Electronic Supplementary Information (ESI)

Bifunctional zinc and magnesium Schiff-base complexes containing quaternary ammonium side-arm for epoxide/CO_2 coupling reaction

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Experimental section

Materials

All operations were carried out in a glove box or using standard Schlenk techniques under nitrogen atmosphere. Toluene, dichloromethane (DCM), and tetrahydrofuran (THF) solvents were dried by a solvent purification system (MB SPS-5, MBraun). Dimethylformamide (DMF) was dried over calcium hydride overnight and distilled under nitrogen atmosphere. Zinc *bis*(*bis*(trimethylsilyl))amide ($Zn(N(SiMe_3)_2)_2$),[1] magnesium *bis*(*bis*(trimethylsilyl))amide ($Mg(N(SiMe_3)_2)_2$),[2] 2,4-di-tert-butyl-6-(((2-(diethylamino)ethyl)imino)methyl)phenol (**HL^1**),[3] 2,4-di-tert-butyl-6-(((2-(diethylamino)ethyl)amino)methyl)phenol (**HL^2**),[4] and 2,4-di-tert-butyl-6-(((2-(diethylamino)ethyl)(methyl)amino)methyl)phenol (**HL^3**)[5] were synthesized according to the reported procedures. Propylene oxide (PO) and cyclohexene oxide (CHO) were dried over calcium hydride overnight, distilled under nitrogen atmosphere, and stored in a freezer at -30 °C in a glove box. Epichlorohydrin (ECH), phenyl glycidyl ether (PGE), 1,3-butadiene monoepoxide (BME), 1,2-epoxyhexane (EH), styrene oxide (SO), cyclopentene oxide (CPO) were obtained from Tokyo Chemical Industry (TCI) Co., Ltd. and used as received. Carbon dioxide gas (99.5% purity) was obtained from Bangkok Industrial Gas (BIG) Co., Ltd. Other reagents were obtained from Sigma-Aldrich, Acros Organics, and Tokyo Chemical Industry (TCI) Co., Ltd.

Measurements

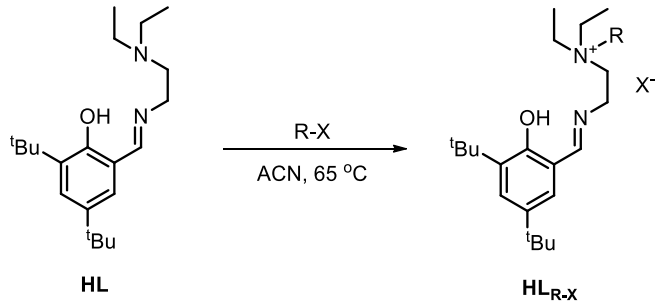
^1H and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker AVANCE III HD-600 MHz spectrometer and referenced to protio impurity of commercial benzene-*d*6 (C_6D_6, δ 7.16 ppm), chloroform-*d* ($CDCl_3$, δ 7.26 ppm), and dimethylsulfoxide-*d*6 (DMSO-*d*6, δ 2.50 ppm) as internal standards. Mass spectrometry of ligands and complexes were acquired by matrix-assisted laser desorption and ionization time-of-flight (MALDI-TOF) mass spectrometry using a Bruker Daltonics Autoflex speed TM mass spectrometer, equipped with laser frequency at 2000 Hz. Solutions of *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2- propylidene]-malononitrile (DCTB) as matrix (40 μL of a 40 g/L DCM solution) and complex (40 μL of a 2.0 g/L DCM solution) were mixed before handed spot to the target followed by solvent

evaporation to prepare a thin film. The samples were measured in refractive positive mode and calibrated by comparison to 5 and 20 kg/mol protein calibration standards I.

X-ray crystallography

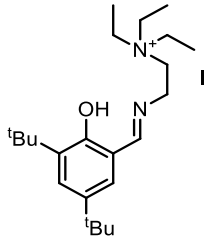
The X-ray crystallographic data were collected on a Bruker D8 Venture using Photon II detector and IμS 3.0 Microfocus Source, Mo Kα radiation (λ= 0.71073 Å). Data collection was carried out using the Bruker software suite APEX3. Data integration was performed with the SAINT software, and intensity data were corrected based on the intensities symmetry-related reflections measured at different angular settings (SADABS). The space group was determined with the XPREP software. The crystal structure was solved by a direct method using intrinsic phasing (SHELXT program)[6] and refined by full-matrix least-squares against F2 using the program SHELXL[7] base on ShelXle engine or Olex2 software package.[8] All non-hydrogen atoms were refined anisotropically while the hydrogen atoms were placed in calculated positions and not refined. The crystallographic images were processed by Ortep3 program.[9]

Synthesis of 2-((3,5-di-tert-butyl-2-hydroxybenzylidene)amino)-*N,N,N*-diethylalkylethanaminium halide ($HL_{R\text{-}X}$)



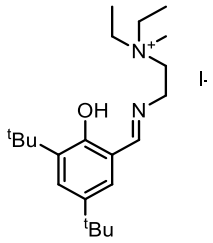
Compound $\mathbf{HL_{R\text{-}X}}$ was synthesized from the applied method from the previous work.[10] The following procedure is for the synthesis of $\mathbf{HL^{1}_{Et\text{-}I}}$. The synthesis of complexes $\mathbf{HL^{1}_{Me\text{-}I}}$, $\mathbf{HL^{1}_{Pr\text{-}I}}$, $\mathbf{HL^{1}_{Et\text{-}Br}}$, $\mathbf{HL^{2}_{Et\text{-}I}}$, $\mathbf{HL^{3}_{Et\text{-}I}}$, and $\mathbf{HL^{4}_{Et\text{-}I}}$ can be carried out similarly using the corresponding Schiff base precursors and alkylhalides (R-X).

Compound $\mathbf{HL^{1}}$ (1.16 g, 5.0 mmol, 1.0 equiv.) was dissolved in acetonitrile (25mL). Iodoethane (1.17g, 7.5 mmol, 1.5 equiv.) was added into a solution. The solution was stirred at 60 °C overnight. Next, the volatile component was evaporated under vacuum and washed with cold diethyl ether (3 x 50 mL) resulting in a yellow powder. The resulting powder was dissolved in dichloromethane (50 mL), extracted with DI water, and dried over anhydrous $NaSO_4$. The volatile components were removed under reduced pressure giving a yellow powder.

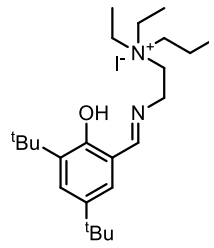


Compound $\mathbf{HL^{1}_{Et\text{-}I}}$ (yellow powder, 77.4 %). ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 12.73 (s, 1H, O*H*), 8.76 (s, 1H, N=C*H*Ar), 7.40 (d, *J* = 2.4 Hz, Ar-*H*), 7.18 (d, *J* = 2.4 Hz, 1H, Ar-*H*), 4.25 (t, *J* = 6.3 Hz, 2H, NCH_2-CH_2N), 3.74 (t, *J* = 6.3 Hz, 2H, NCH_2-CH_2N), 3.60 (q, *J* = 7.3 Hz, 6H, N(CH_2CH$_3$)$_3$), 1.43 (t, *J* = 7.3 Hz, 9H, N(CH$_2$CH_3)$_3$), 1.40 (s, 9H, C(CH_3)$_3$), 1.28 (s, 9H, C(CH_3)$_3$). ^{13}C{^{1}H} NMR (600 MHz, $CDCl_3$, 30 °C): δ 170.61 (N=*C*HAr), 157.70, 141.07, 136.77, 128.24,

127.12, 117.62 (Ar*C*), 57.97, 52.53 (N*C*H$_2$*C*H$_2$N), 54.67 (N(*C*H$_2$CH$_3$)$_3$), 35.13, 34.31 (*C*(CH$_3$)$_3$), 31.57, 29.50 (C(*C*H$_3$)$_3$), 8.50 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{23}H_{41}N_2O^+$ $[M - I^-]^+$ = 361.3269, found 361.2087.

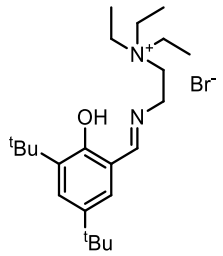


Compound HL^1$_{Me-I}$ (white powder, 99.2 %). ^{1}H NMR (600 MHz, CDCl$_3$, 30 °C): δ 12.72 (s, 1H, O*H*), 8.72 (s, 1H, N=C*H*Ar), 7.41 (d, *J* = 2.4 Hz, Ar-*H*), 7.18 (d, *J* = 2.4 Hz, 1H, Ar-*H*), 4.24 (t, *J* = 6.2 Hz, 2H, NC*H*$_2$-C*H*$_2$N), 3.89 (t, *J* = 6.2 Hz, 2H, NC*H*$_2$-C*H*$_2$N), 3.72 (dt, *J* = 8.6, 6.3 Hz, 4H, N(C*H*$_2$CH$_3$)$_2$), 3.38 (s, 3H, NC*H*$_3$),1.45 (t, *J* = 7.2 Hz, 6H, N(CH$_2$C*H*$_3$)$_2$), 1.40 (s, 9H, C(C*H*$_3$)$_3$), 1.29 (s, 9H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (600 MHz, CDCl$_3$, 30 °C): δ 170.59 (N=*C*HAr), 157.72, 141.12, 136.84, 128.30, 127.10, 117.62 (Ar*C*), 61.10, 52.83 (N*C*H$_2$*C*H$_2$N), 58.03 (N(*C*H$_2$CH$_3$)$_2$), 48.90 (N*C*H$_3$), 35.15, 34.33 (*C*(CH$_3$)$_3$), 31.58, 29.51 (C(*C*H$_3$)$_3$), 8.66 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{22}H_{39}N_2O^+$ $[M - I^-]^+$ = 347.3057, found 347.4467.

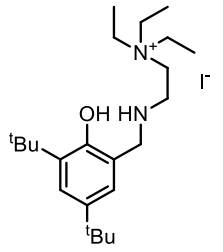


Compound HL^1$_{Pr-I}$ (white powder, 43.0 %). ^{1}H NMR (600 MHz, CDCl$_3$, 30 °C): δ 12.73 (s, 1H, O*H*), 8.76 (s, 1H, N=C*H*Ar), 7.40 (d, *J* = 2.4 Hz, Ar-*H*), 7.19 (s, 1H, Ar-*H*), 4.26 (t, *J* = 6.1 Hz, 2H, NC*H*$_2$-C*H*$_2$N), 3.80 (t, *J* = 6.1 Hz, 2H, NC*H*$_2$-C*H*$_2$N), 3.64 (qd, *J* = 6.9, 3.3 Hz, 4H, N(C*H*$_2$CH$_3$)$_2$), 3.52-3.28 (m, 2H, N(C*H*$_2$CH$_2$CH$_3$)), 1.83 (dt, J = 11.9, 7.4 Hz, 2H, N(CH$_2$C*H*$_2$CH$_3$)), 1.44 (t, *J* = 7.2 Hz, 6H, N(CH$_2$C*H*$_3$)$_2$), 1.40 (s, 9H, C(C*H*$_3$)$_3$), 1.29 (s, 9H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (600 MHz, CDCl$_3$, 30 °C): δ 170.54 (N=*C*HAr), 157.58, 140.99, 136.67, 128.17, 127.01, 117.50 (Ar*C*), 60.60 (N(*C*H$_2$CH$_2$CH$_3$)), 58.53, 52.55 (N*C*H$_2$*C*H$_2$N), 55.04 (N(*C*H$_2$CH$_3$)$_2$), 35.00, 34.21 (*C*(CH$_3$)$_3$), 31.45, 29.38 (C(*C*H$_3$)$_3$), 16.03 (N(CH$_2$*C*H$_2$CH$_3$)), 10.78

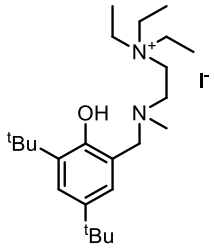
(N($CH_2CH_2CH_3$)), 8.43 (N(CH_2CH_3)$_2$). MALDI-TOF MS calcd. for $C_{24}H_{43}N_2O^+$ [M – I^-]$^+$ = 375.3370, found 375.5120.



