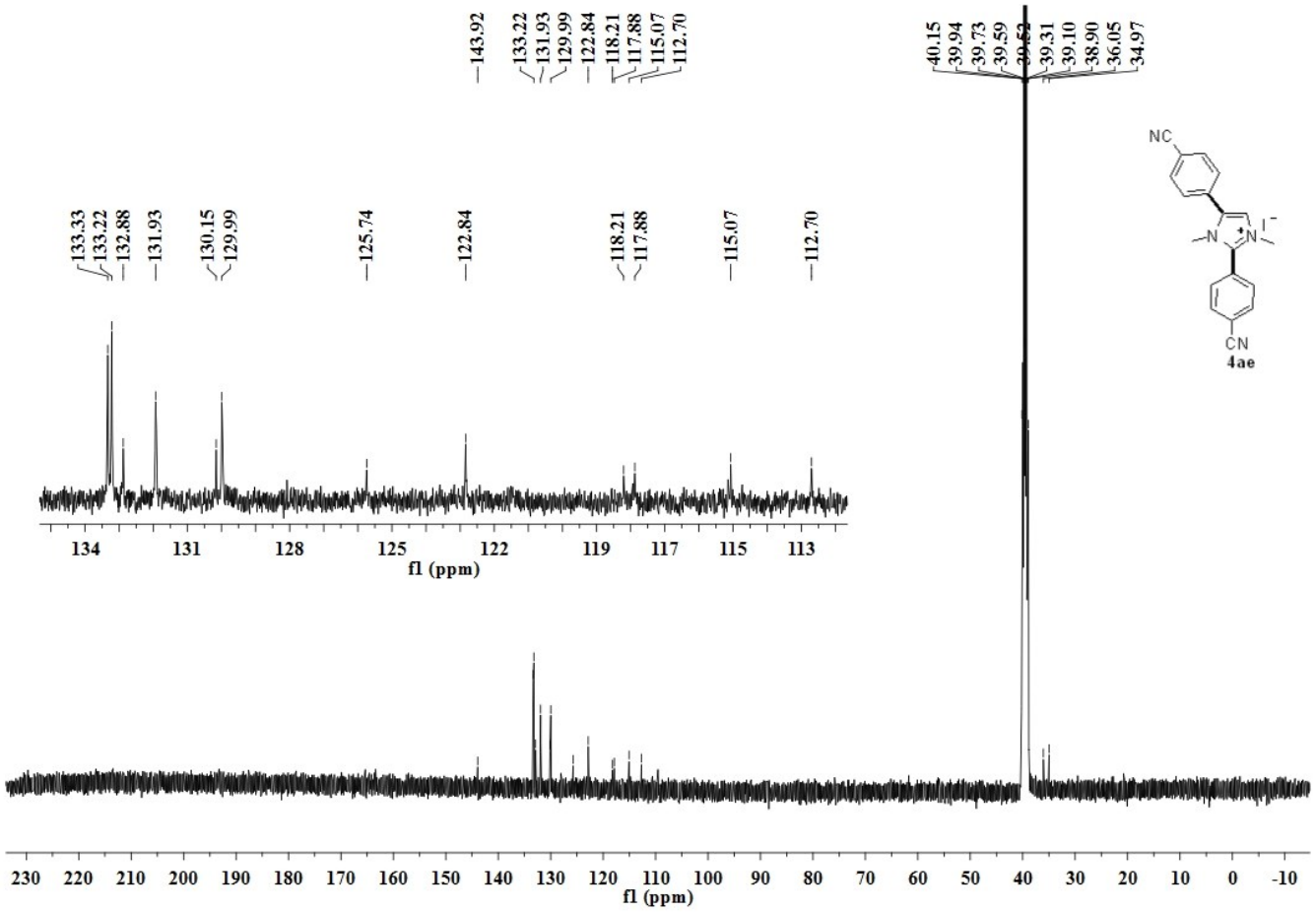
7.549
7.260
7.133
7.112
6.982
6.961
3.882
3.823
3.804
3.602
-0.023
MeO
OMe
4ab
1.99
1.99
0.96
2.11
2.00
3.07
3.14
3.00
3.00
fl (ppm)


162.79
161.25
145.11
133.01
131.83
120.60
117.42
115.40
114.72
112.89
77.48
77.16
76.84
55.80
55.57
36.70
34.94
MeO
OMe
4ab
fl (ppm)