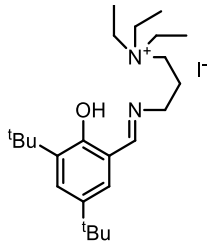
Compound HL^1$_{Et-Br}$ (yellow powder, 37.1 %). ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 12.78 (s, 1H, O*H*), 8.72 (d, J = 1.3 Hz, 1H, N=C*H*Ar), 7.42 (d, *J* = 2.4 Hz, Ar-*H*), 7.17 (d, *J* = 2.4 Hz, 1H, Ar-*H*), 4.28 (t, *J* = 6.3 Hz, 2H, NCH_2-CH_2N), 3.79 (t, *J* = 6.3 Hz, 2H, NCH_2-CH_2N), 3.63 (q, *J* = 7.3 Hz, 6H, N(C$H_2$$CH_3$)$_3$), 1.44 (t, *J* = 7.3 Hz, 9H, N(CH_2CH_3)$_3$), 1.41 (s, 9H, C(CH_3)$_3$), 1.30 (s, 9H, C(CH_3)$_3$). ^{13}C{^{1}H} NMR (600 MHz, $CDCl_3$, 30 °C): δ 170.69 (N=*C*HAr), 157.72, 141.12, 136.79, 128.25, 127.12, 117.66 (Ar*C*), 57.99, 52.51 (N*C*H_2*C*H_2N), 54.44 (N(*C*$H_2$$CH_3$)$_3$), 35.15, 34.33 (*C*($CH_3$)$_3$), 31.58, 29.52 (C(*C*$H_3$)$_3$), 8.28 (N($CH_2$*C*$H_3$)$_3$). MALDI-TOF MS calcd. for $C_{23}H_{41}N_2O^+$ [M – Br^-]$^+$ = 361.3269, found 361.4918.



Compound HL^2$_{Et-I}$ (white powder, 99 %). ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): 7.21 (d, *J* = 2.4 Hz, Ar-*H*), 6.91 (s, 1H, Ar-*H*), 4.06 (s, 2H ArCH_2NH), 3.61 (t, *J* = 7.1 Hz, 2H, NCH_2-CH_2N), 3.09 (t, *J* = 7.3 Hz, 2H, NCH_2-CH_2N), 3.38 (q, *J* = 7.3 Hz, 6H, N(C$H_2$$CH_3$)$_3$), 1.34 (t, *J* = 7.3 Hz, 9H, N(CH_2CH_3)$_3$), 1.39 (s, 9H, C(CH_3)$_3$), 1.27 (s, 9H, C(CH_3)$_3$). ^{13}C{^{1}H} NMR (600 MHz, $CDCl_3$, 30 °C): 153.80, 141.52, 136.06, 124.40, 123.53, 120.92 (Ar*C*), 56.80, 53.08 (N*C*H_2*C*H_2N), 54.37 (N(*C*$H_2$$CH_3$)$_3$), 40.95 (Ar*C*$H_2$NH) 35.03, 34.35 (*C*($CH_3$)$_3$), 31.82, 29.78 (C(*C*$H_3$)$_3$), 8.26 (N($CH_2$*C*$H_3$)$_3$). MALDI-TOF MS calcd. for $C_{23}H_{43}N_2O^+$ [M – I^-]$^+$ = 363.3370 found 363.3247.

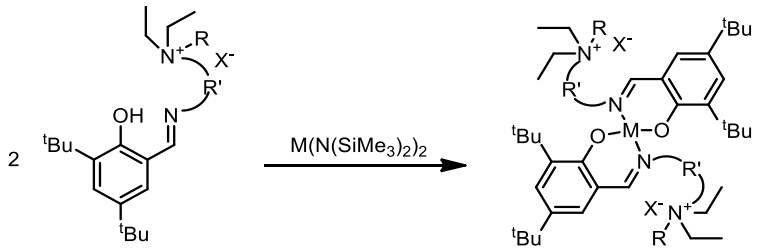


Compound HL$^{3}_{Et-I}$ (white powder, 67.4 %). ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 9.58 (s, 1H, O*H*), 7.26 (d, *J* = 2.4 Hz, Ar-*H*), 6.93 (d, *J* = 2.4 Hz, 1H, Ar-*H*), 3.81 (s, 2H, ArC*H*$_2$NCH$_3$), 3.44 – 2.95 (m, *J* = 7.3 Hz, 10H, N(C*H*$_2$CH$_3$)$_3$ + NC*H*$_2$-C*H*$_2$N), 2.62 (s, 3H, ArCH$_2$NC*H*$_3$) 1.40 (s, 9H, C(C*H*$_3$)$_3$), 1.29 – 1.26 (m, 18H, N(CH$_2$C*H*$_3$)$_3$ + C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (600 MHz, $CDCl_3$, 30 °C): 153.44, 142.00, 136.08, 124.14, 123.92, 120.80 (Ar*C*), 62.67, 55.29 (N*C*H$_2$*C*H$_2$N), 54.45 (N(*C*H$_2$CH$_3$)$_3$), 48.61 (ArCH$_2$N*C*H$_3$), 44.03 (Ar*C*H$_2$NCH$_3$), 35.01, 34.39 (*C*(CH$_3$)$_3$), 31.79, 29.72 (C(*C*H$_3$)$_3$), 8.23 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{24}H_{45}N_2O^+$ [M – I$^-$]$^+$ = 377.3562, found 377.6838.



Compound HL$^{4}_{Et-I}$ (yellow powder, 92.3 %). ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 13.34 (s, 1H, O*H*), 8.53 (s, 1H, N=C*H*Ar), 7.39 (d, *J* = 2.4 Hz, Ar-*H*), 7.14 (d, *J* = 2.4 Hz, 1H, Ar-*H*), 3.84 (t, *J* = 6.3 Hz, 2H, NC*H*$_2$-C*H*$_2$N), 3.53 (t, 2H, NC*H*$_2$CH$_2$C*H*$_2$N), 3.48 (q, *J* = 7.3 Hz, 6H, N(C*H*$_2$CH$_3$)$_3$), 2.21 (m, 2H, NCH$_2$C*H*$_2$CH$_2$N), 1.41 – 1.38 (m, 18H, N(CH$_2$C*H*$_3$)$_3$ + C(C*H*$_3$)$_3$), 1.30 (s, 9H, C(C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (600 MHz, $CDCl_3$, 30 °C): δ 168.66 (N=*C*HAr), 157.92, 140.83, 136.78, 127.68, 126.63, 117.68 (Ar*C*), 55.98, 55.49 (N*C*H$_2$CH$_2$*C*H$_2$N), 54.01 (N(*C*H$_2$CH$_3$)$_3$), 35.15, 34.32 (*C*(CH$_3$)$_3$), 31.61, 29.51 (C(*C*H$_3$)$_3$), 24.02 (NCH$_2$*C*H$_2$CH$_2$N) 8.31 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{24}H_{43}N_2O^+$ [M – I$^-$]$^+$ = 375.3370, found 375.4977

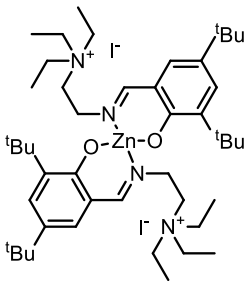
General method for synthesis of Schiff-base zinc and magnesium complexes with quaternary ammonium iodide side-arm (1–5)



The following procedure is for the synthesis of zinc complex **1Et-I**. The synthesis of other complexes can be carried out similarly by using corresponding Schiff-base ligand and $Zn(N(SiMe_3)_2)_2$ or $Mg(N(SiMe_3)_2)_2$.

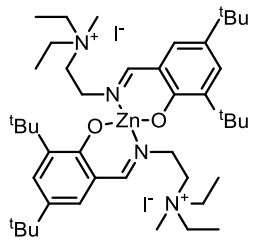
Synthesis of complex 1Et-I

Dichloromethane (30 mL) was added to a mixture of ligand $\mathbf{HL^1_{Et\text{-}I}}$ (0.488 g, 1.0 mmol, 2.0 equiv.) and $Zn((N(SiMe_3)_2)_2$ (0.193 g, 0.5 mmol, 1.0 equiv.). The solution was stirred at room temperature overnight. The volatile components were subsequently removed under vacuum. The solid was washed with dry hexane and dried under vacuum for 2 h giving a yellow powder. Crystals suitable for X-ray crystallography were grown by a slow evaporation in concentrated toluene solution.

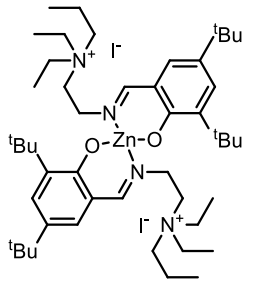


Complex 1Et-I. Yellow powder (81.7 %) ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 8.91 (s, 2H, N=C*H*Ar), 7.45 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 7.21 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 4.59 (t, *J* = 12.3, 2H, NCH_2CH_2N), 4.11 (t, *J* = 12.2, 2H, NCH_2CH_2N), 3.97 – 3.81 (m, 2H, NCH_2CH_2N), 3.45 (m, 12H, N(CH_2CH$_3$)$_3$), 3.26 (t, *J* = 12.7, 2H, , NCH_2CH_2N), 1.37 (s, 18H, C(CH_3)$_3$), 1.28 (s, 18H, C(CH_3)$_3$), 1.21 (t, *J* = 7.2 Hz, 18H, N(CH$_2$CH_3)$_3$).^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 176.88 (N=*C*HAr), 168.55, 141.07, 137.02, 131.32,

131.00, 117.40 (Ar*C*), 55.61, 53.45 (N*C*H_2*C*H_2N), 55.00 (N(*C*H_2CH$_3$)$_3$), 35.70, 34.15 (*C*(CH$_3$)$_3$), 31.55, 29.59 (C(*C*H$_3$)$_3$), 8.38 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{46}H_{80}N_4O_2ZnI^+$ $[M - I^-]^+$ = 911.4617, found 911.5478.

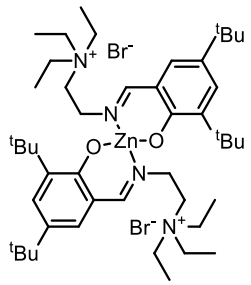


Complex 1Me-I. Yellow powder (68.5 %) ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ 8.93 (s, 2H, N=C*H*Ar), 7.51 – 7.42 (m, *J* = 2.6 Hz, 2H, Ar-*H*),7.25 – 7.21 (m, 2H, Ar-*H*), 4.11 – 3.55 (m, 8H, NC*H*$_2$C*H*$_2$N), 3.50 – 3.25 (m, 8H, N(C*H*$_2$CH$_3$)$_2$), 3.14 (s, 6H, NC*H*$_3$) 1.39 (s, 18H, C(C*H*$_3$)$_3$), 1.29 (s, 18H, C(C*H*$_3$)$_3$), 1.16 (m, *J* = 7.2 Hz, 12H, N(CH$_2$C*H*$_3$)$_2$).^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 176.89 (N=*C*HAr), 168.44, 141.18, 137.11, 131.30, 131.07, 117.33 (Ar*C*), 58.29, 57.73 (N*C*H$_2$*C*H$_2$N), 58.56, 53.11 (N(*C*H$_2$CH$_3$)$_2$), 48.58 (N*C*H$_3$), 35.74, 34.17 (*C*(CH$_3$)$_3$), 31.56, 29.64 (C(*C*H$_3$)$_3$), 8.42, 8.32 – 3.81 (N(CH$_2$*C*H$_3$)$_2$). MALDI-TOF MS calcd. for $C_{44}H_{76}N_4O_2ZnI^+$ $[M - I^-]^+$ = 883.4299, found 883.5854.