8.292
8.260
8.140
8.122
8.064
8.046
7.874
7.855
3.778
3.634
3.339
2.500
-0.008
NC
CN
4ae
3.01
2.02
2.03
2.00
3.00
3.00
fl (ppm)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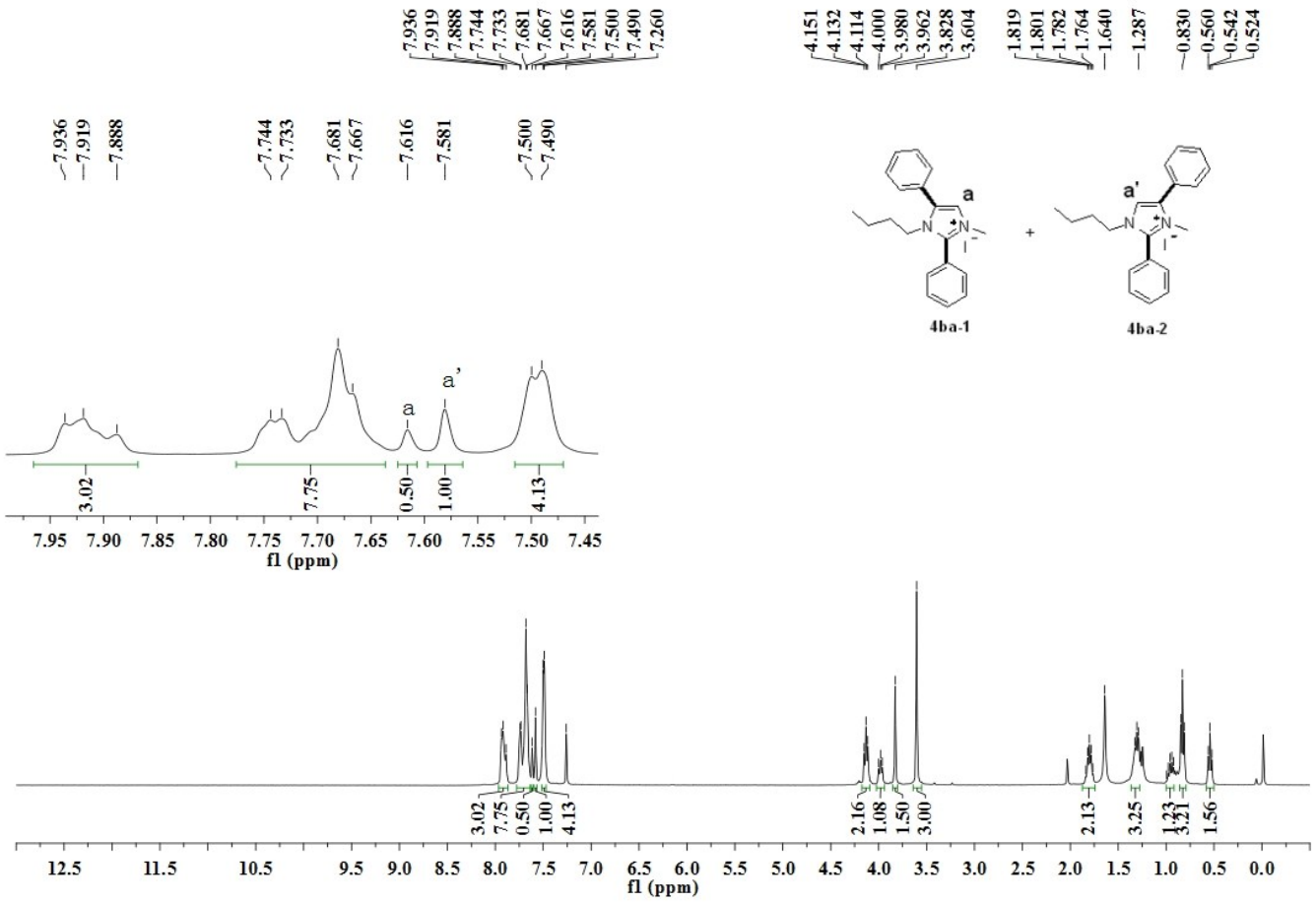
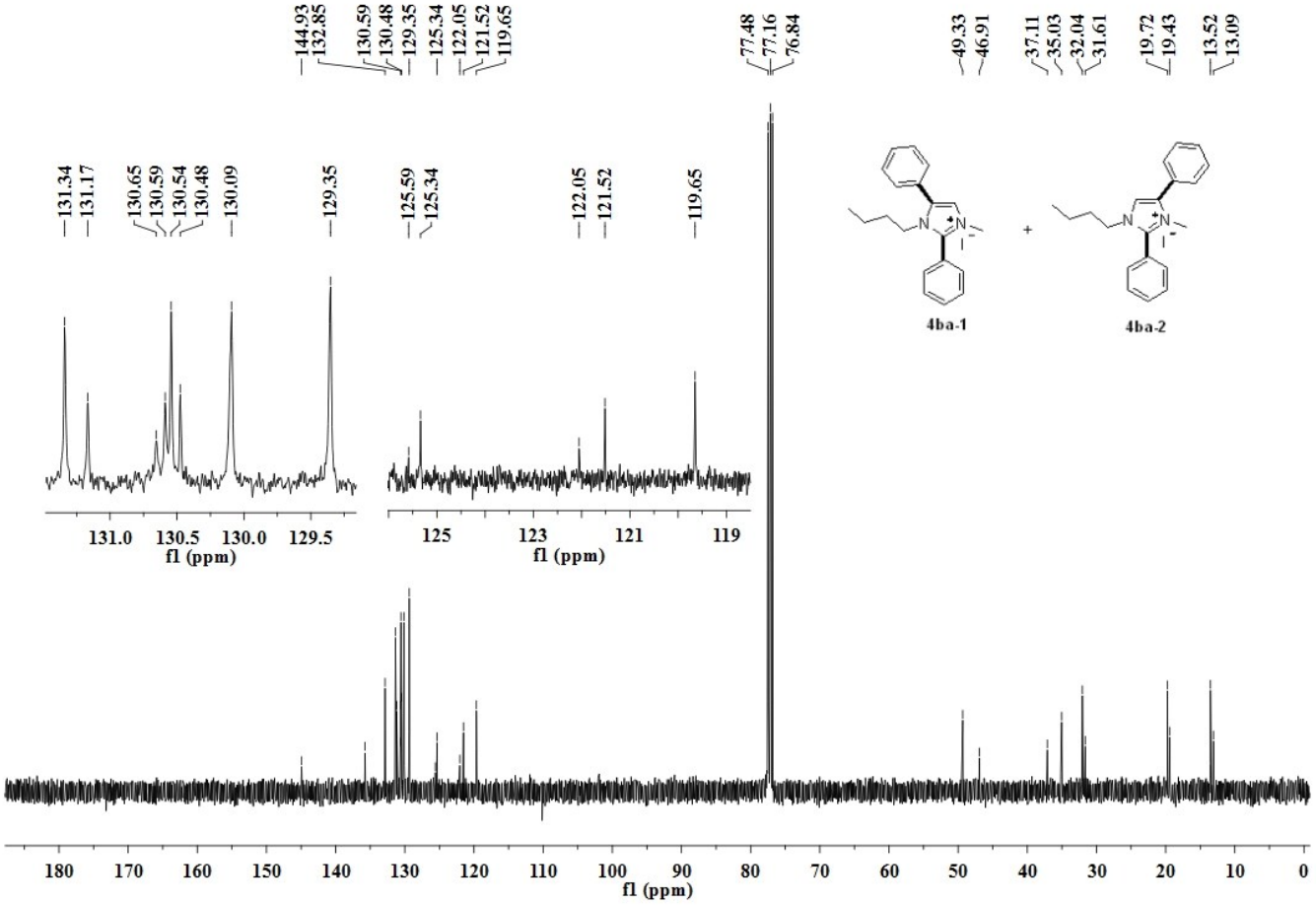
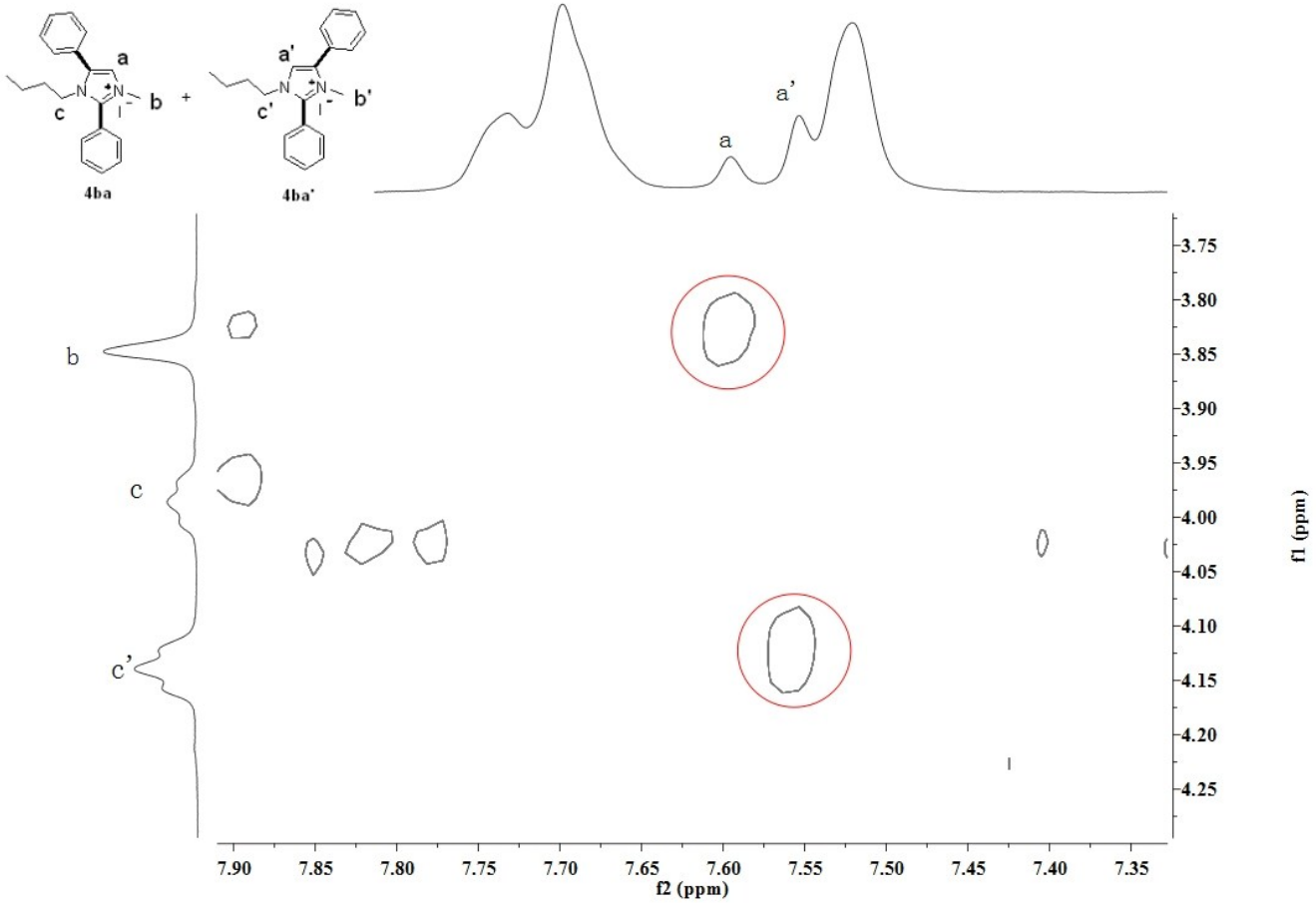
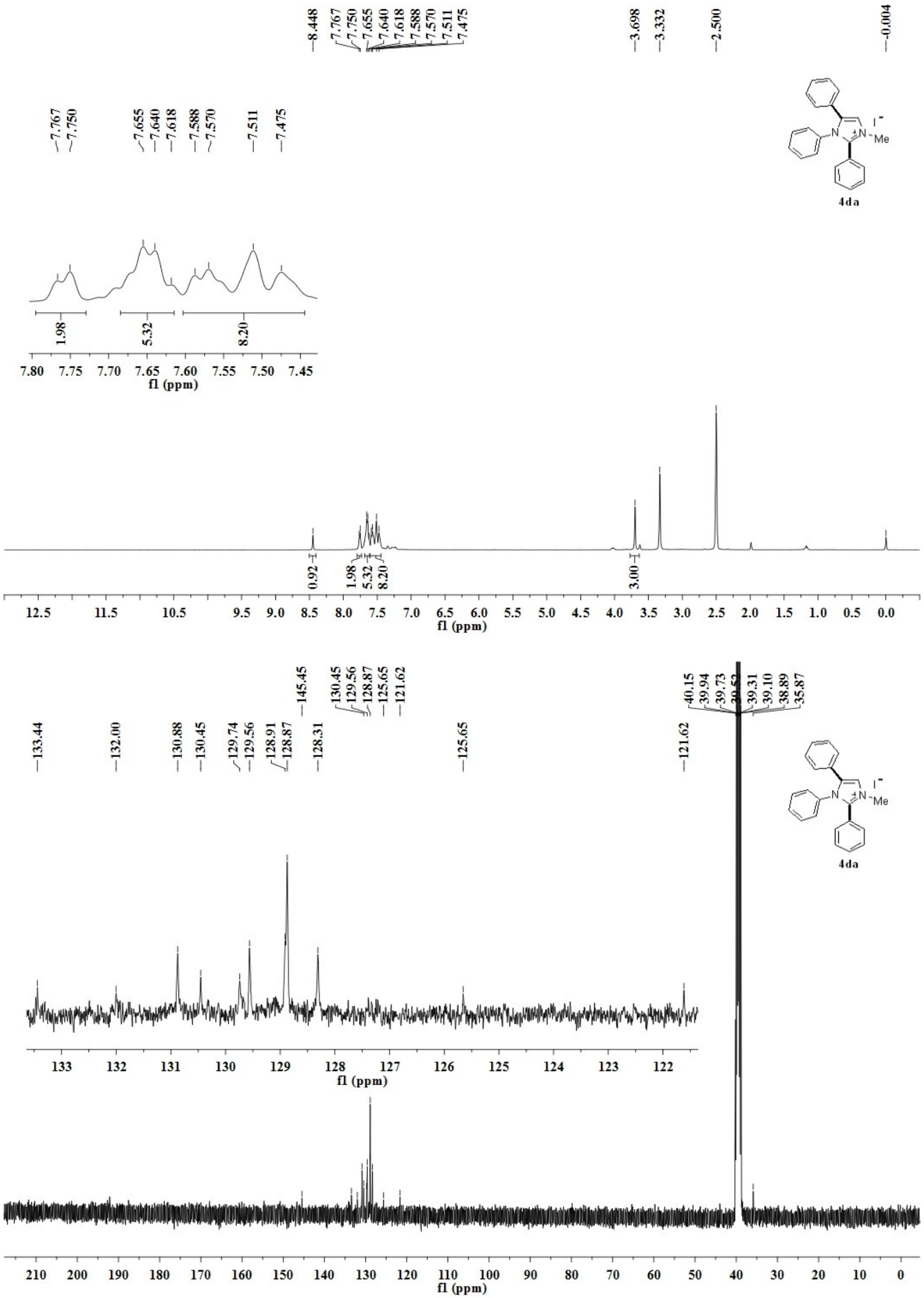
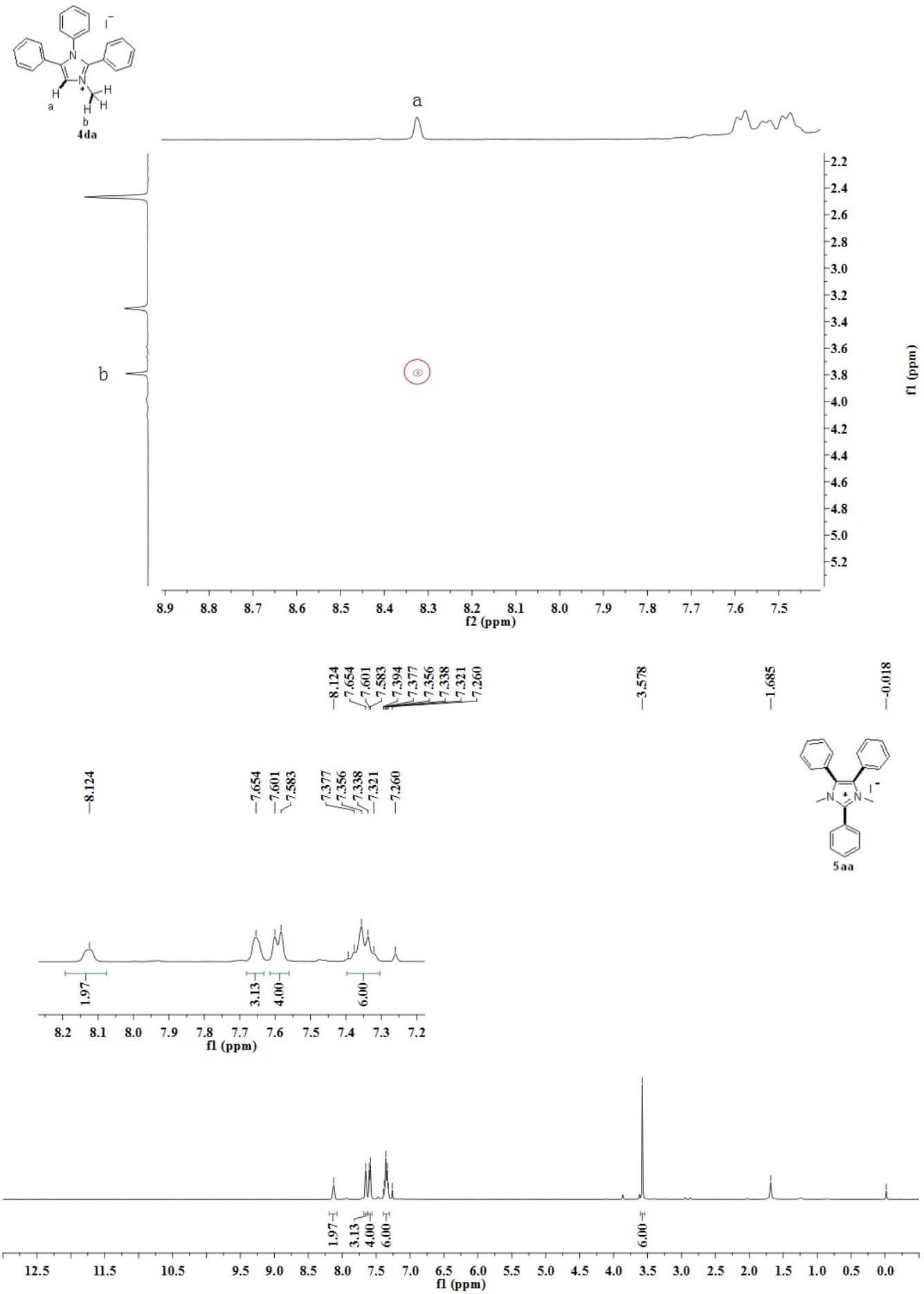
118.21
117.88
115.07
112.70
40.15
39.94
39.73
39.59
39.31
39.10
38.90
36.05
34.97
NC
CN
4ae
fl (ppm)

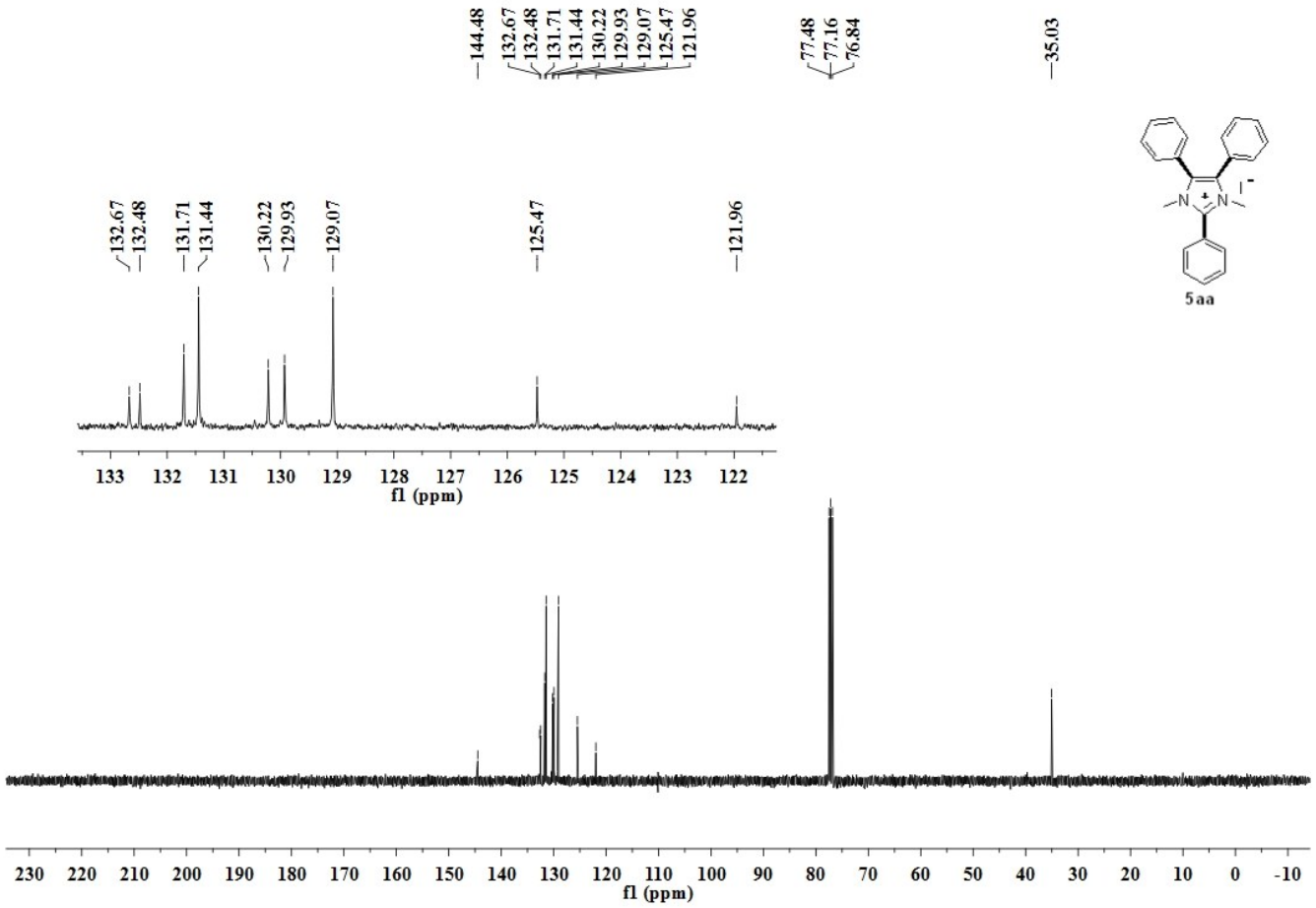

7.936
7.919
7.888
7.744
7.733
7.681
7.667
7.616
7.581
7.500
7.490
7.260
4.151
4.132
4.114
4.000
3.980
3.962
3.828
3.604
1.819
1.801
1.782
1.764
1.640
1.287
0.830
0.560
0.542
0.524
a
a'
4ba-1
4ba-2
3.02
7.75
0.50
1.00
4.13
2.16
1.08
1.50
3.00
2.13
3.25
1.33
3.21
1.56
fl (ppm)

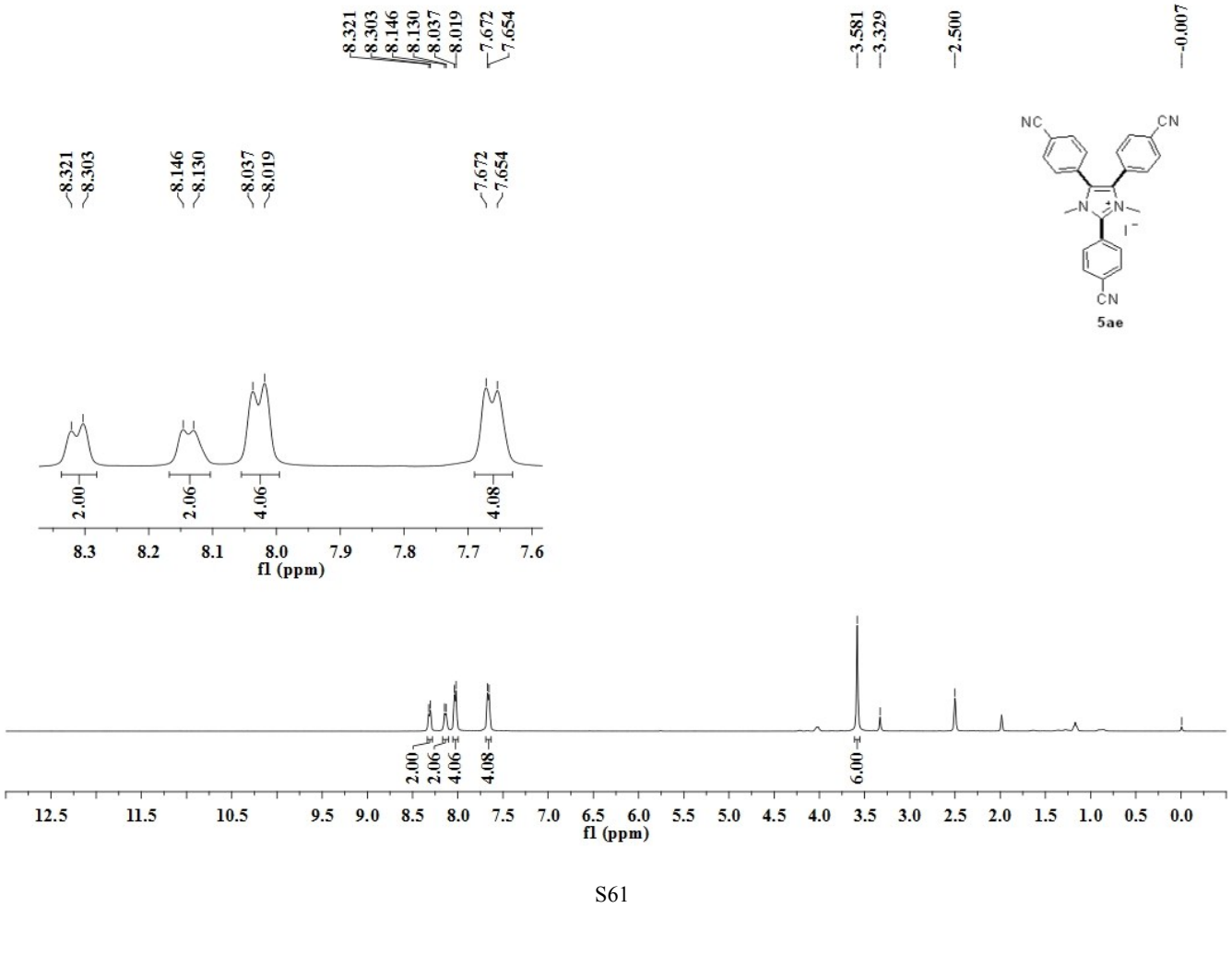

144.93
132.85
130.59
130.48
129.35
125.34
122.05
121.52
119.65
77.48
77.16
76.84
49.33
46.91
37.11
35.03
32.04
31.61
19.72
19.43
13.52
13.09
131.34
131.17
130.65
130.59
130.54
130.48
130.09
129.35
125.59
125.34
122.05
121.52
119.65
4ba-1
4ba-2
131.0 130.5 130.0 129.5
f1 (ppm)
125 123 121 119
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

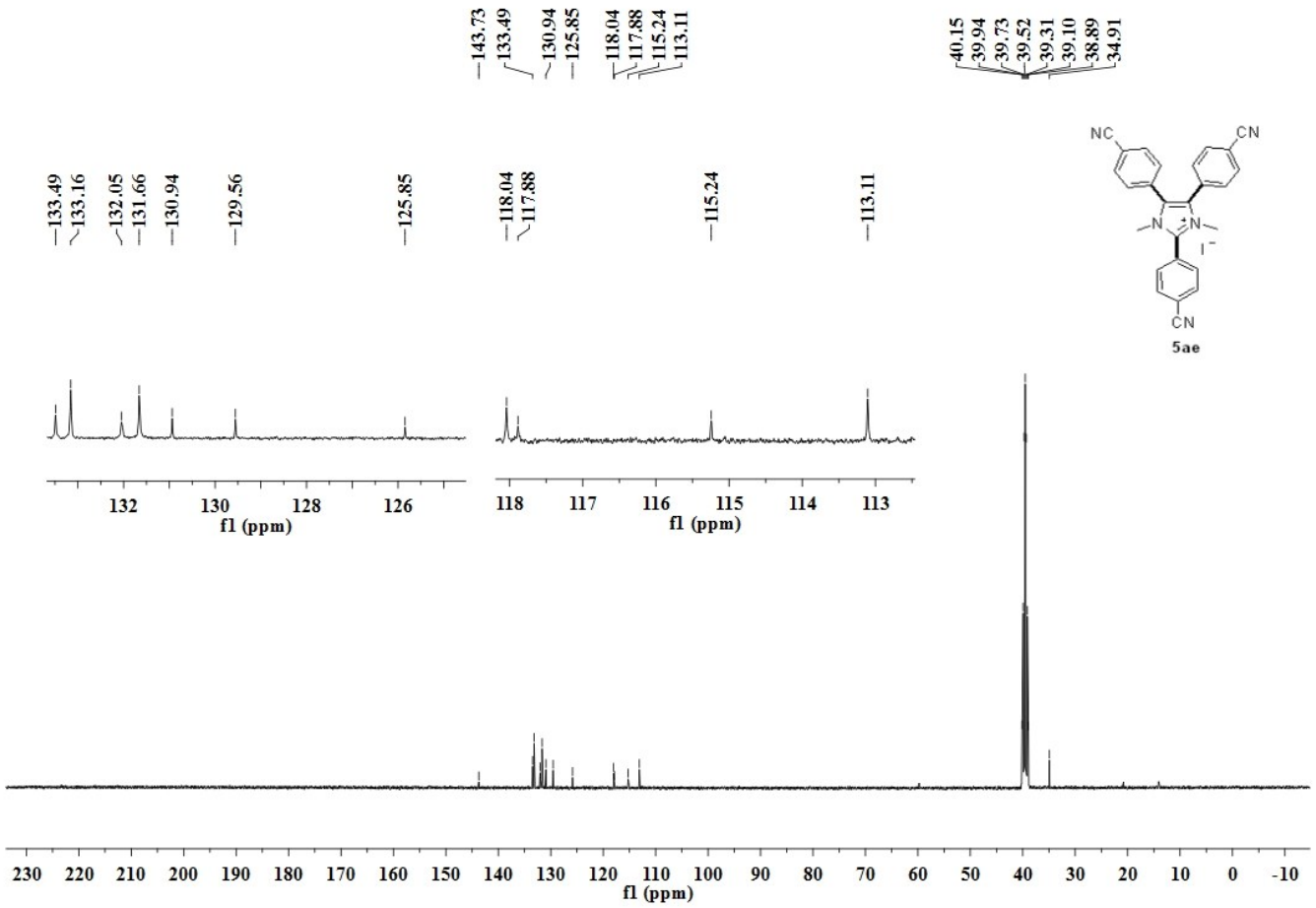

a
b
c
4ba
a'
b'
c'
4ba'
a
a'
b
c
c'
3.75
3.80
3.85
3.90
3.95
4.00
4.05
4.10
4.15
4.20
4.25
f1 (ppm)
7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35
f2 (ppm)

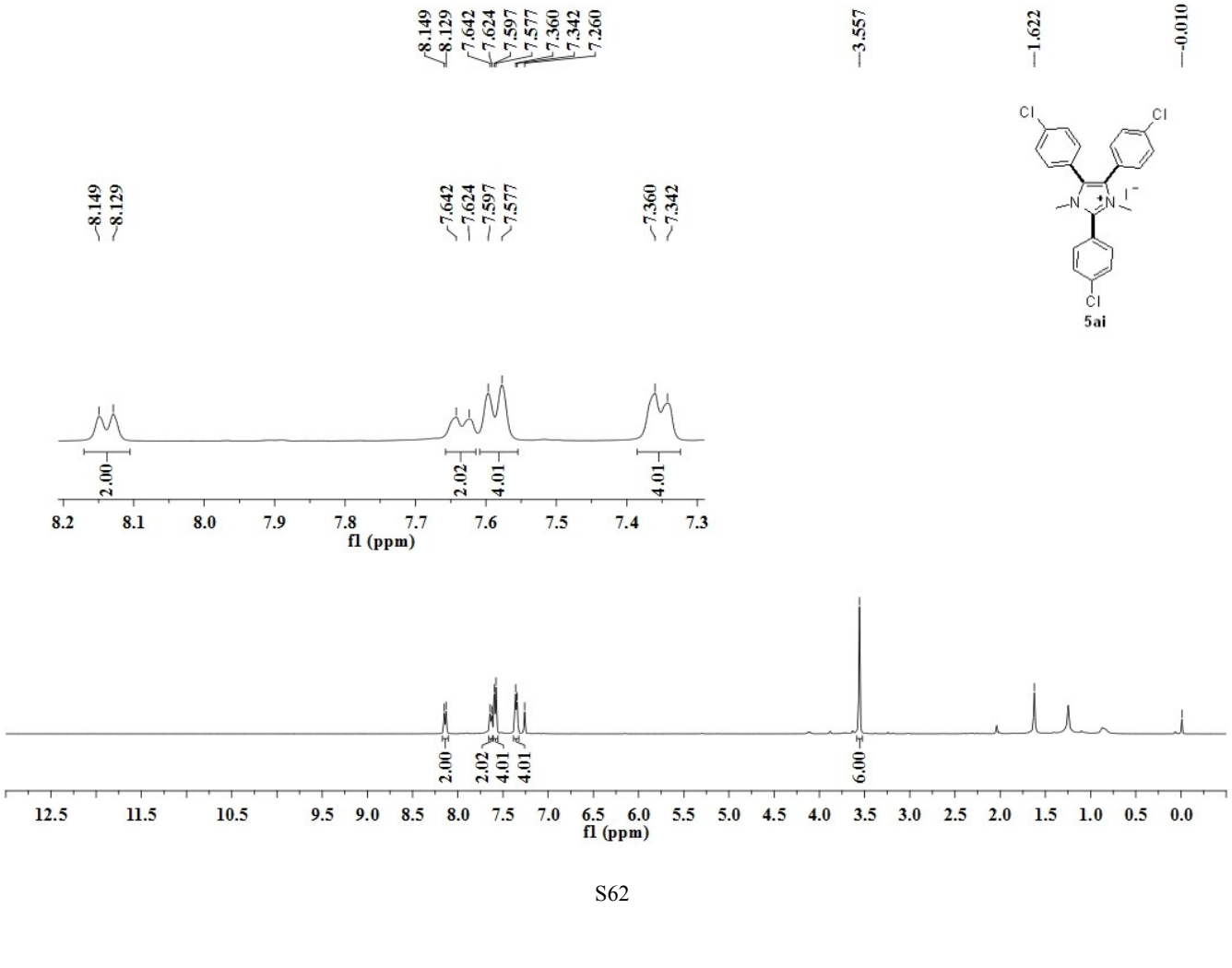

8.448
7.767
7.750
7.655
7.640
7.618
7.588
7.570
7.511
7.475
3.698
3.332
2.500
-0.004
4da
1.98
5.32
8.20
fl (ppm)
0.92
1.98
5.32
8.20
3.00
fl (ppm)
145.45
130.45
129.56
128.87
125.65
121.62
40.15
39.94
39.73
39.31
39.10
38.89
35.87
133.44
132.00
130.88
130.45
129.74
129.56
128.91
128.87
128.31
125.65
121.62
4da
fl (ppm)
fl (ppm)