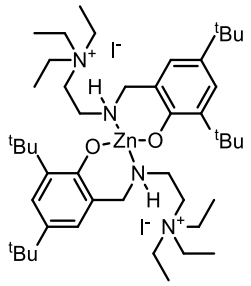


Complex 1Pr-I. Yellow powder (49.0 %) ^{1}H NMR (600 MHz, $CDCl_3$, 30 °C): δ – 3.81 8.94 (s, 2H, N=C*H*Ar), 7.46 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 7.23 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 4.56 (s, 2H, NC*H*$_2$C*H*$_2$N), 4.10 – 4.04 (br, 4H, NC*H*$_2$C*H*$_2$N), 3.51 – 3.16 (br, 14H, NC*H*$_2$C*H*$_2$N+N(C*H*$_2$CH$_3$)$_2$+N(C*H*$_2$CH$_2$CH$_3$), 1.6 (s, 2H, N(CH$_2$C*H*$_2$CH$_3$)), 1.48 (s, 2H, N(CH$_2$C*H*$_2$CH$_3$)), 1.37 (s, 18H, C(C*H*$_3$)$_3$), 1.29 – 1.25 (s, 30H, C(C*H*$_3$)$_3$ + N(CH$_2$C*H*$_3$)$_2$), 0.81 (t, *J* = 7.2 Hz, 6H, N(CH$_2$C*H*$_3$)$_2$).^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 30 °C): δ 177.06 (N=*C*HAr), 168.59, 141.04, 137.02, 131.30, 131.14, 117.42 (Ar*C*), 60.91, 56.04 (N*C*H$_2$*C*H$_2$N), 55.4 – 55.8 (br, N(*C*H$_2$CH$_3$)$_2$), 53.41(N*C*H$_2$CH$_2$CH$_3$) 35.71, 34.16

(*C*(CH_3)$_3$), 31.55, 29.58 (C(*C*H_3)$_3$), 16.05, 8.52 (N(CH_2*C*H_2*C*H_3)), 10.86 (N(CH_2*C*H_3)$_2$) . MALDI-TOF MS calcd. for $C_{48}H_{84}N_4O_2ZnI^+$ $[M - I^-]^+$ = 939.4925, found 939.6238.

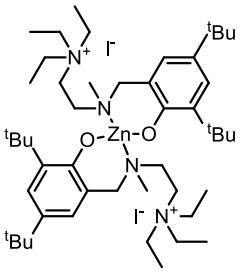


Complex 1Et-Br. Yellow powder (74.4 %) ^{1}H NMR (600 MHz, DMSO-*d6*, 30 °C): δ 8.64 (s, 2H, N=C*H*Ar), 7.37 (s, 2H, Ar-*H*), 7.09 (s, 2H, Ar-*H*), 4.07 – 3.92 (m, 4H, NC*H*$_2$C*H*$_2$N), 3.35 (d, *J* = 7.3, 4H, NC*H*$_2$C*H*$_2$N), 3.22 (d, 12H, N(C*H*$_2$CH$_3$)$_3$), 1.36 (s, 18H, C(C*H*$_3$)$_3$), 1.26 (s, 18H, C(C*H*$_3$)$_3$), 1.06 (t, *J* = 7.2 Hz, 18H, N(CH$_2$C*H*$_3$)$_3$).^{13}C{^{1}H} NMR (150 MHz, DMSO-*d6*, 30 °C): δ 176.32 (N=*C*HAr), 167.69, 139.94, 135.08, 130.03, 129.42, 117.31 (Ar*C*), 54.63, 51.49 (N*C*H$_2$*C*H$_2$N), 52.97 (N(*C*H$_2$CH$_3$)$_3$), 35.06, 33.53 (*C*(CH$_3$)$_3$), 31.20, 29.23 (C(*C*H$_3$)$_3$), 6.97 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{46}H_{80}N_4O_2ZnBr^+$ $[M - Br^-]^+$ = 865.4731, found 865.5880.

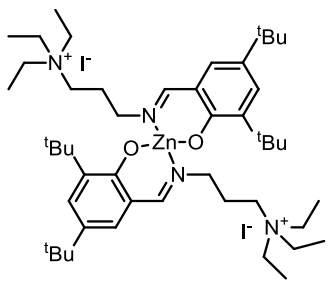


Complex 2. Yellow powder (44.4 %) ^{1}H NMR (600 MHz, DMSO-*d6*, 30 °C): δ 7.09 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 6.93 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 4.98 (t, *J* = 5.9 Hz, 2H, ArCH$_2$N*H*), 3.94 (d, *J* = 4.4 Hz, 4H, ArC*H*$_2$NH), 3.43 (t, J = 8.2 Hz, 4H, NC*H*$_2$C*H*$_2$N), 3.22 (q, J = 7.2 Hz, 12H, N(CH$_2$C*H*$_3$)$_3$) 3.16 – 3.05 (m, 4H, NC*H*$_2$C*H*$_2$N), 1.33 (s, 18H, C(C*H*$_3$)$_3$), 1.24 (s, 18H, C(C*H*$_3$)$_3$), 1.13 (t, *J* = 7.2 Hz, 18H, N(CH$_2$C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (150 MHz, DMSO-*d6*, 30 °C): δ 163.60, 137.33, 134.65, 126.12, 123.67, 121.51 (Ar*C*), 53.81, 53.46 (N*C*H$_2$*C*H$_2$N + Ar*C*H$_2$NH), 53.41 (N(*C*H$_2$CH$_3$)$_3$), 35.29, 34.00 (*C*(CH$_3$)$_3$), 32.25, 30.18

(C(*C*H$_3$)$_3$), 7.69 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{46}H_{84}N_4O_2ZnI^+$ [M – I$^-$]$^+$ = 915.4925, found 915.5941.

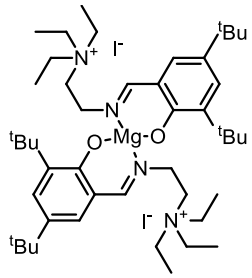


Complex 3. Yellow powder (51.8 %) ^{1}H NMR (600 MHz, DMSO-*d6*, 30 °C): δ 7.10 (m, 2H, Ar-*H*), 6.93 (m, 2H, Ar-*H*), 3.92 (s, 4H, ArC*H*$_2$NCH$_3$), 3.55 – 3.42 (m, 4H, NC*H*$_2$C*H*$_2$N), 3.11 (t, J = 7.5 Hz, 4H, NC*H*$_2$C*H*$_2$N), 3.17 (d, J = 7.5 Hz, 12H, N(C*H*$_2$CH$_3$)$_3$), 2.70 (s, 6H, , ArCH$_2$NC*H*$_3$), 1.23 (s, 18H, C(C*H*$_3$)$_3$), 1.10 (s, 18H, C(C*H*$_3$)$_3$), 1.10 (t, *J* = 7.2 Hz, 18H, N(CH$_2$C*H*$_3$)$_3$). ^{13}C{^{1}H} NMR (150 MHz, DMSO-*d6*, 30 °C): δ 162.63, 136.75, 134.57, 125.36, 123.25, 120.11 (Ar*C*), 60.48, 49.60 (N*C*H$_2$*C*H$_2$N), 52.87 (N(*C*H$_2$CH$_3$)$_3$), 46.51 (Ar*C*H2NCH$_3$), 42.58 (ArCH$_2$N*C*H$_3$), 34.71, 33.50 (*C*(CH$_3$)$_3$), 31.70, 29.59 (C(*C*H$_3$)$_3$), 7.17 (N(CH$_2$*C*H$_3$)$_3$). MALDI-TOF MS calcd. for $C_{48}H_{88}N_4O_2ZnI^+$ [M – I$^-$]$^+$ = 943.5238, found 943.8280.



Complex 4. Yellow powder (52.4 %) ^{1}H NMR (600 MHz, CDCl$_3$, 30 °C): δ 8.84 (s, 2H, N=C*H*Ar), 7.41 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 7.14 (d, *J* = 2.6 Hz, 2H, Ar-*H*), 4.17 (td, *J* = 11.9, 4.1 Hz, 2H, NC*H*$_2$C*H*$_2$N), 3.77 (td, *J* = 12.7, 5.0 Hz, 2H, NC*H*$_2$CH$_2$C*H*$_2$N), 3.55 (td, J = 12.0, 4.5 Hz, 2H, NC*H*$_2$CH$_2$C*H*$_2$N), 3.16 (dp, J = 41.6, 7.2 Hz, 12H, N(C*H*$_2$CH$_3$)$_3$), 2.58 (td, *J* = 13.0, 3.2 Hz, 2H, NC*H*$_2$CH$_2$C*H*$_2$N), 2.29 (dt, J = 11.2, 5.3 Hz, 2H, NCH$_2$C*H*$_2$CH$_2$N), 1.81 – 1.68 (m, 2H, NCH$_2$C*H*$_2$CH$_2$N), 1.41 (s, 18H, C(C*H*$_3$)$_3$), 1.27 (s, 18H, C(C*H*$_3$)$_3$), 1.12 (t, *J* = 7.2 Hz, 18H, N(CH$_2$C*H*$_3$)$_3$).^{13}C{^{1}H} NMR (150 MHz, CDCl$_3$, 30 °C): δ 173.60

(N=*C*HAr), 168.22, 141.50, 136.14, 130.50, 129.98, 117.13 (Ar*C*), 56.46, 54.73 (N*C*H_2CH_2*C*H_2N), 54.18 (N(*C*H_2CH_3)$_3$), 35.78, 34.11 (*C*(CH_3)$_3$), 31.70, 29.63 (C(*C*H_3)$_3$), 23.44 (NCH_2*C*H_2CH_2N), 7.87 (N(CH_2*C*H_3)$_3$). MALDI-TOF MS calcd. for $C_{48}H_{84}N_4O_2ZnI^+$ $[M - I^-]^+$ = 939.4925, found 939.6513.



Complex 5. Yellow powder (74 %) ^{1}H NMR (600 MHz, DMSO-*d6*, 30 °C): *δ* 8.20 (s, 2H, N=C*H*Ar), 7.22 (d, J_{HH} = 2.7 Hz, 2H, Ar*H*), 6.95 (d, J_{HH} = 2.7 Hz, 2H, Ar*H*), 3.35 – 3.30, (broad, 4H, NCH_2CH_2N), 2.92-2.75 (broad, 4H, NCH_2CH_2N), 3.25-2.92 (broad, 12H, N(CH_2CH_3)$_3$), 1.43 (s, 18H, C(CH_3)$_3$), 1.24 (s, 18H, C(CH_3)$_3$), 0.98 (d, J_{HH} = 7.2 Hz, 18H, N(CH_2CH_3)$_3$). ^{13}C{^{1}H} NMR (150 MHz, DMSO-*d6*, 30 °C): δ 172.46 (N=*C*HAr), 168.38, 139.22, 131.16, 129.05, 127.40, 119.08 (Ar*C*), 56.92, 51.85 (N*C*H_2*C*H_2N), 53.03 (N(*C*H_2CH_3)$_3$), 35.07, 33.37 (*C*(CH_3)$_3$), 31.50, 29.78 (C(*C*H_3)$_3$), 7.30 (N(CH_2*C*H_3)$_3$). MALDI-TOF MS calcd. for $C_{46}H_{80}N_4O_2MgI^+$ $[M - I^-]^+$ = 871.5176 found 871.6613.