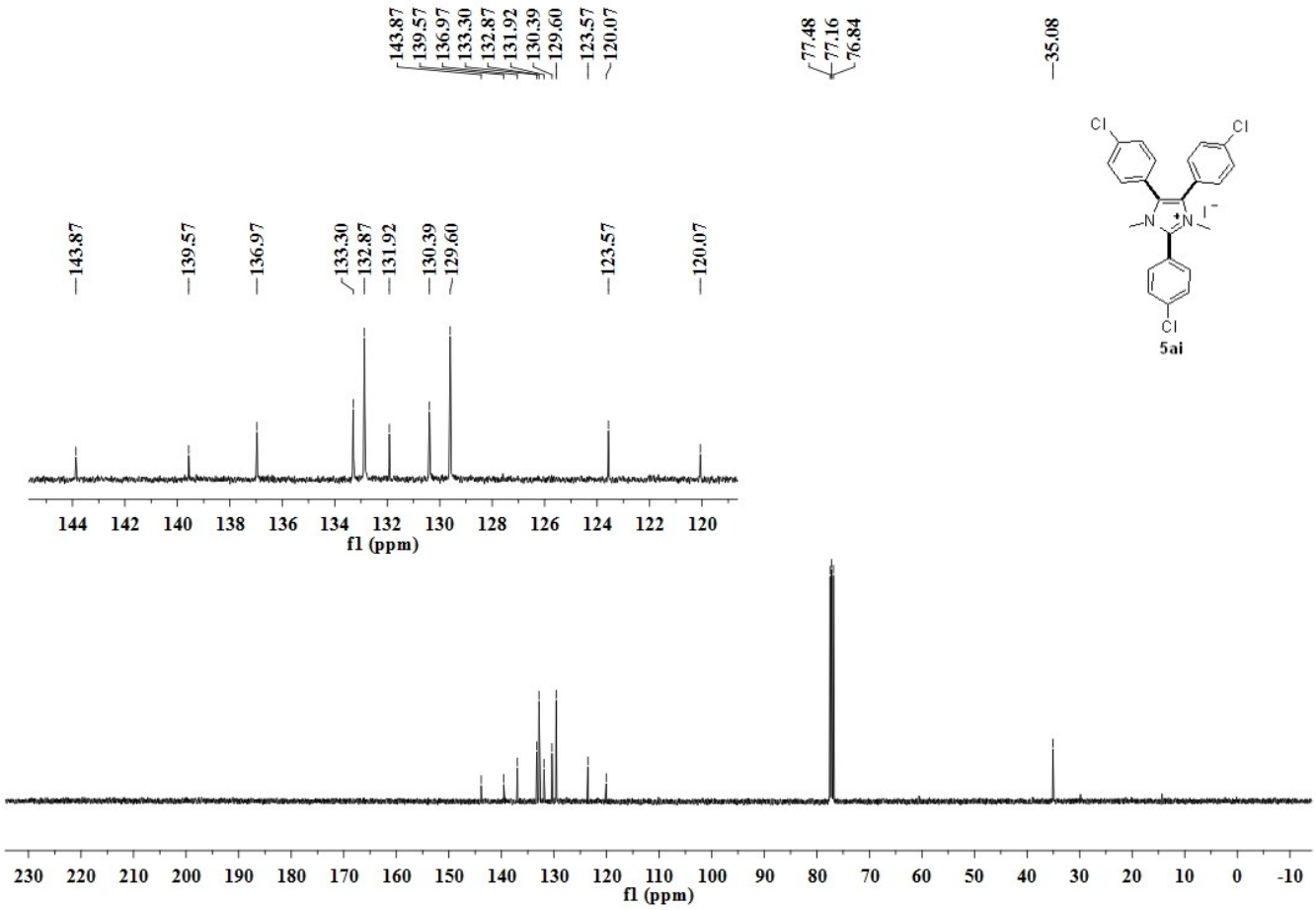

4da
a
b
f2 (ppm)
f1 (ppm)
8.124
7.654
7.601
7.583
7.394
7.377
7.356
7.338
7.321
7.260
3.578
1.685
0.018
5aa
1.97
3.13
4.00
6.00
f1 (ppm)

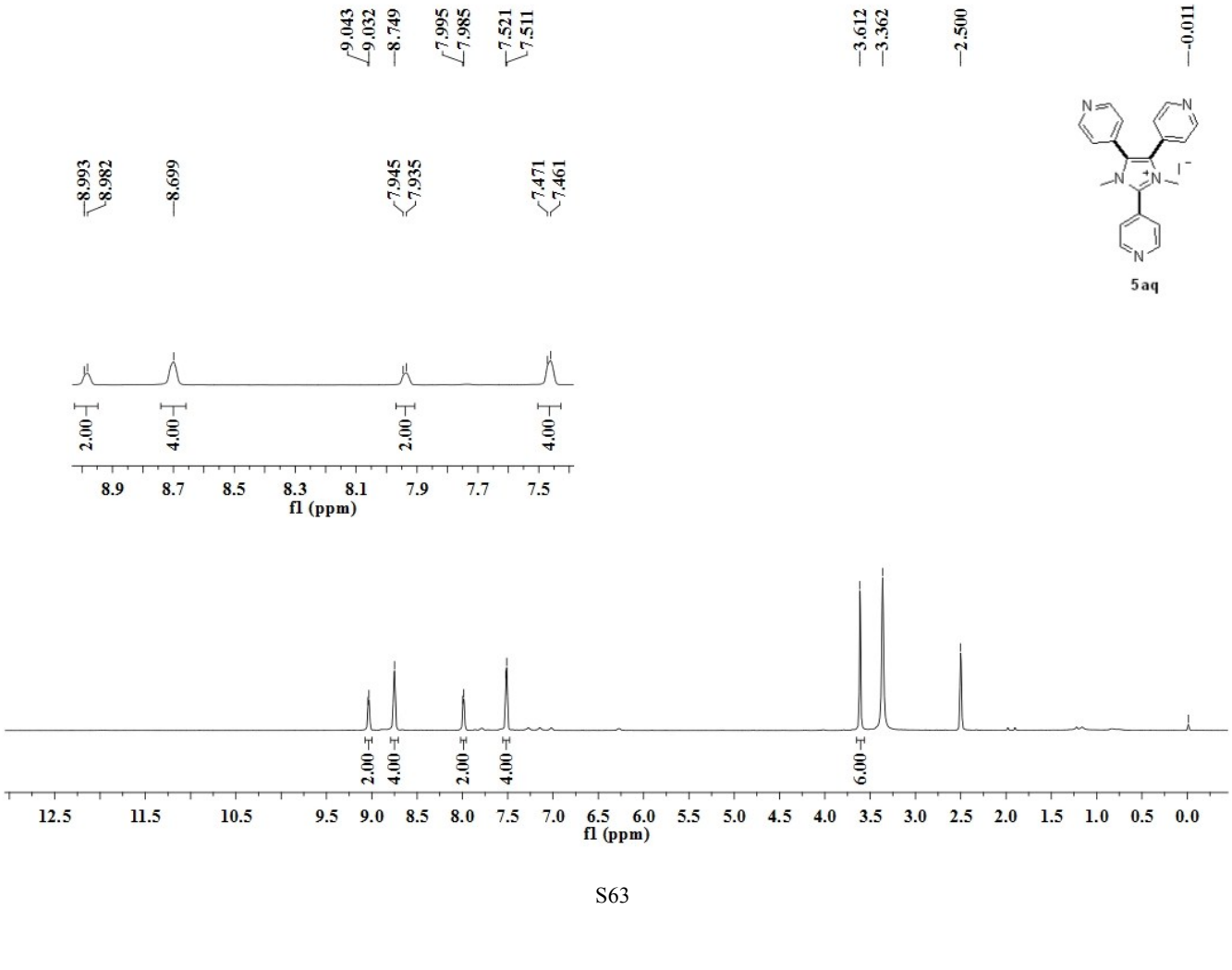

144.48
132.67
132.48
131.71
131.44
130.22
129.93
129.07
125.47
121.96
77.48
77.16
76.84
35.03
5aa
fl (ppm)

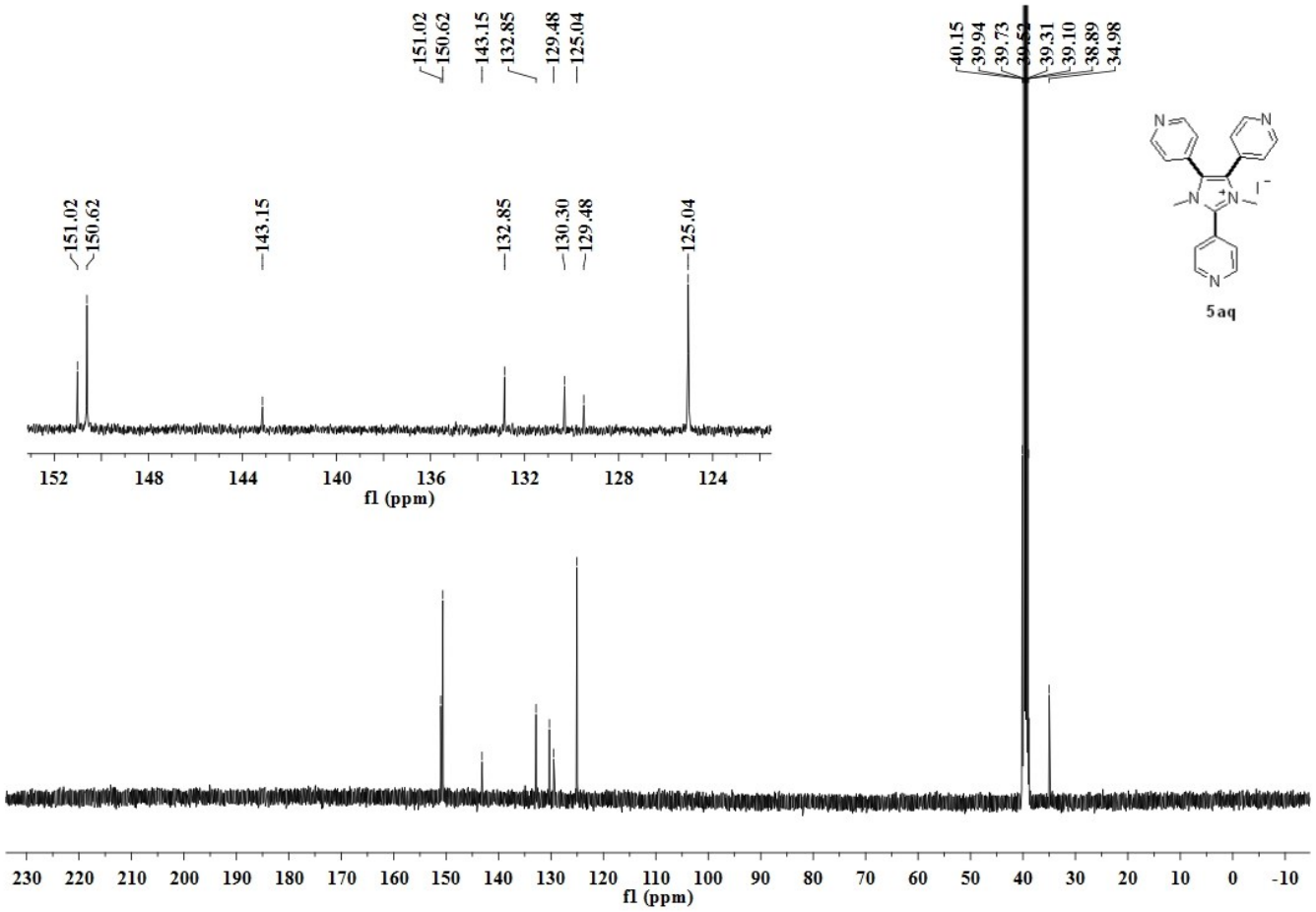

8.321
8.303
8.146
8.130
8.037
8.019
7.672
7.654
3.581
3.329
2.500
0.007
5ae
2.00
2.06
4.06
4.08
6.00
fl (ppm)

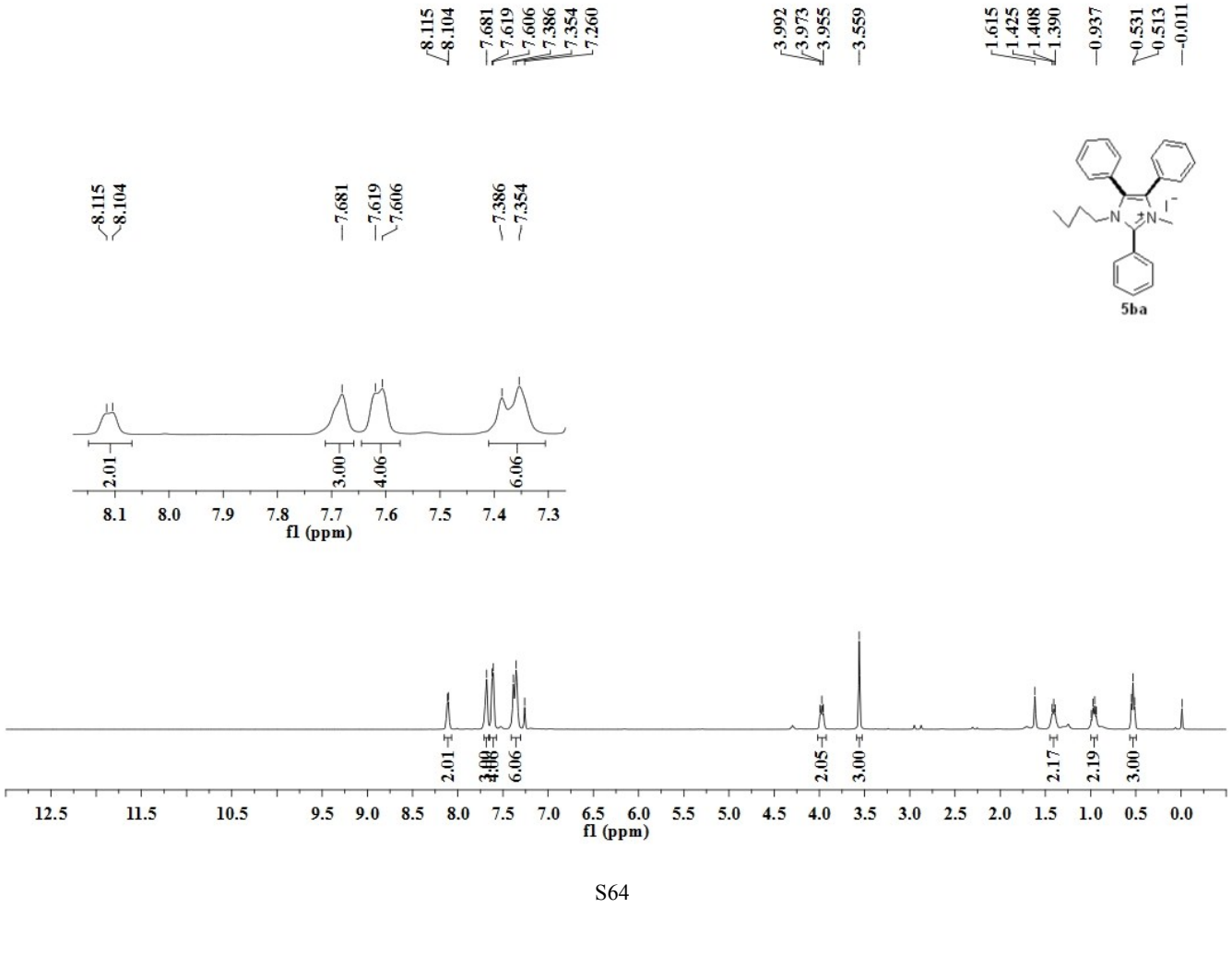

143.73
133.49
130.94
125.85
118.04
117.88
115.24
113.11
40.15
39.94
39.73
39.52
39.31
39.10
38.89
34.91
NC
CN
CN
I⁻
5ae
fl (ppm)

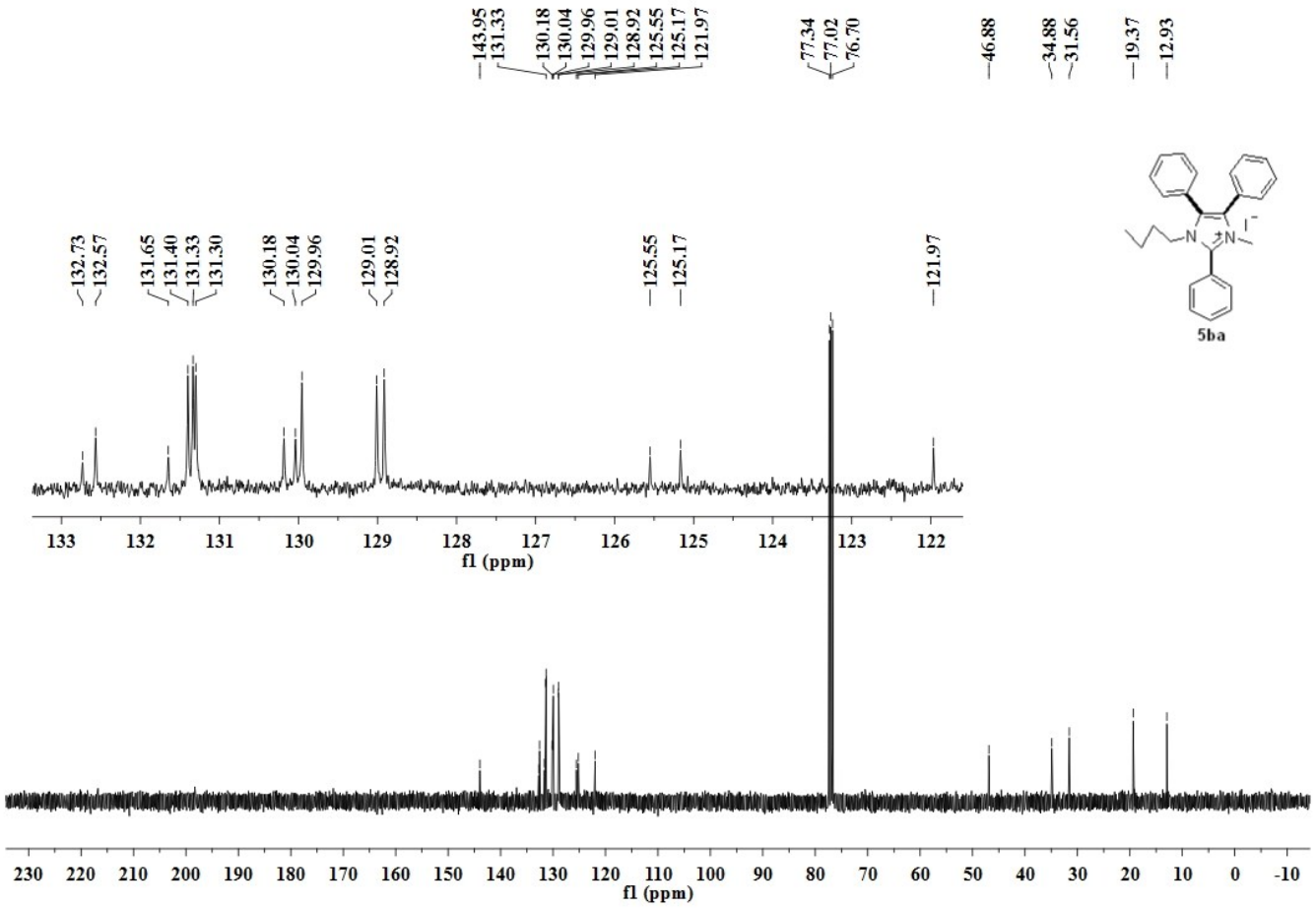

8.149
8.129
7.642
7.624
7.597
7.577
7.360
7.342
7.260
3.557
1.622
0.010
Cl
Cl
Cl
I⁻
5ai
2.00
2.02
4.01
4.01
6.00
fl (ppm)

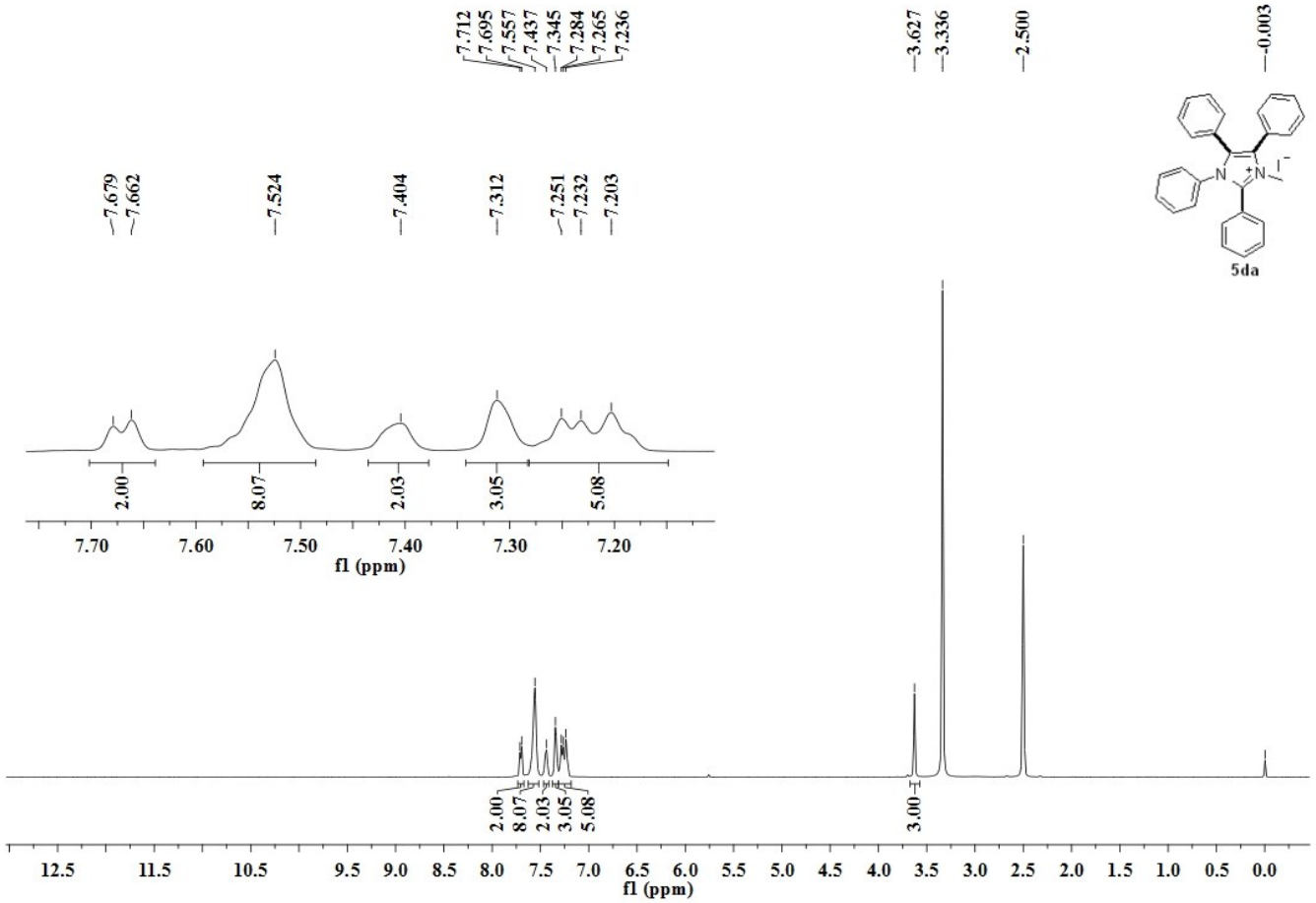

143.87
139.57
136.97
133.30
132.87
131.92
130.39
129.60
123.57
120.07
77.48
77.16
76.84
35.08
5ai
fl (ppm)

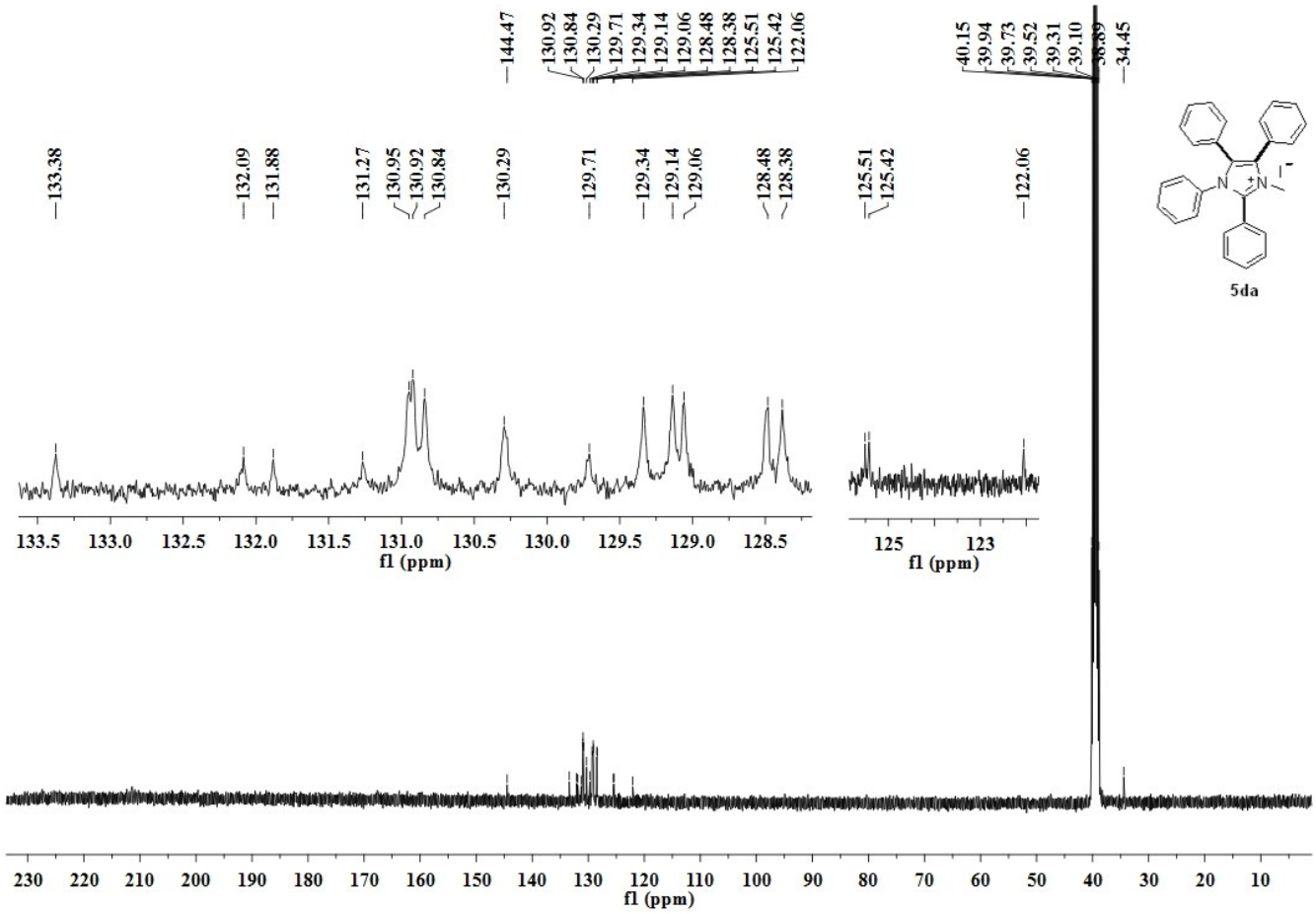

9.043
9.032
8.749
7.995
7.985
7.521
7.511
3.612
3.362
2.500
0.011
8.993
8.982
8.699
7.945
7.935
7.471
7.461
5aq
2.00
4.00
2.00
4.00
fl (ppm)
2.00
4.00
2.00
4.00
6.00
fl (ppm)