Synthesis of Schiff-base zinc complex with tertiary amine side arm (7)

Compound **HL^1** (0.332 g, 1.00 mmol, 2.0 equiv.) was dissolved in dichloromethane (30 mL). Zn((N(SiMe$_3$)$_2$)$_2$ (0.193 g, 0.500 mmol, 1.0 equiv.) was added into a solution. The solution was stirred at room temperature for 6 h. Then the volatile component was evaporated under vacuum and washed with dry hexane. The resulting product was dried under vacuum giving a yellow powder (0.237 g, 65%).^{1}H NMR (600 MHz, C_6D_6, 30 °C): δ 7.82 (s, 1H, N=C*H*Ar), 7.67 (d, *J* = 2.7 Hz, 1H, Ar-*H*), 6.91 (d, *J* = 2.6 Hz, 1H, Ar-*H*), 3.30 (tq, *J* = 12.0, 6.8, 6.2 Hz, 2H, NCH_2CH_2N), 2.60 – 2.45 (m, 2H, NCH_2CH_2N), 2.31 (qt, *J* = 13.0, 7.0 Hz, 4H, N(CH_2CH$_3$)$_2$), 1.73 (s, 9H, C(CH_3)$_3$), 1.38 (s, 9H, C(CH_3)$_3$), 0.80 (t, *J* = 7.1 Hz, 6H, N(CH$_2$CH_3)$_2$). ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 30 °C): δ 172.48 (N=*C*HAr), 169.62, 141.84, 135.03, 129.86, 129.63, 117.94 (Ar*C*), 59.17, 53.92 (N*C*H_2*C*H_2N), 57.54

(N(CH_2CH_3)$_3$), 36.03, 34.06 (C(CH_3)$_3$), 31.79, 30.07 (C(CH_3)$_3$), 11.99 (N(CH_2CH_3)$_3$). Anal. Calcd for $C_{42}H_{70}N_4O_2Zn$: C,69.25; H, 9.69; N, 7.69. Found: C, 69.25; H, 9.65; N, 7.64.

Representative procedures for epoxide/CO_2 coupling reaction

The following representative reaction is for PO:**1Et-I** ratio of 2000:1, P_{CO2} = 100 psi, 75 °C. For other epoxides, the volume of epoxides was fixed to 2.0 mL and the amount of catalyst was adjusted according to molar ratios of epoxide and catalyst. For the study of solvent effect, 1.0 mL of solvent was added into the solution.

The coupling reaction of PO and CO_2 was carried out by charging magnetic bar, complex **1Et-I** (15.4 mg, 14.7 μmol, 1.0 equiv.), and PO (2.0 mL, 29.5 mmol, 2000 equiv.) into a stainless-steel pressure reactor. Then the reaction was pressurized to 100 psi of CO_2 and submerged with continuous stirring into a preheated oil bath at 75 °C. After a specific time, the reactor was taken out of the oil bath and cooled with ice bath. The excess CO_2 was vented very slowly, and a small amount of sample was taken for ^{1}H-NMR analysis to calculate conversion. The pure product can be purified using column chromatography (EtOAc/hexanes).

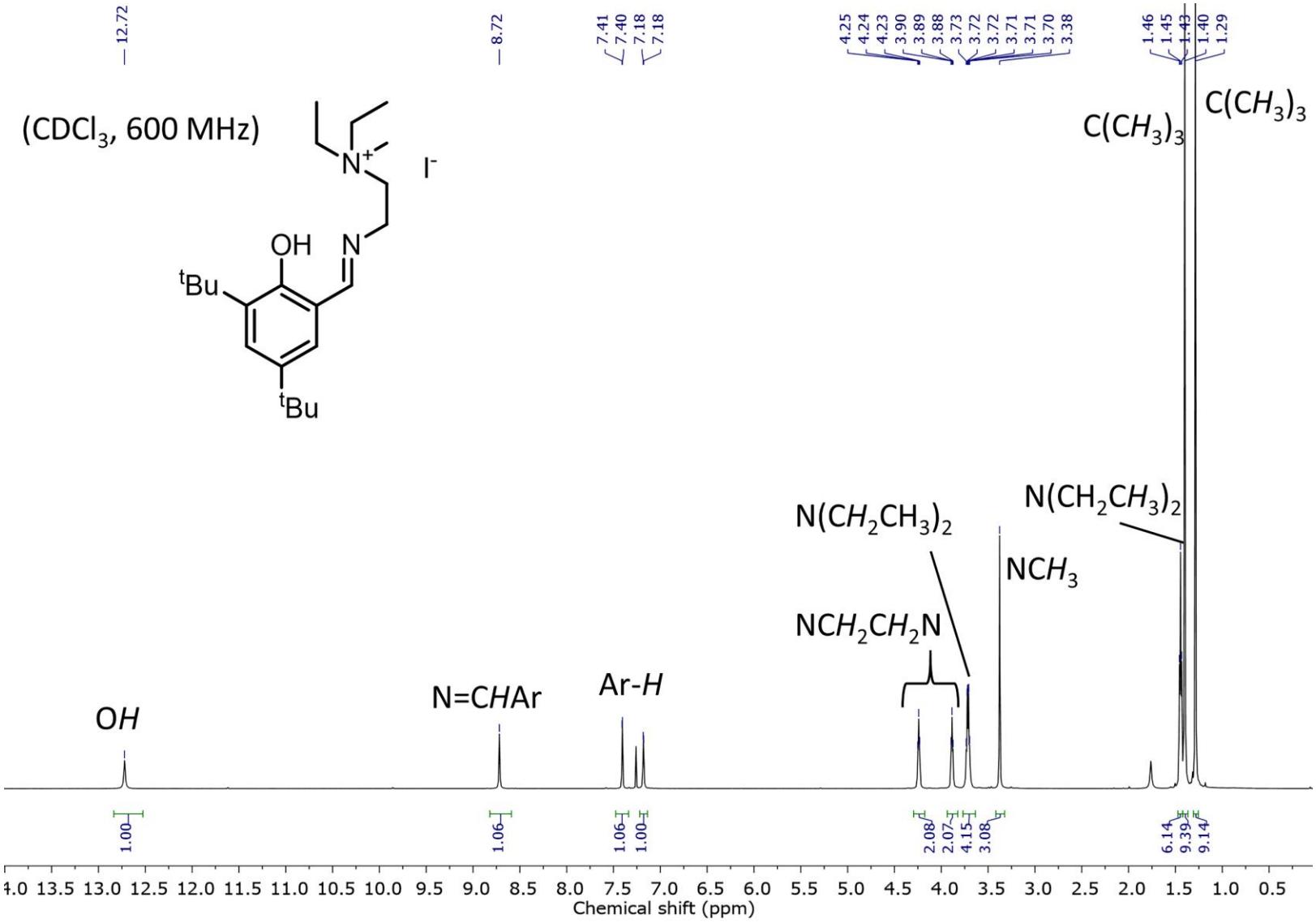


Figure. S1 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^{1}_{Me\text{-}I}}$.

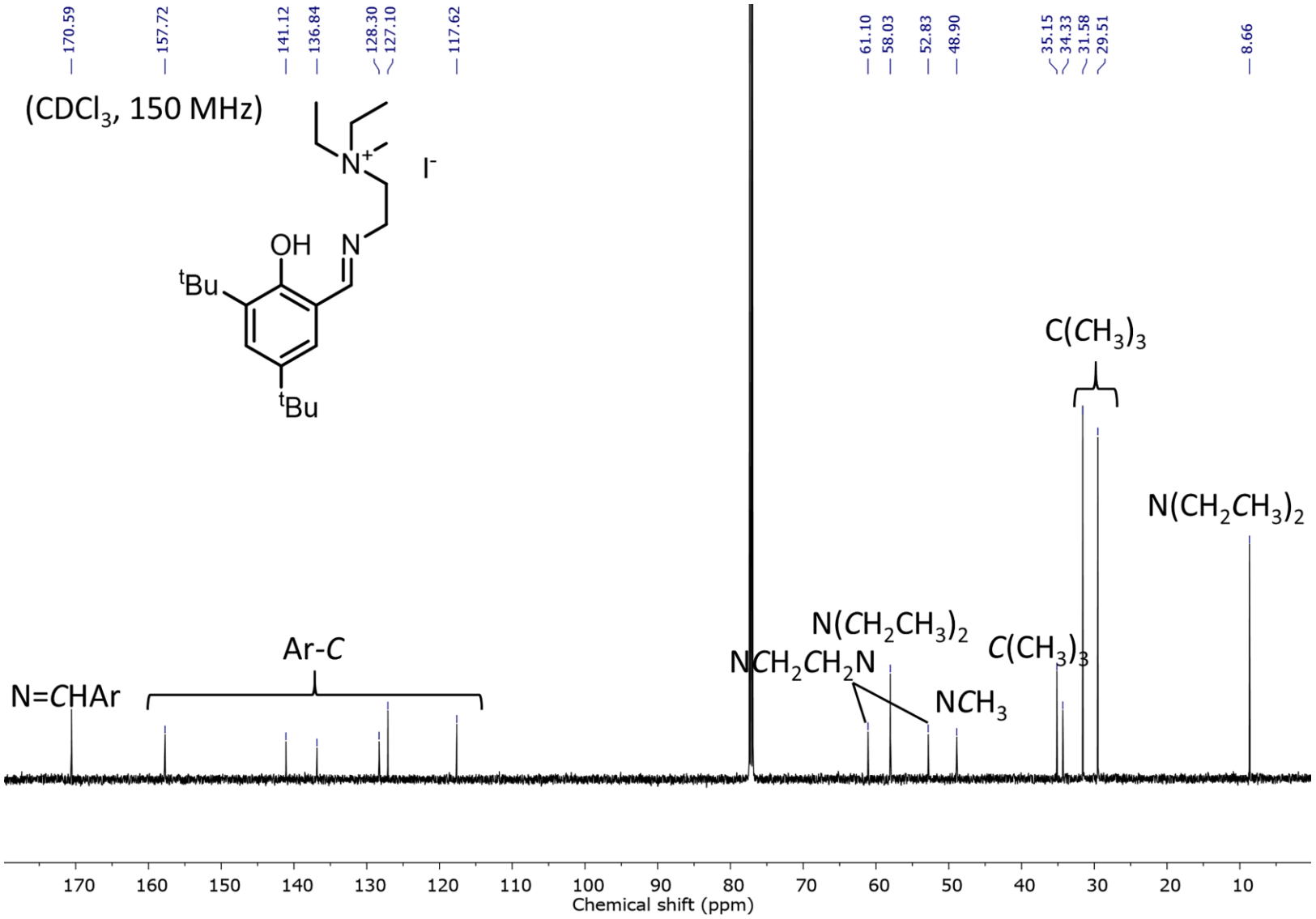


Figure. S2 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^1_{Me\text{-}I}}$.

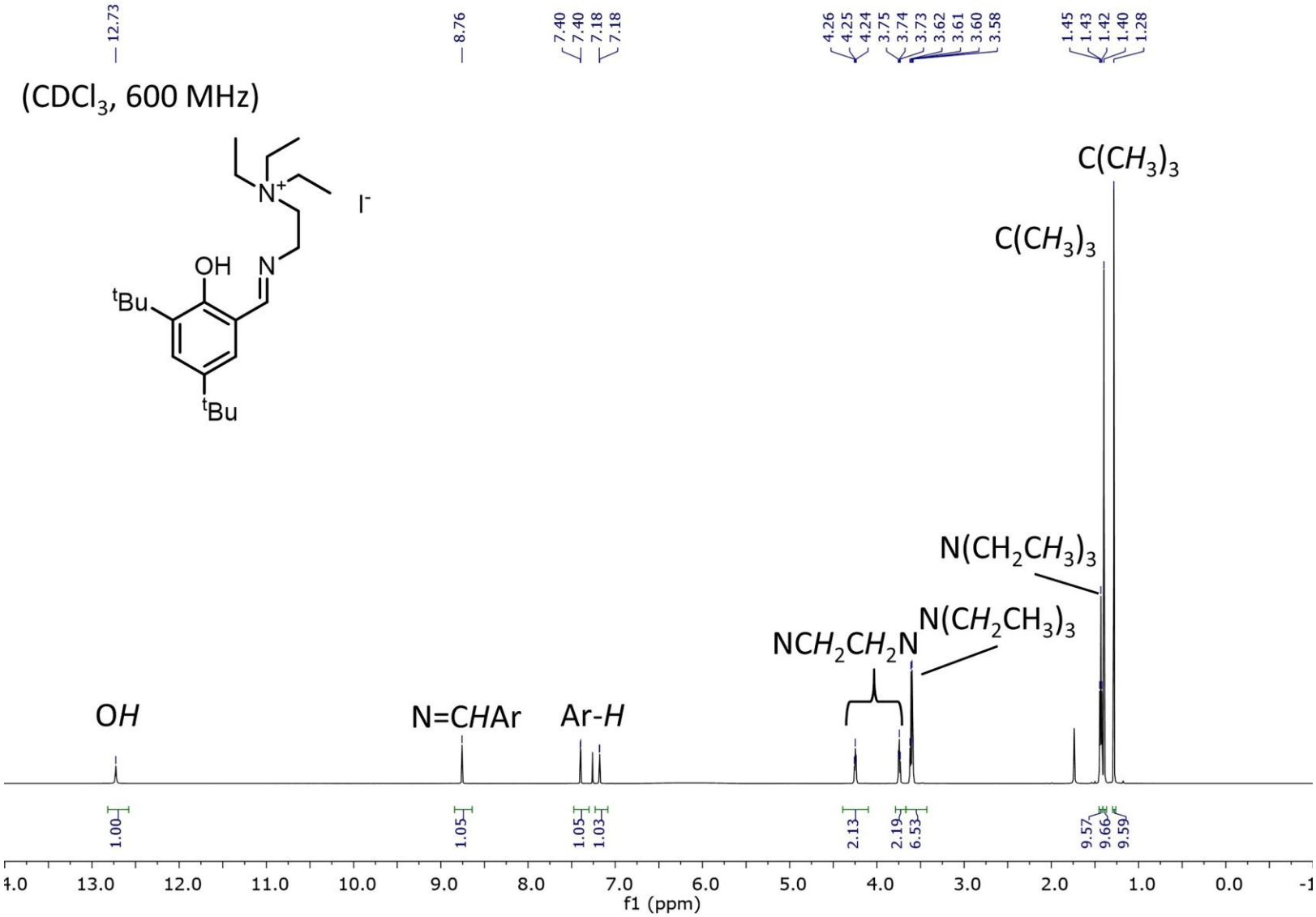


Figure. S3 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^{1}_{Et\text{-}I}}$.

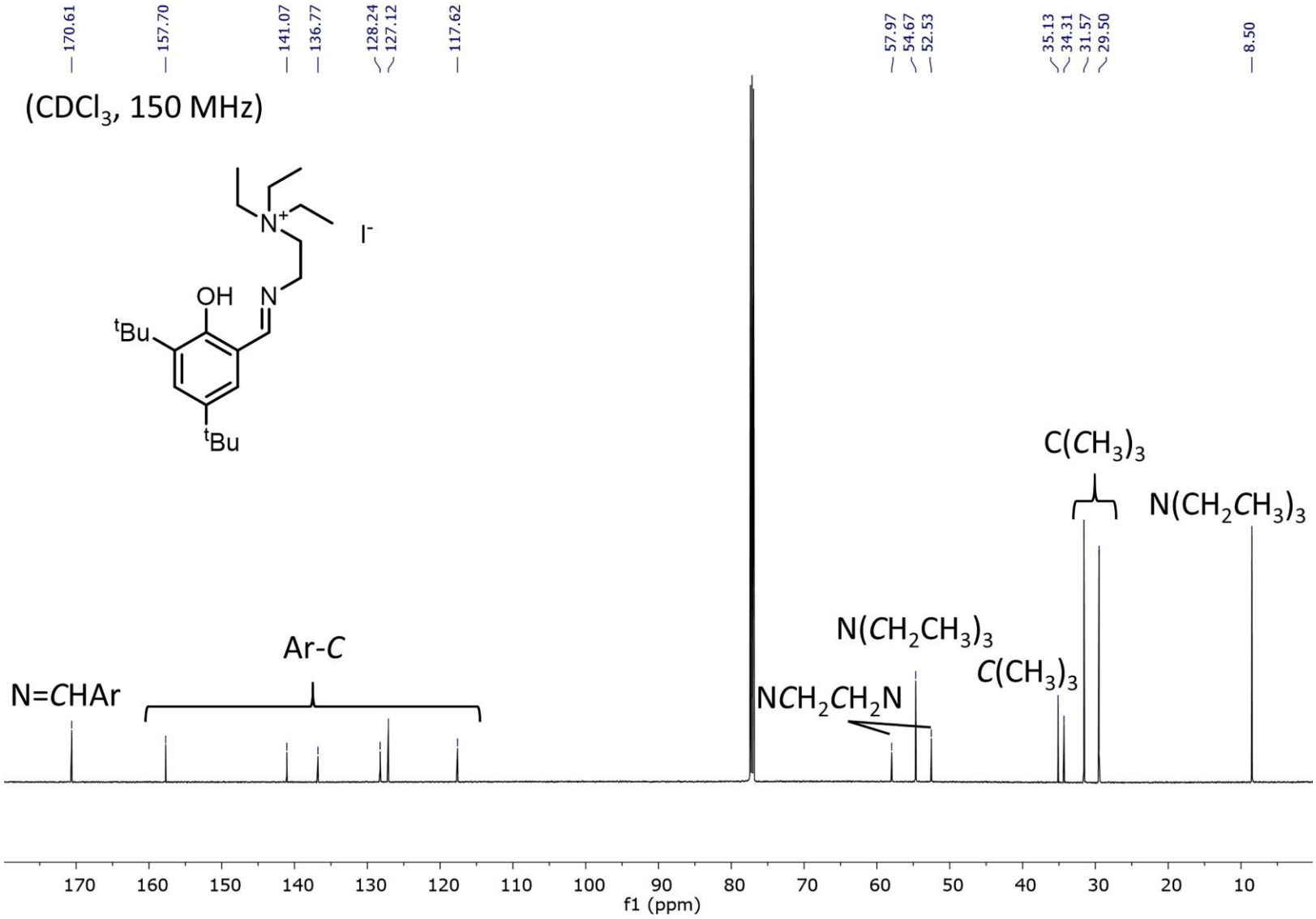


Figure. S4 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^1_{Et\text{-}I}}$.

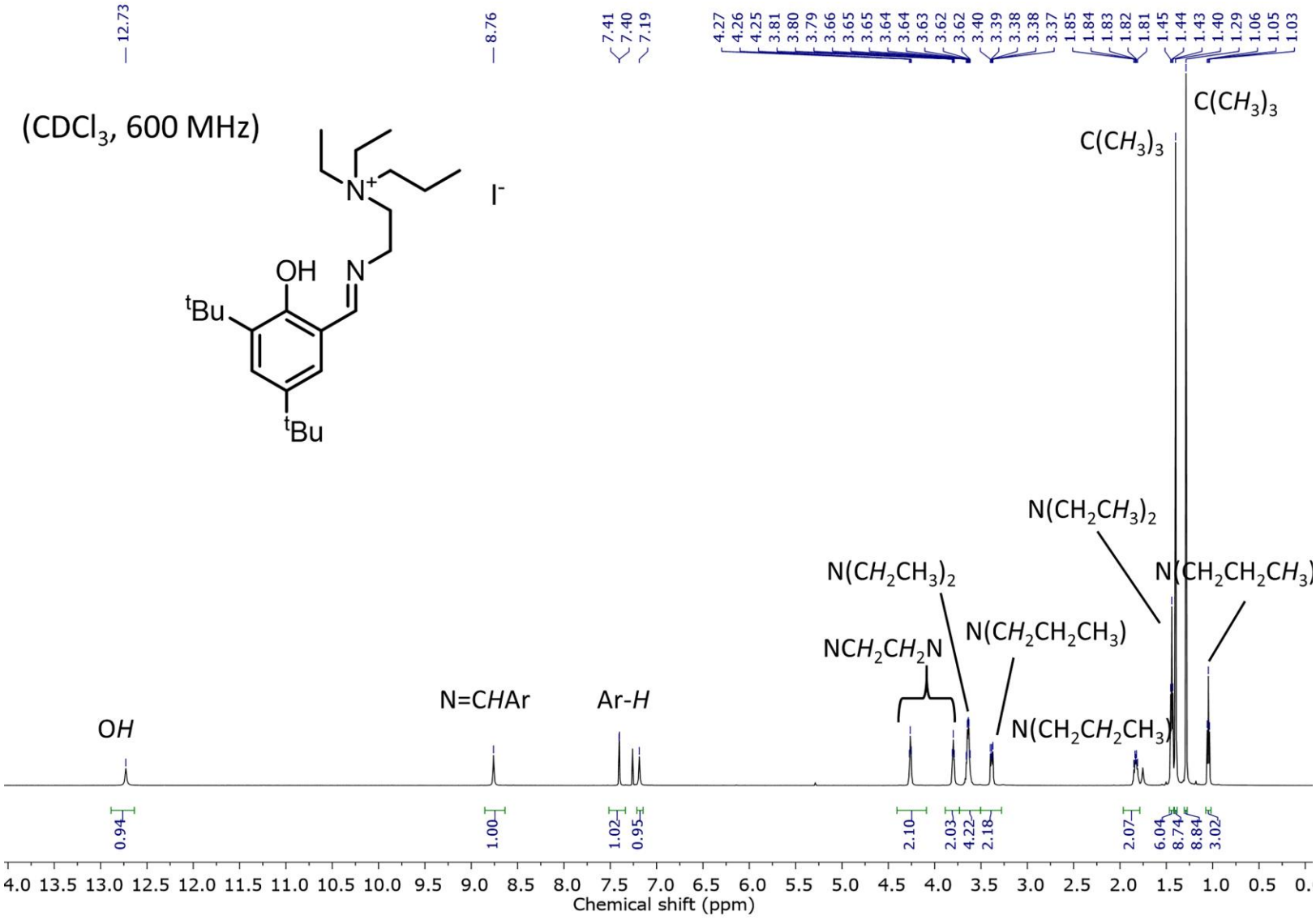


Figure. S5 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^{1}_{Pr\text{-}I}}$.