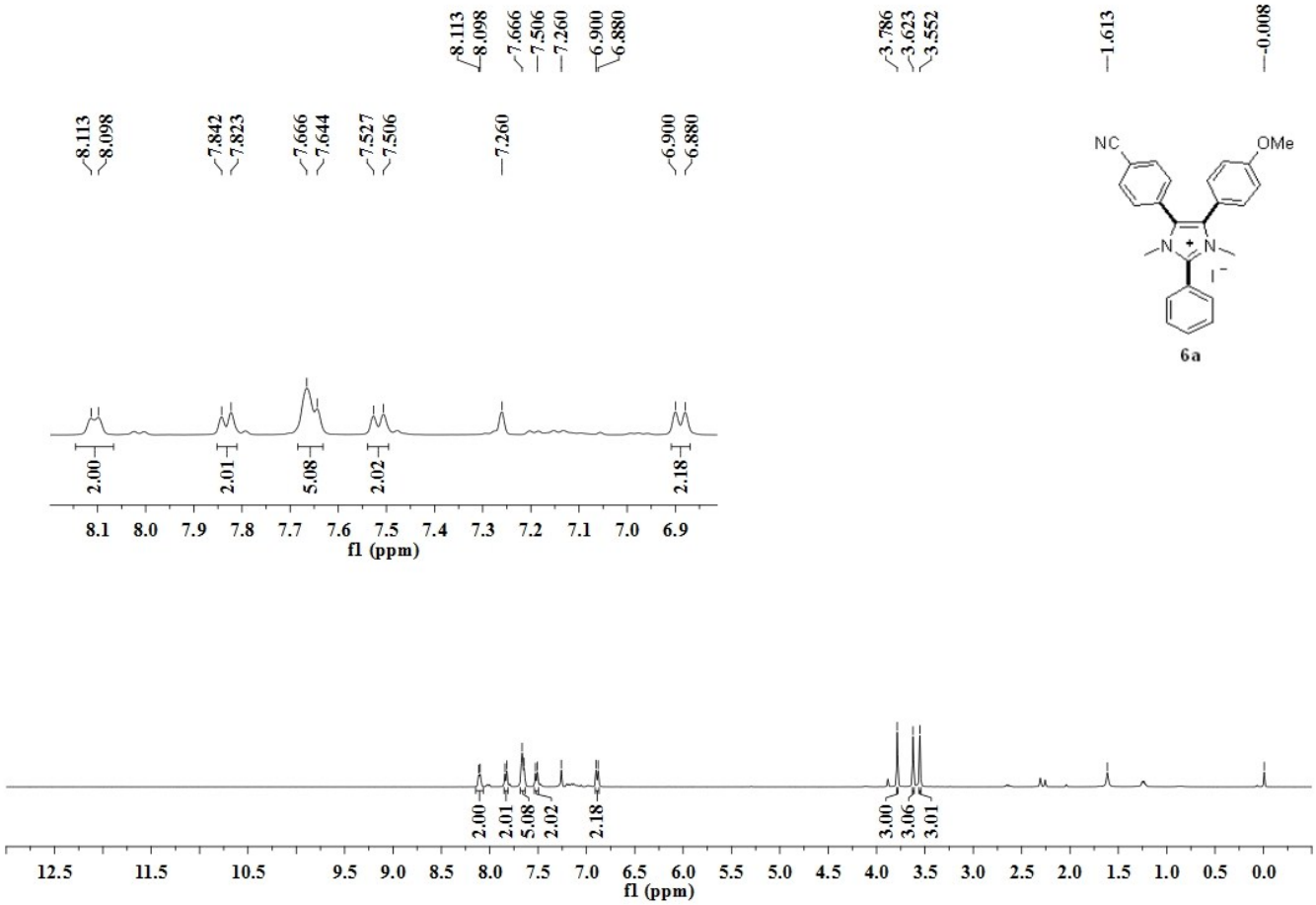

151.02
150.62
143.15
132.85
129.48
125.04
40.15
39.94
39.73
39.52
39.31
39.10
38.89
34.98
5aq
fl (ppm)


8.115
8.104
7.681
7.619
7.606
7.386
7.354
7.260
3.992
3.973
3.955
3.559
1.615
1.425
1.408
1.390
0.937
0.531
0.513
0.011
5ba
2.01
3.00
4.06
6.06
2.05
3.00
2.17
2.19
3.00
fl (ppm)


143.95
131.33
130.18
130.04
129.96
129.01
128.92
125.55
125.17
121.97
77.34
77.02
76.70
46.88
34.88
31.56
19.37
12.93
5ba
fl (ppm)


7.712
7.695
7.557
7.437
7.345
7.284
7.265
7.236
3.627
3.336
2.500
0.003
7.679
7.662
7.524
7.404
7.312
7.251
7.232
7.203
5da
2.00
8.07
2.03
3.05
5.08
3.00
fl (ppm)


144.47
130.92
130.84
130.29
129.71
129.34
129.14
129.06
128.48
128.38
125.51
125.42
122.06
40.15
39.94
39.73
39.52
39.31
39.10
38.89
34.45
133.38
132.09
131.88
131.27
130.95
130.92
130.84
130.29
129.71
129.34
129.14
129.06
128.48
128.38
125.51
125.42
122.06
5da
fl (ppm)
fl (ppm)
fl (ppm)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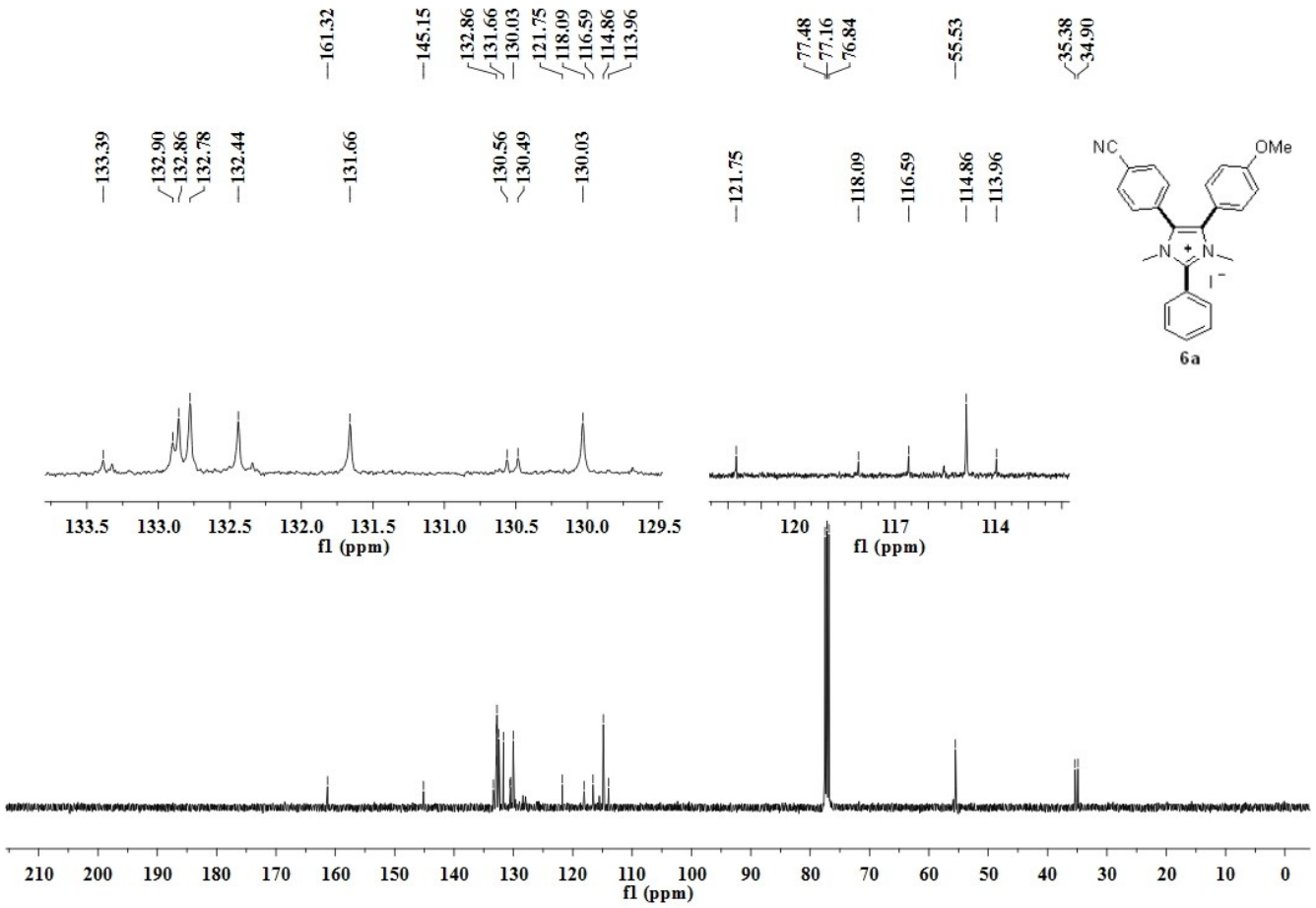
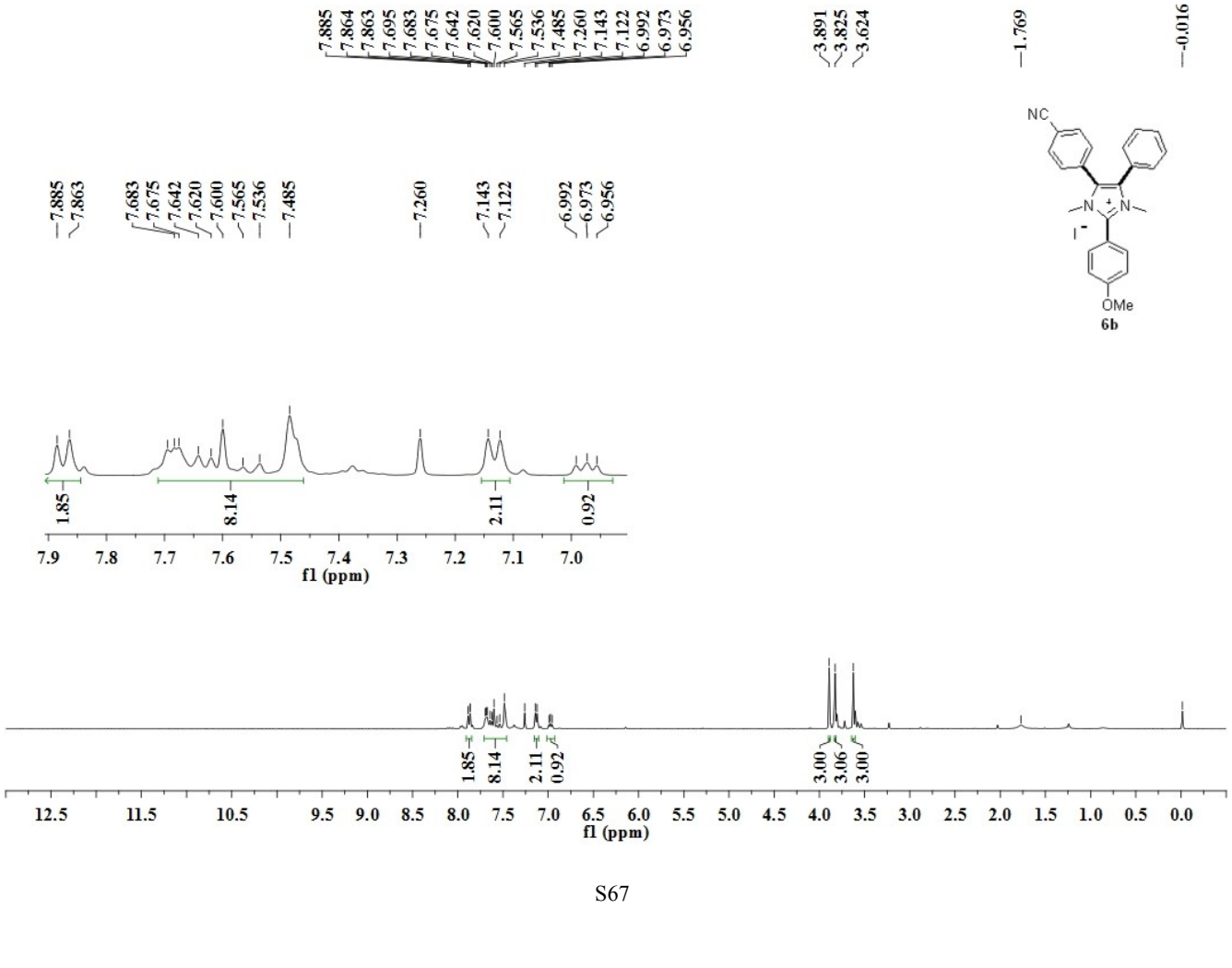
8.098
7.666
7.506
7.260
6.900
6.880
3.786
3.623
3.552
1.613
0.008
8.113
8.098
7.842
7.823
7.666
7.644
7.527
7.506
7.260
6.900
6.880
NC
OMe
6a
2.00
2.01
5.08
2.02
2.18
fl (ppm)
2.00
2.01
5.08
2.02
2.18
3.00
3.06
3.01
fl (ppm)