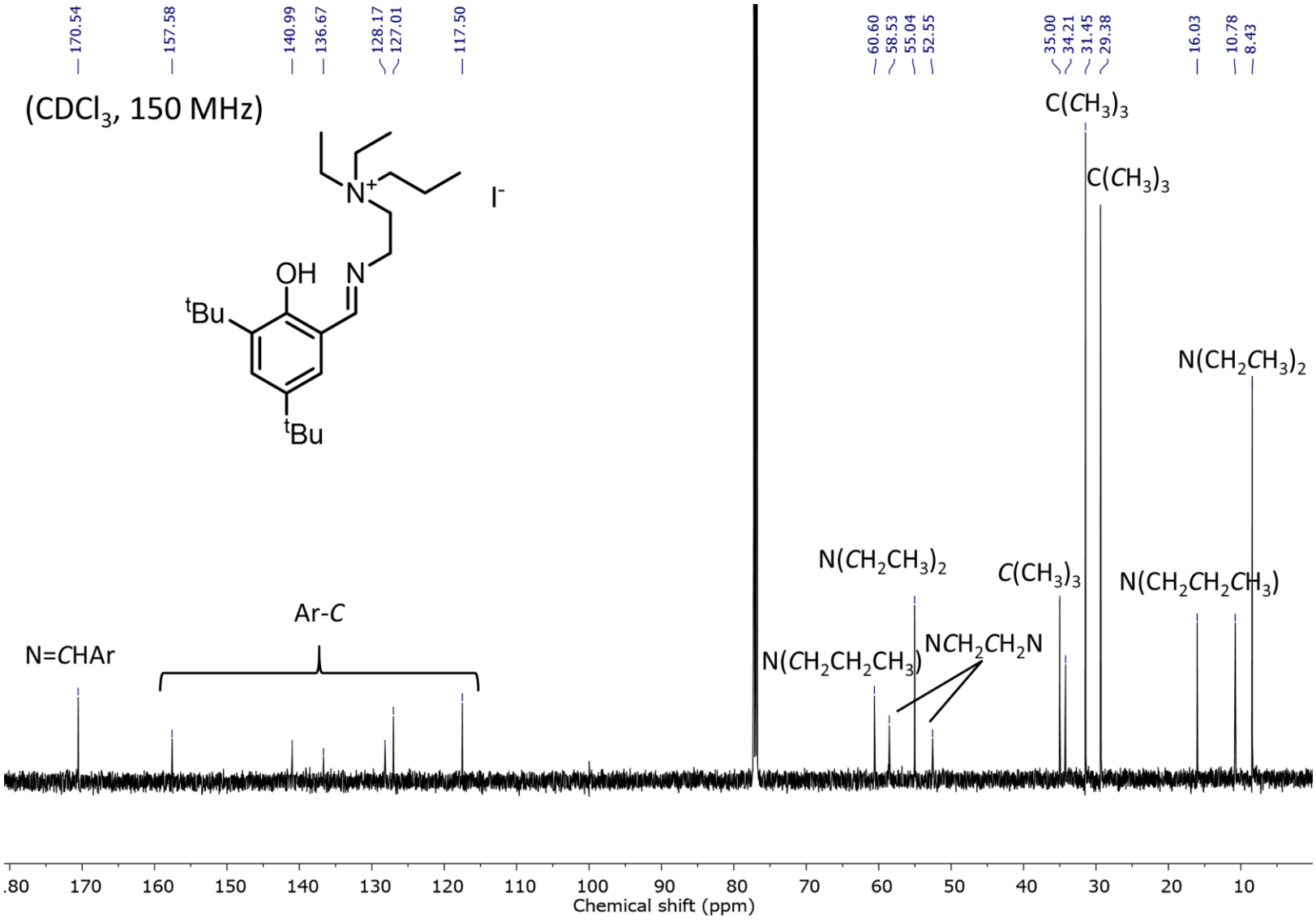


Figure. S6 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^1_{Pr\text{-}I}}$.

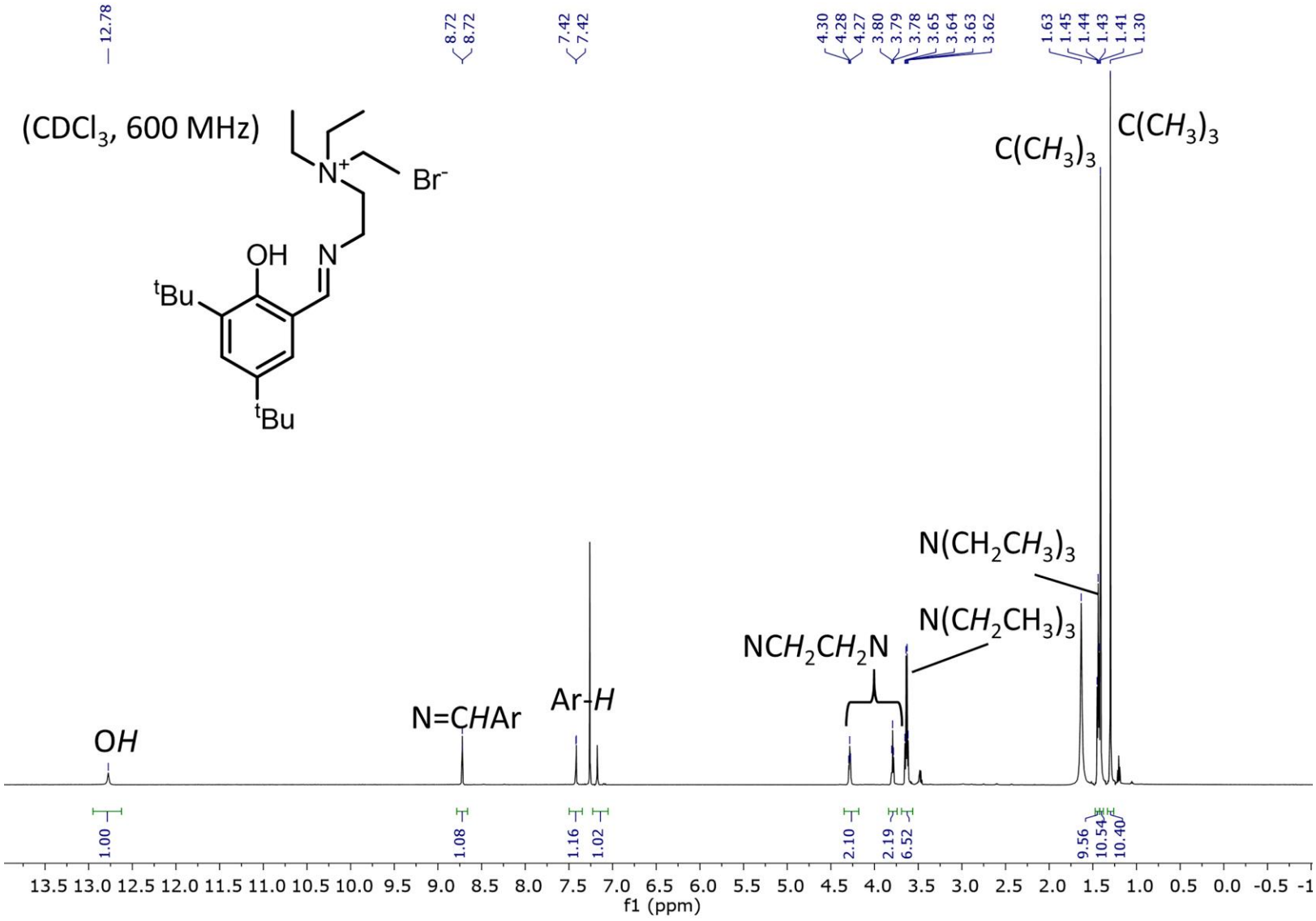


Figure. S7 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^{1}_{Et\text{-}Br}}$.

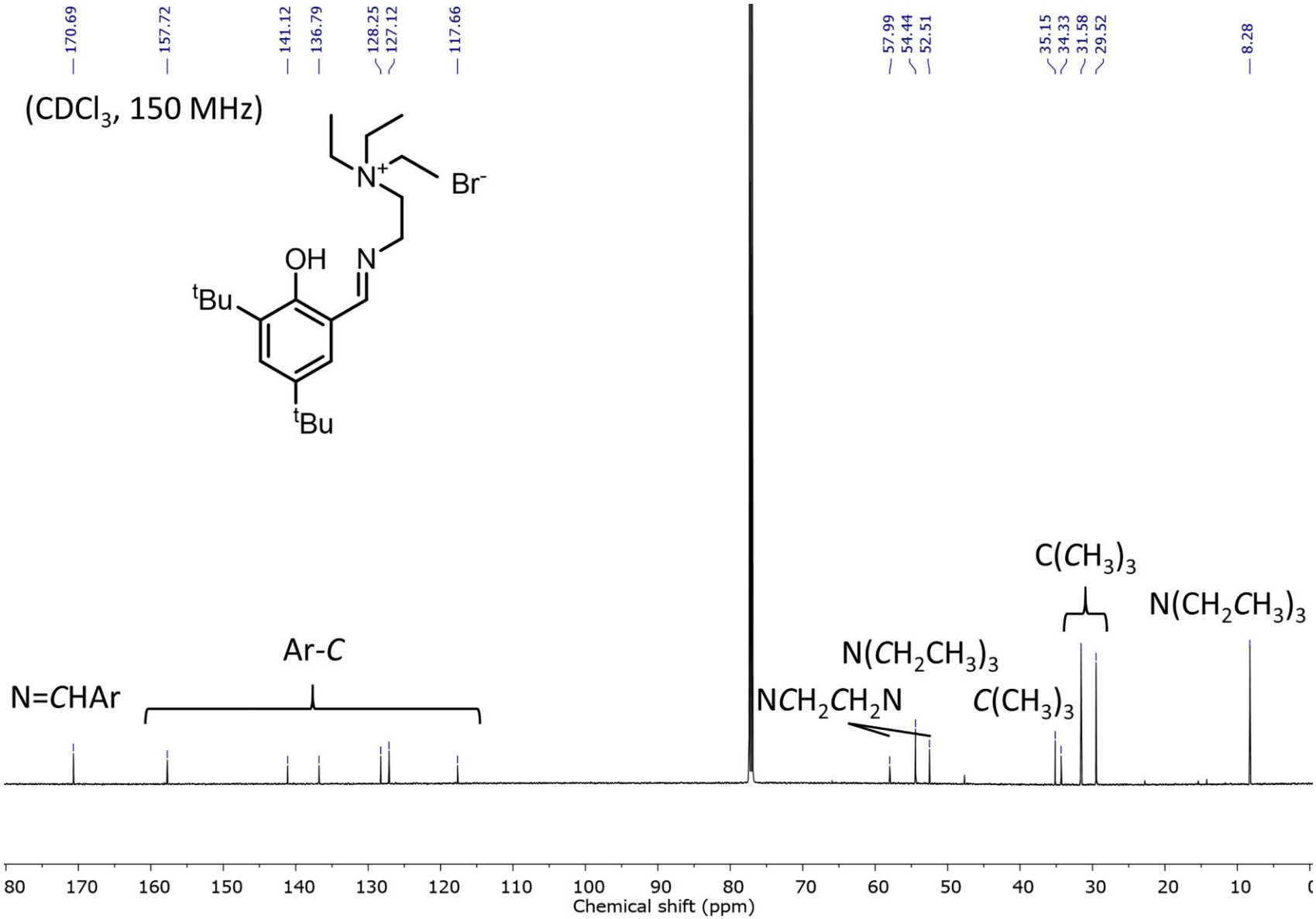


Figure. S8 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^1_{Et\text{-}Br}}$.