161.32
145.15
132.86
131.66
130.03
121.75
118.09
116.59
114.86
113.96
77.48
77.16
76.84
55.53
35.38
34.90
NC
OMe
I⁻
6a
fl (ppm)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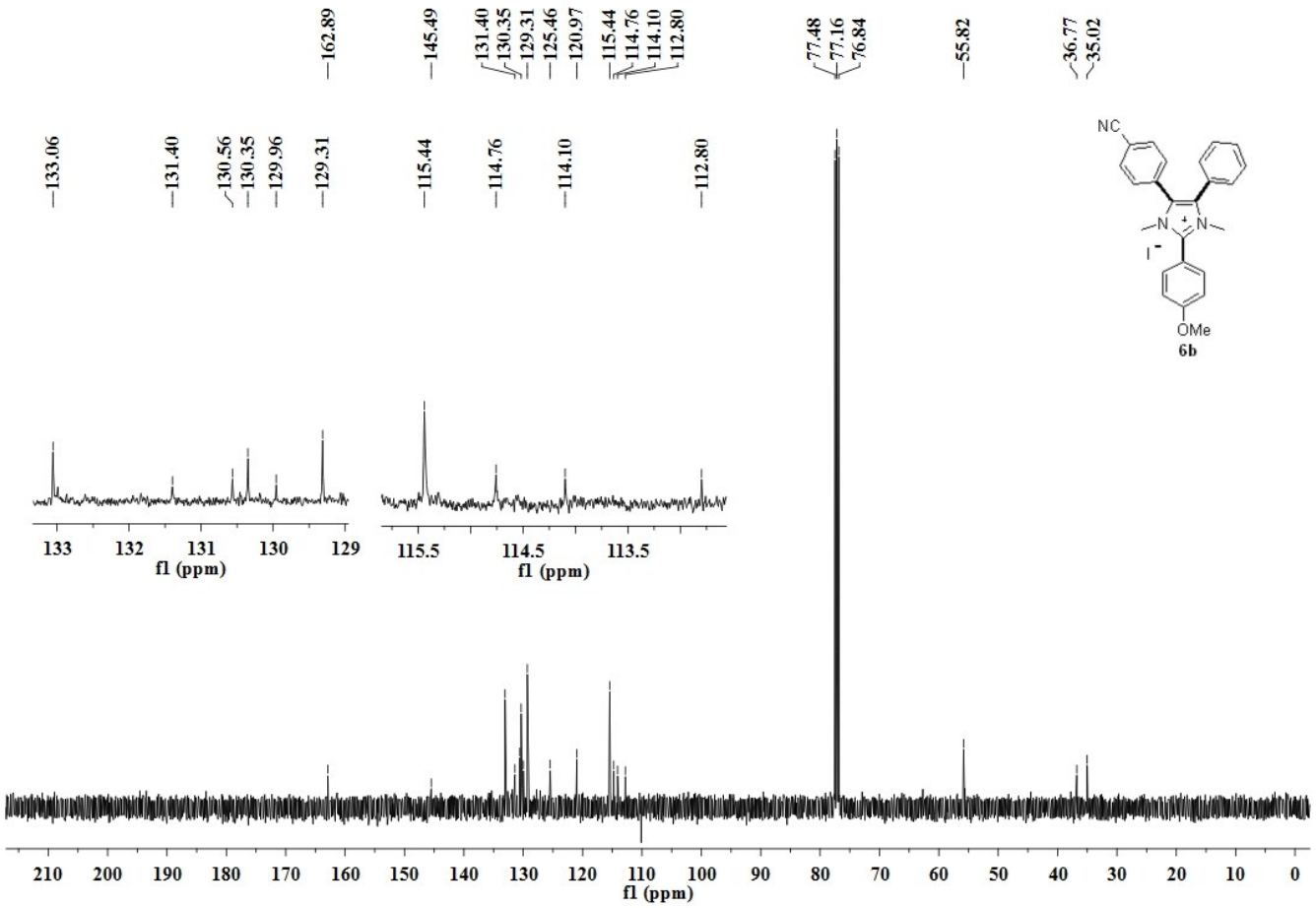
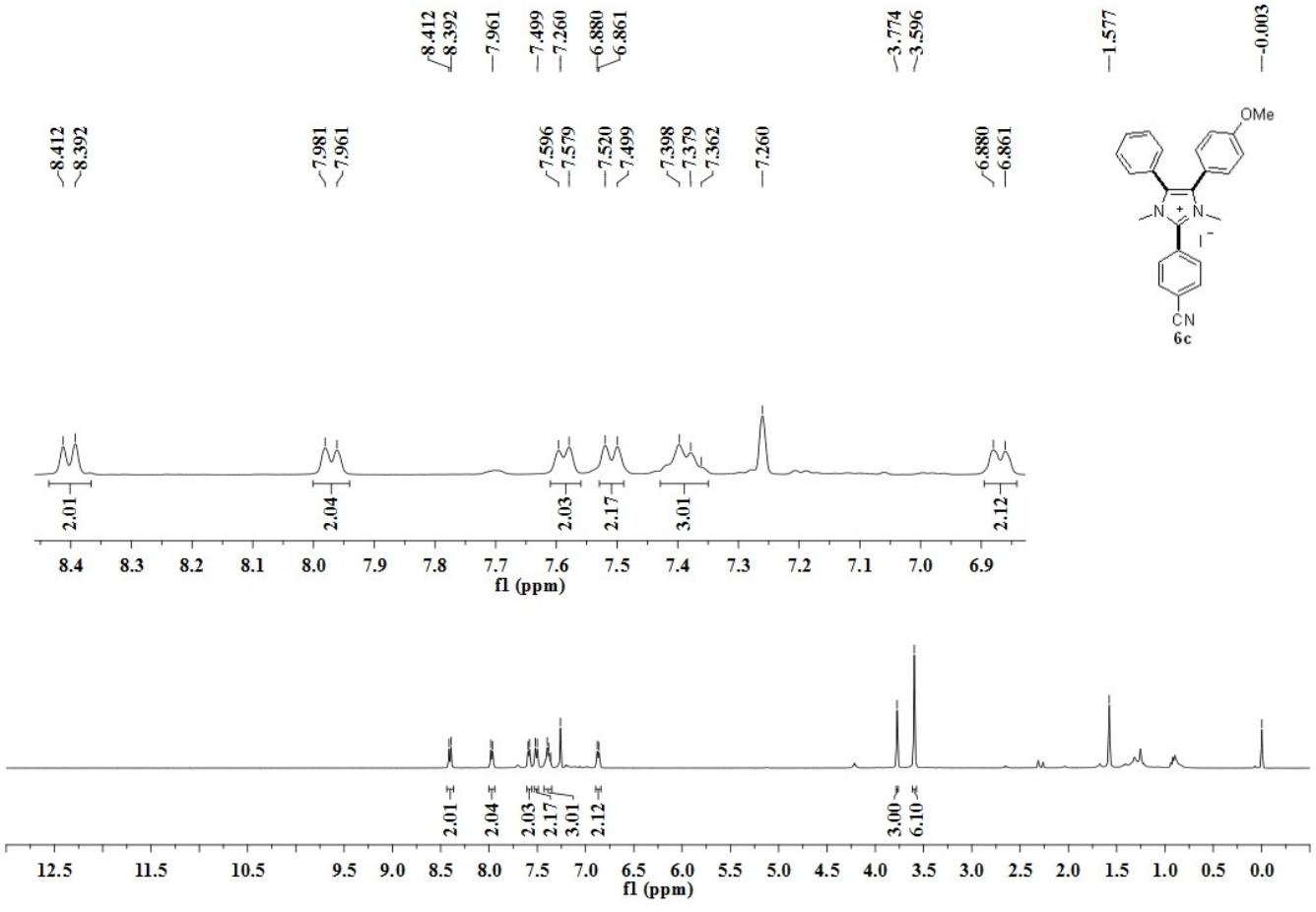
7.864
7.863
7.695
7.683
7.675
7.642
7.620
7.600
7.565
7.536
7.485
7.260
7.143
7.122
6.992
6.973
6.956
3.891
3.825
3.624
1.769
0.016
NC
I⁻
OMe
6b
1.85
8.14
2.11
0.92
3.00
3.06
3.00
fl (ppm)


162.89
145.49
131.40
130.35
129.31
125.46
120.97
115.44
114.76
114.10
112.80
77.48
77.16
76.84
55.82
36.77
35.02
133.06
131.40
130.56
130.35
129.96
129.31
115.44
114.76
114.10
112.80
NC
OMe
6b
133
132
131
130
129
fl (ppm)
115.5
114.5
113.5
fl (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
fl (ppm)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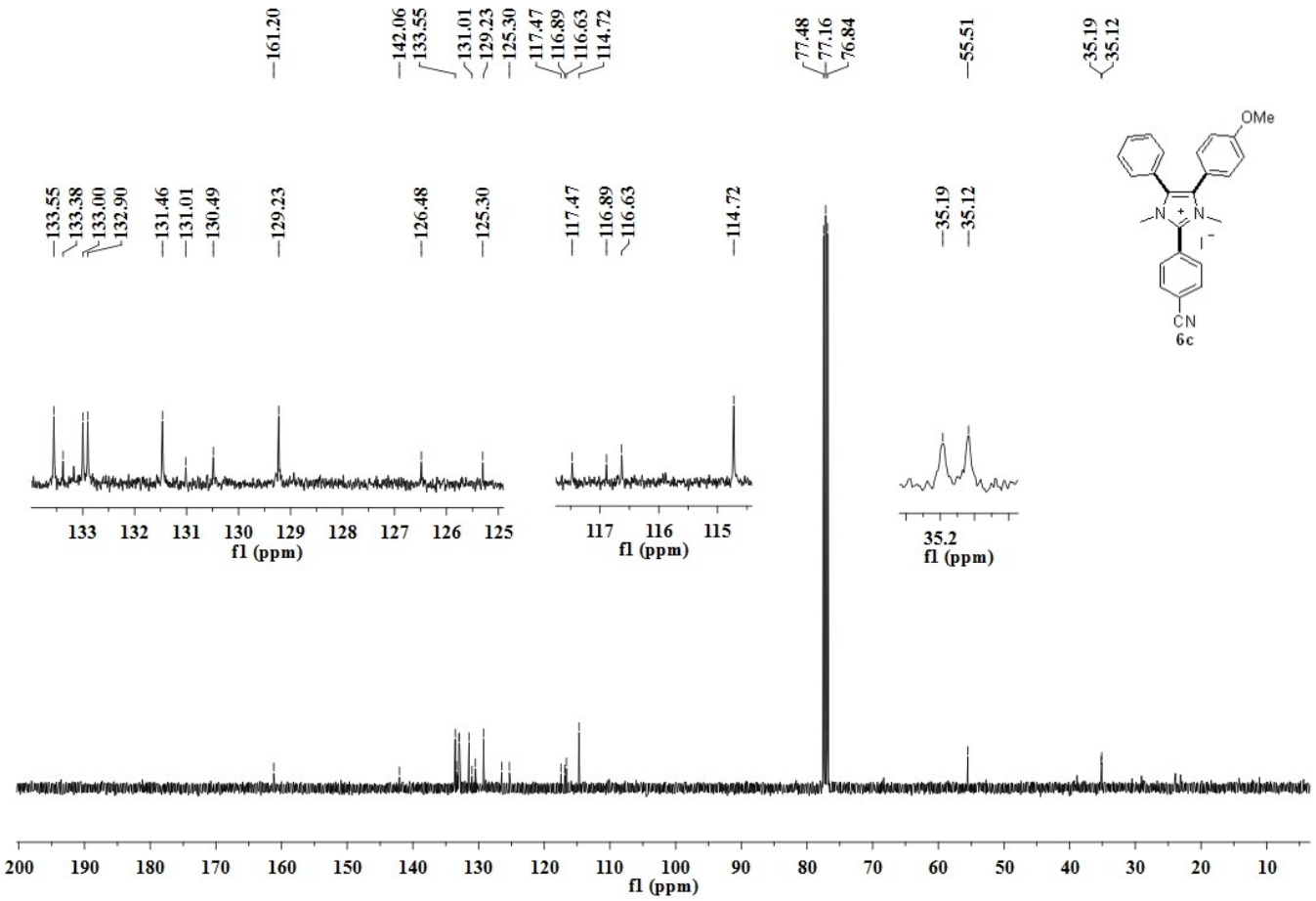
7.499
7.260
6.880
6.861
3.774
3.596
1.577
0.003
8.412
8.392
7.981
7.961
7.596
7.579
7.520
7.499
7.398
7.379
7.362
7.260
6.880
6.861
OMe
CN
6c
2.01
2.04
2.03
2.17
3.01
2.12
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
fl (ppm)
2.01
2.04
2.03
2.17
3.01
2.12
3.00
6.10
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
fl (ppm)