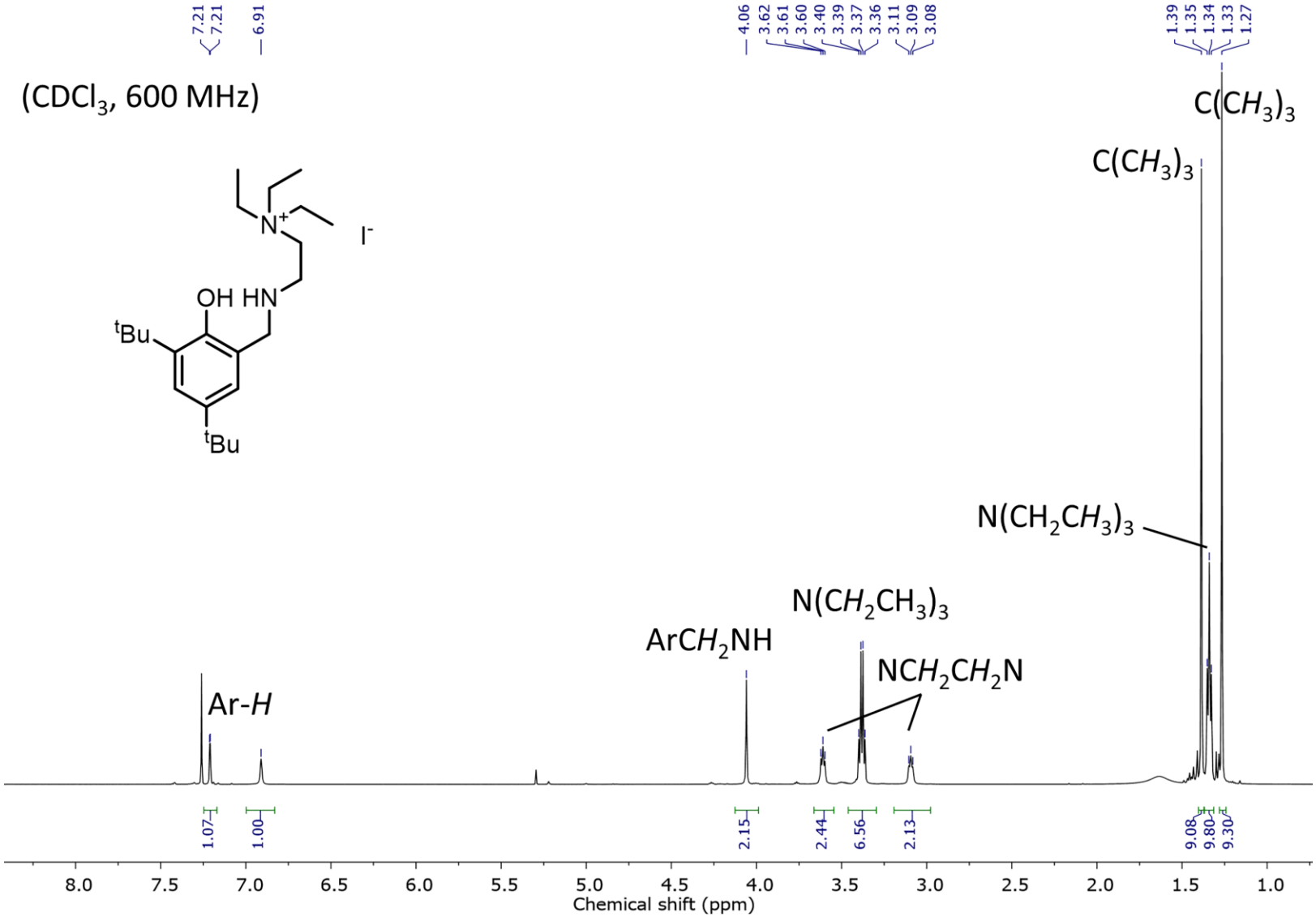


Figure. S9 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^2_{Et\text{-}I}}$.

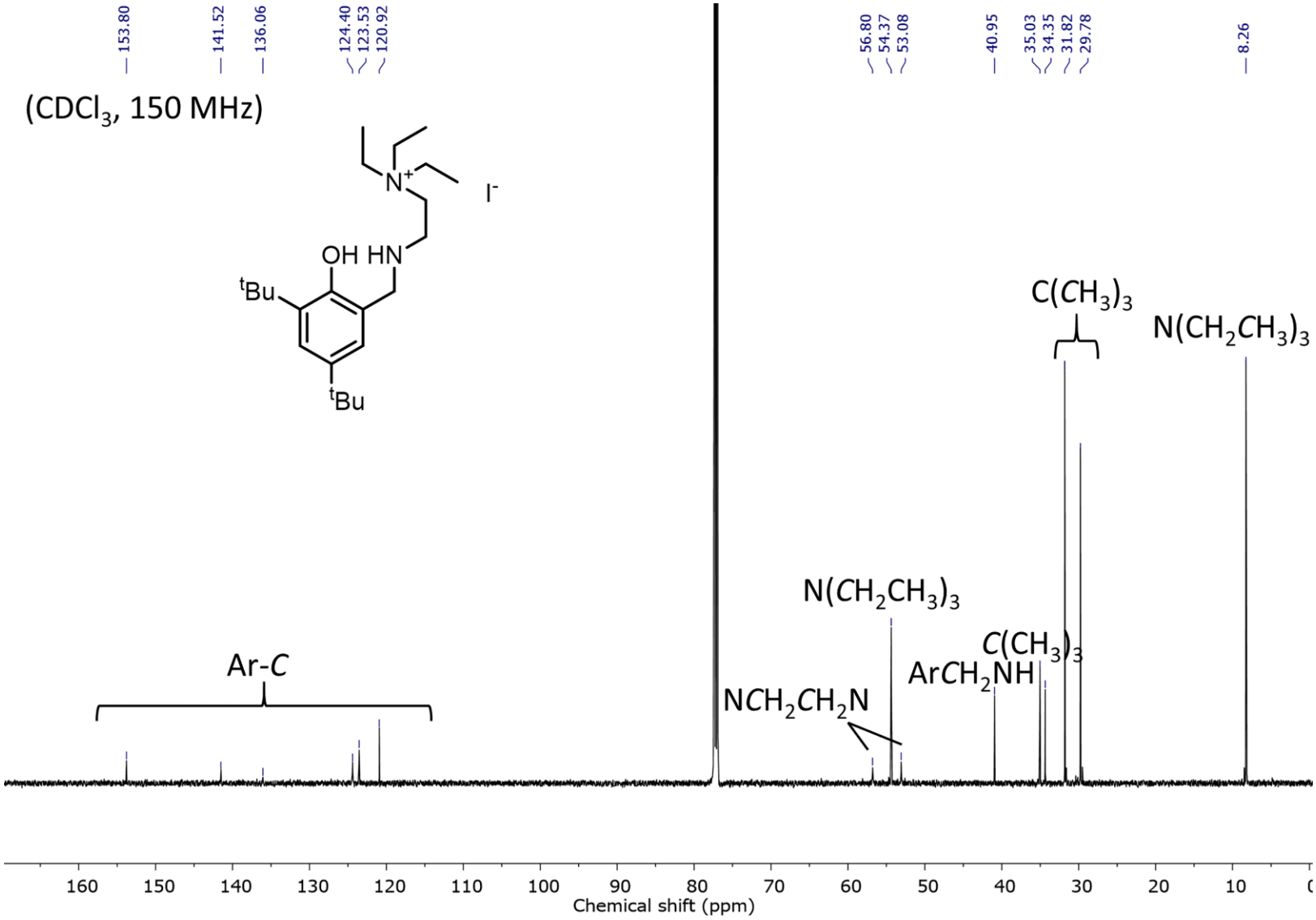


Figure. S10 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^2_{Et\text{-}I}}$.

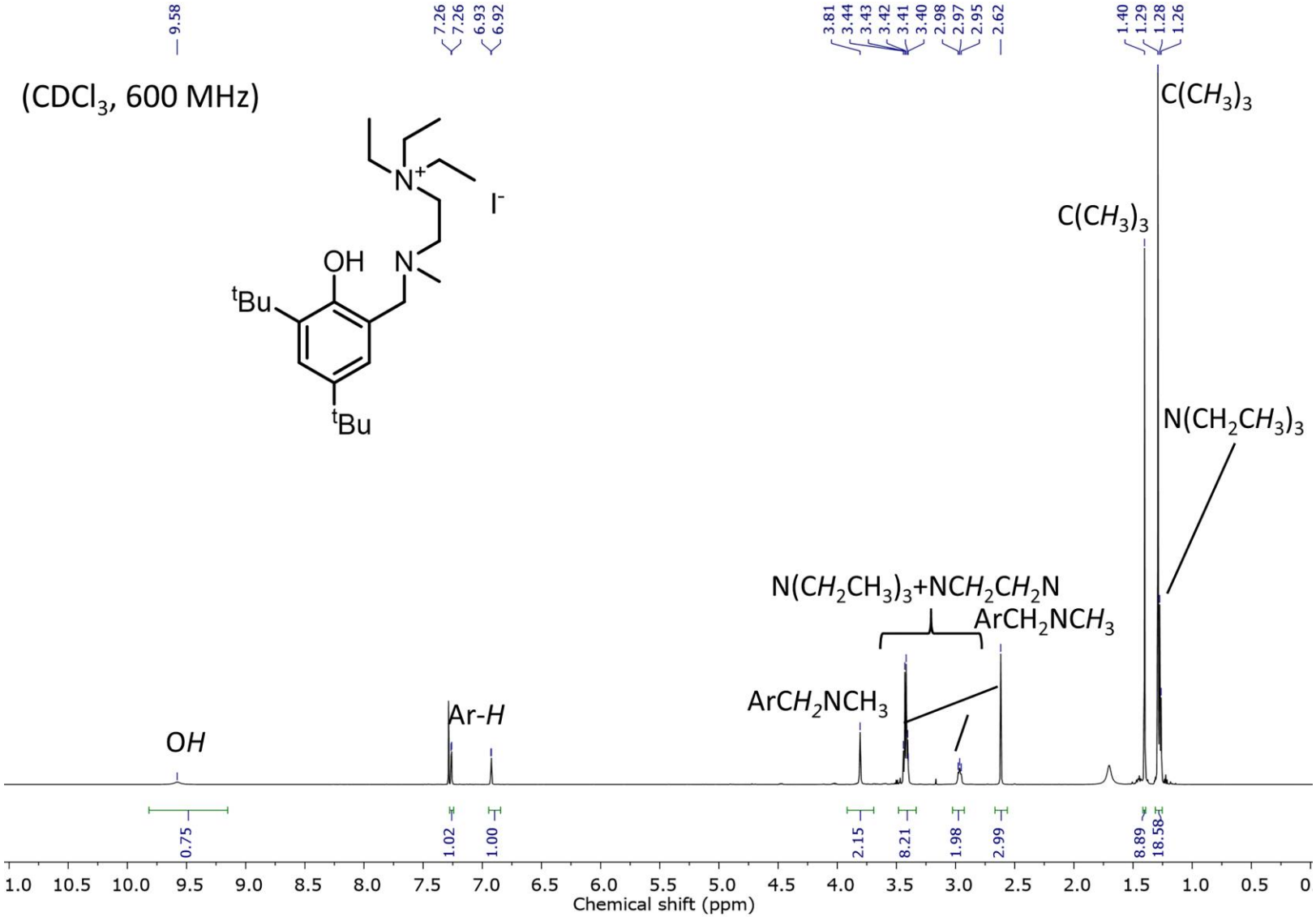


Figure. S11 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^3_{Et\text{-}I}}$.