161.20
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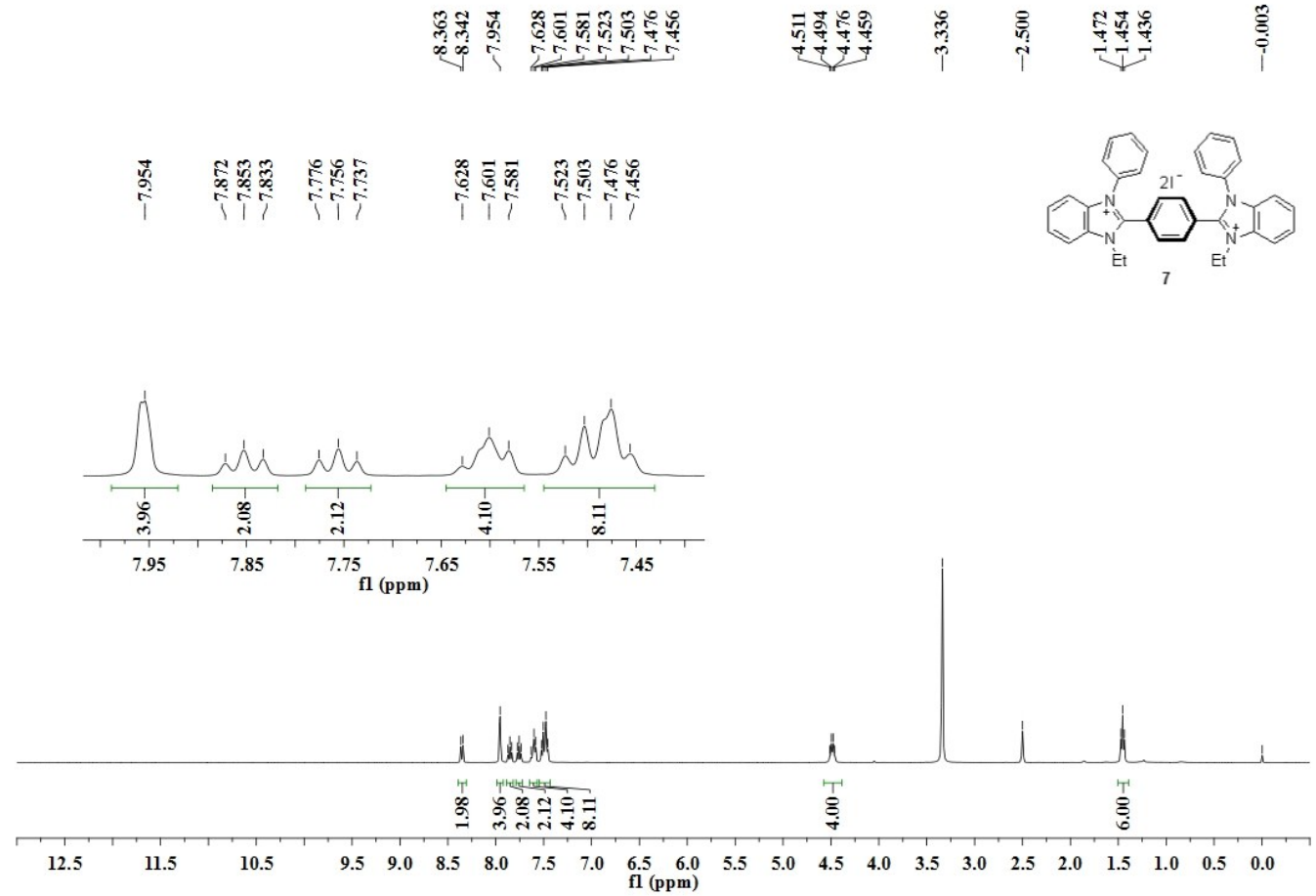
131.01
129.23
125.30
117.47
116.89
116.63
114.72
77.48
77.16
76.84
55.51
35.19
35.12
OMe
I⁻
CN
6c
133.55
133.38
133.00
132.90
131.46
131.01
130.49
129.23
126.48
125.30
117.47
116.89
116.63
114.72
35.19
35.12
133 132 131 130 129 128 127 126 125
f1 (ppm)
117 116 115
f1 (ppm)
35.2
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.342
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7.628
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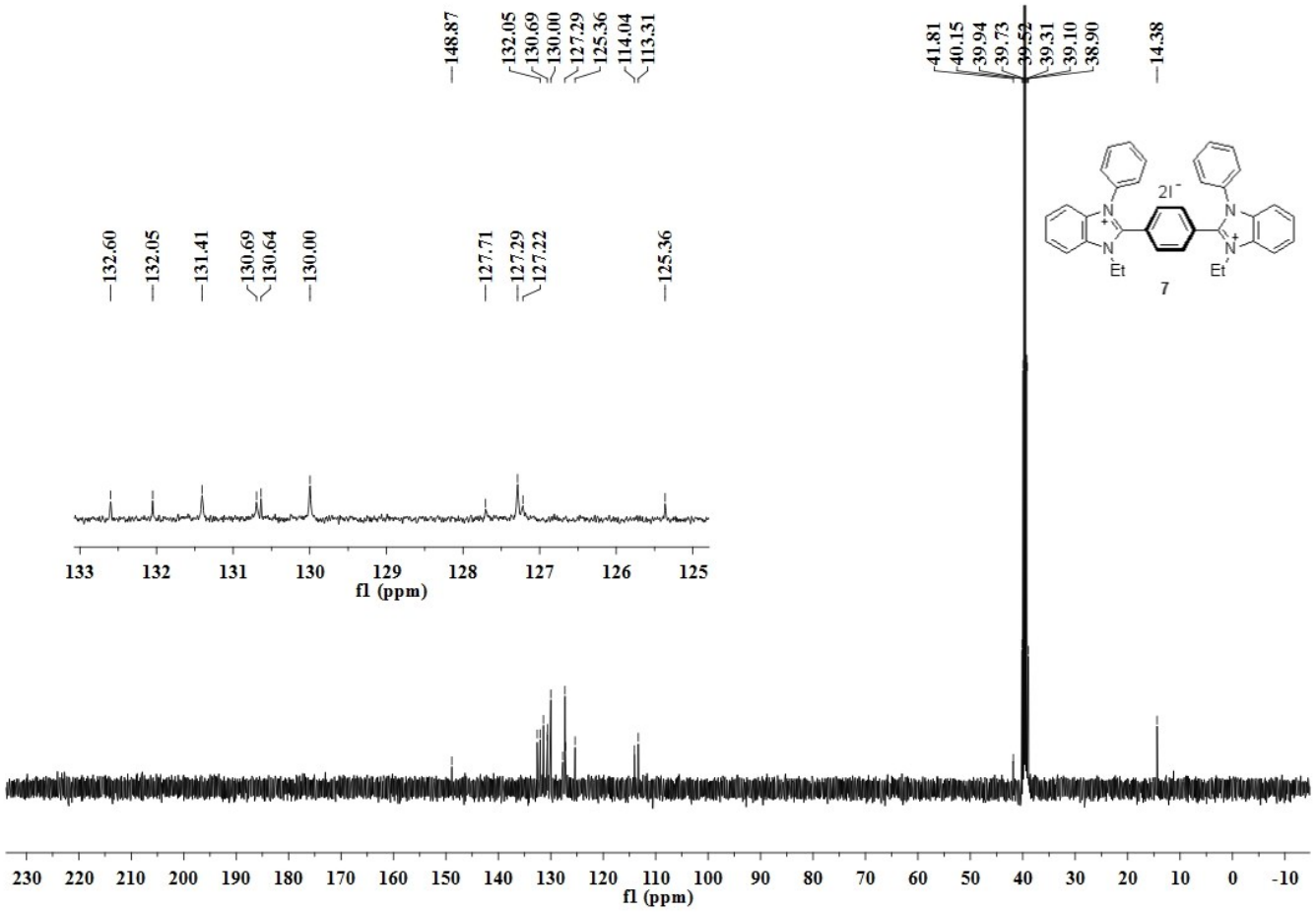
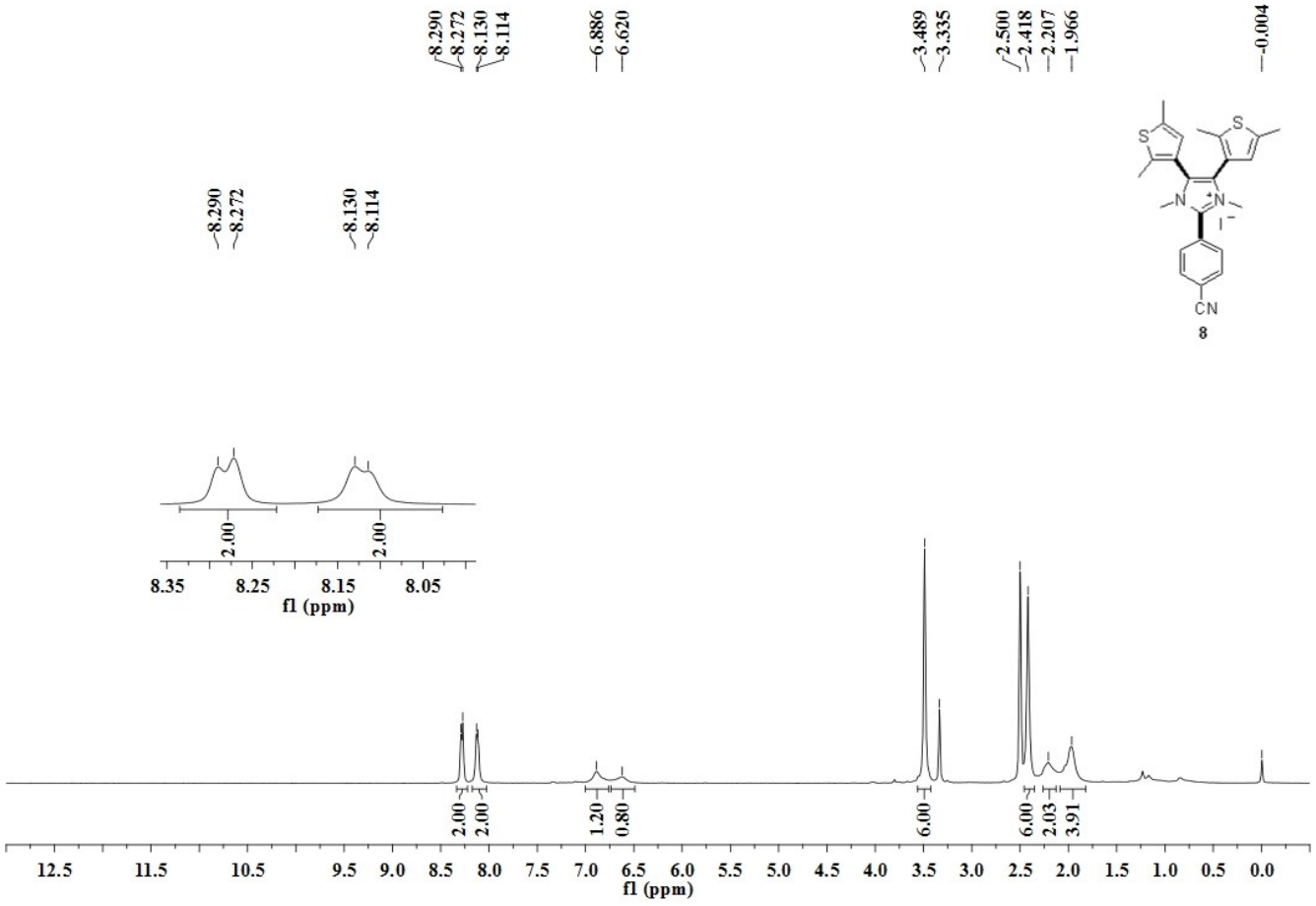
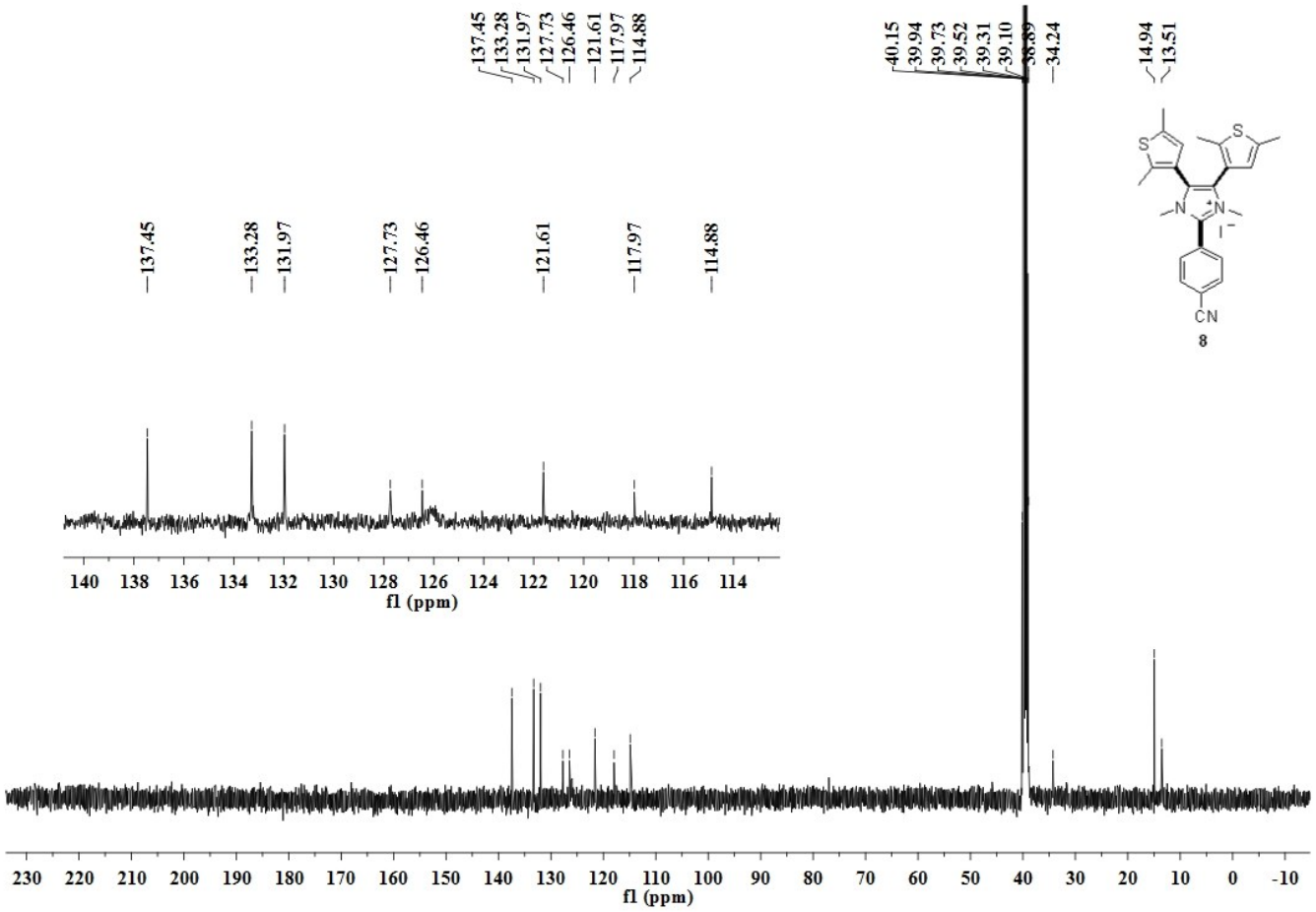
7.581
7.523
7.503
7.476
7.456
4.511
4.494
4.476
4.459
3.336
2.500
1.472
1.454
1.436
-0.003
2I⁻
N
N
Et
Et
7
7.954
7.872
7.853
7.833
7.776
7.756
7.737
7.628
7.601
7.581
7.523
7.503
7.476
7.456
3.96
2.08
2.12
4.10
8.11
7.95 7.85 7.75 7.65 7.55 7.45
f1 (ppm)
1.98
3.96
2.08
2.12
4.10
8.11
4.00
6.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.87
132.05
130.69
130.00
127.29
125.36
114.04
113.31
41.81
40.15
39.94
39.73
39.52
39.31
39.10
38.90
14.38
132.60
132.05
131.41
130.69
130.64
130.00
127.71
127.29
127.22
125.36
2I⁻
Et
Et
7
133 132 131 130 129 128 127 126 125
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.290
8.272
8.130
8.114
6.886
6.620
3.489
3.335
2.500
2.418
2.207
1.966
-0.004
8.290
8.272
8.130
8.114
S
S
N
N
I⁻
CN
8
2.00
2.00
8.35 8.25 8.15 8.05
f1 (ppm)
2.00
2.00
1.20
0.80
6.00
6.00
2.03
3.91
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.45
133.28
131.97
127.73
126.46
121.61
117.97
114.88
40.15
39.94
39.73
39.52
39.31
39.10
38.89
34.24
14.94
13.51
S
S
N
N
I⁻
CN
8
140 138 136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)