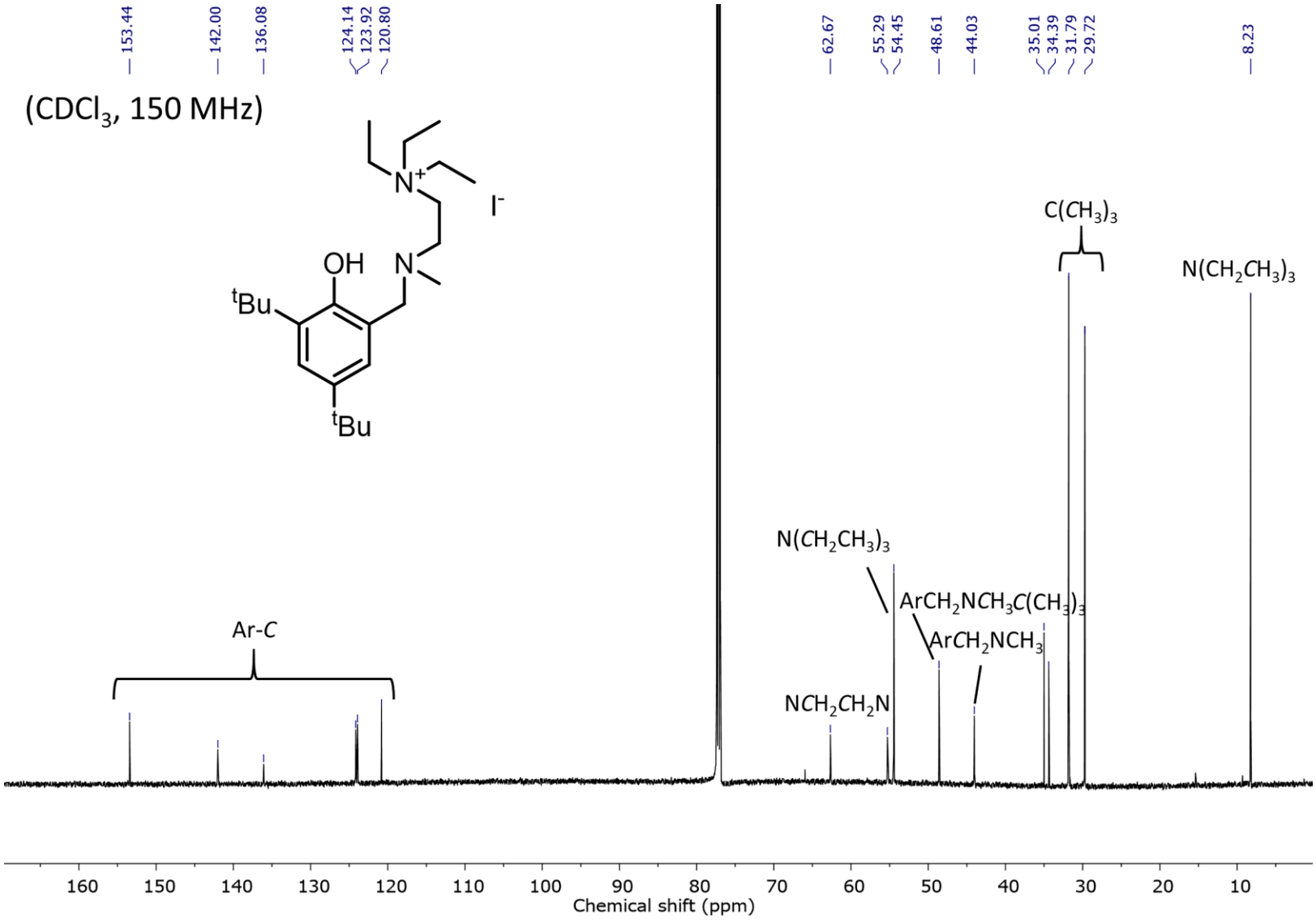


Figure. S12 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^3_{Et\text{-}I}}$.

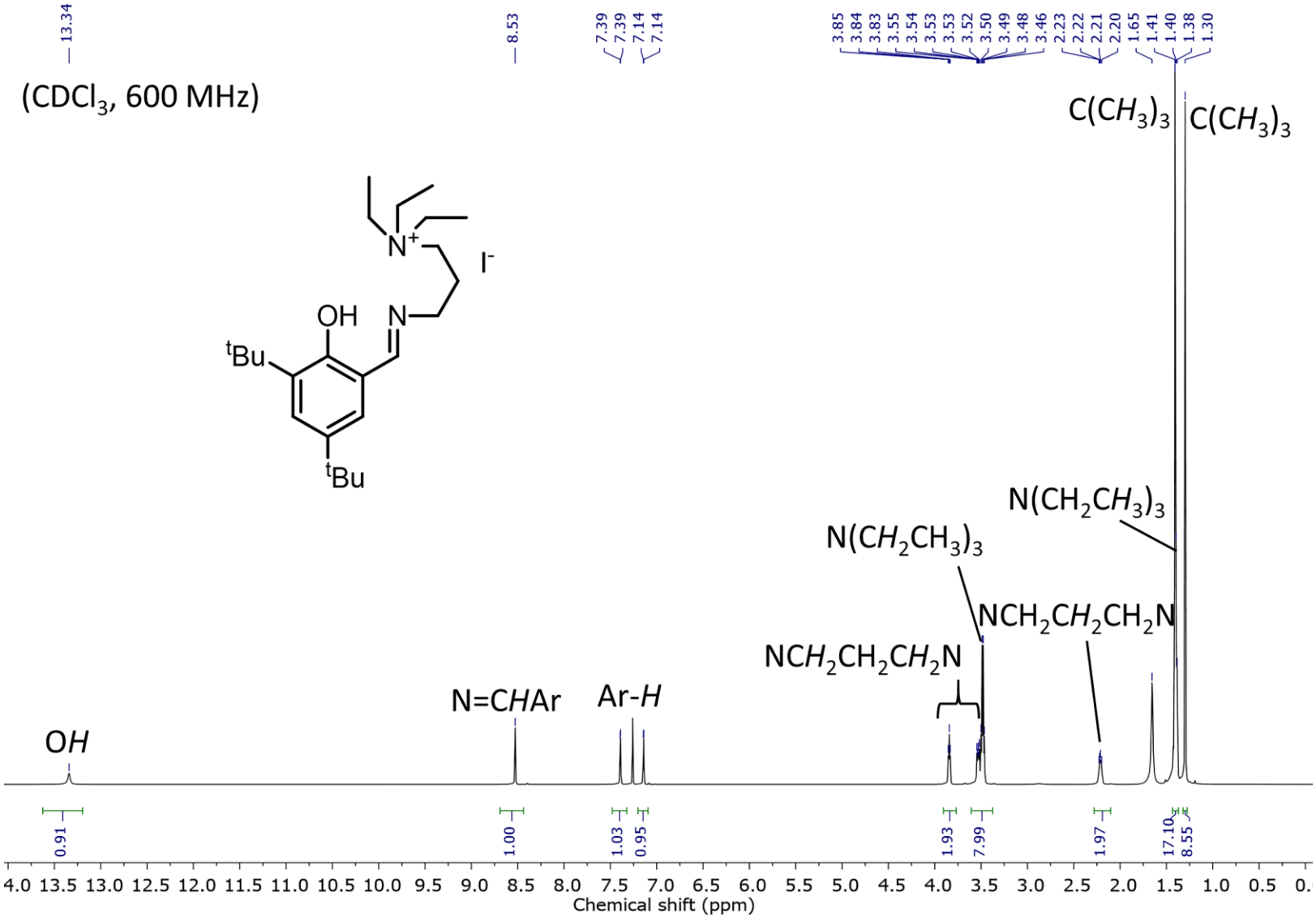


Figure. S13 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of ligand $\mathbf{HL^4_{Et\text{-}I}}$.

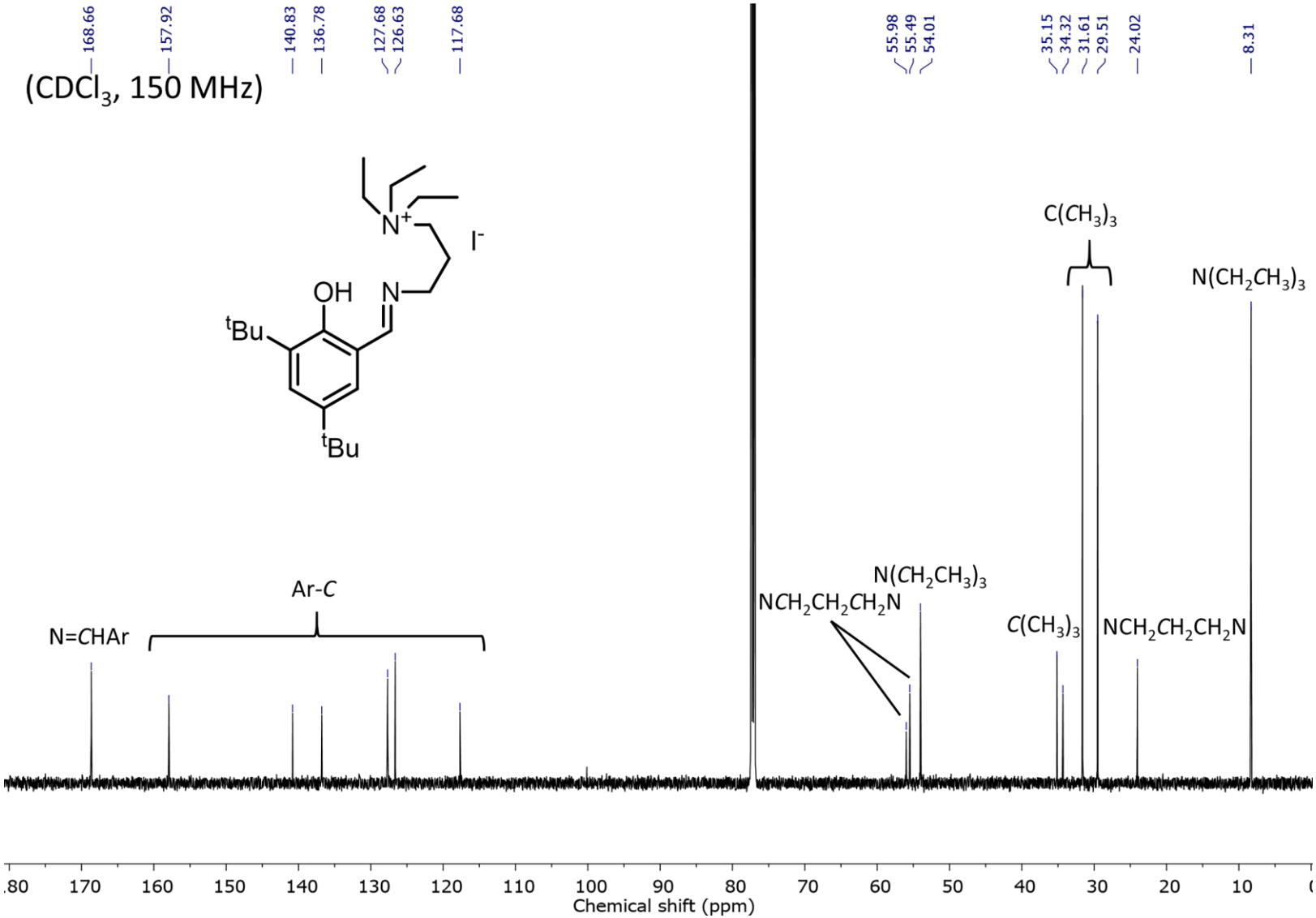


Figure. S14 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of ligand $\mathbf{HL^4_{Et\text{-}I}}$.

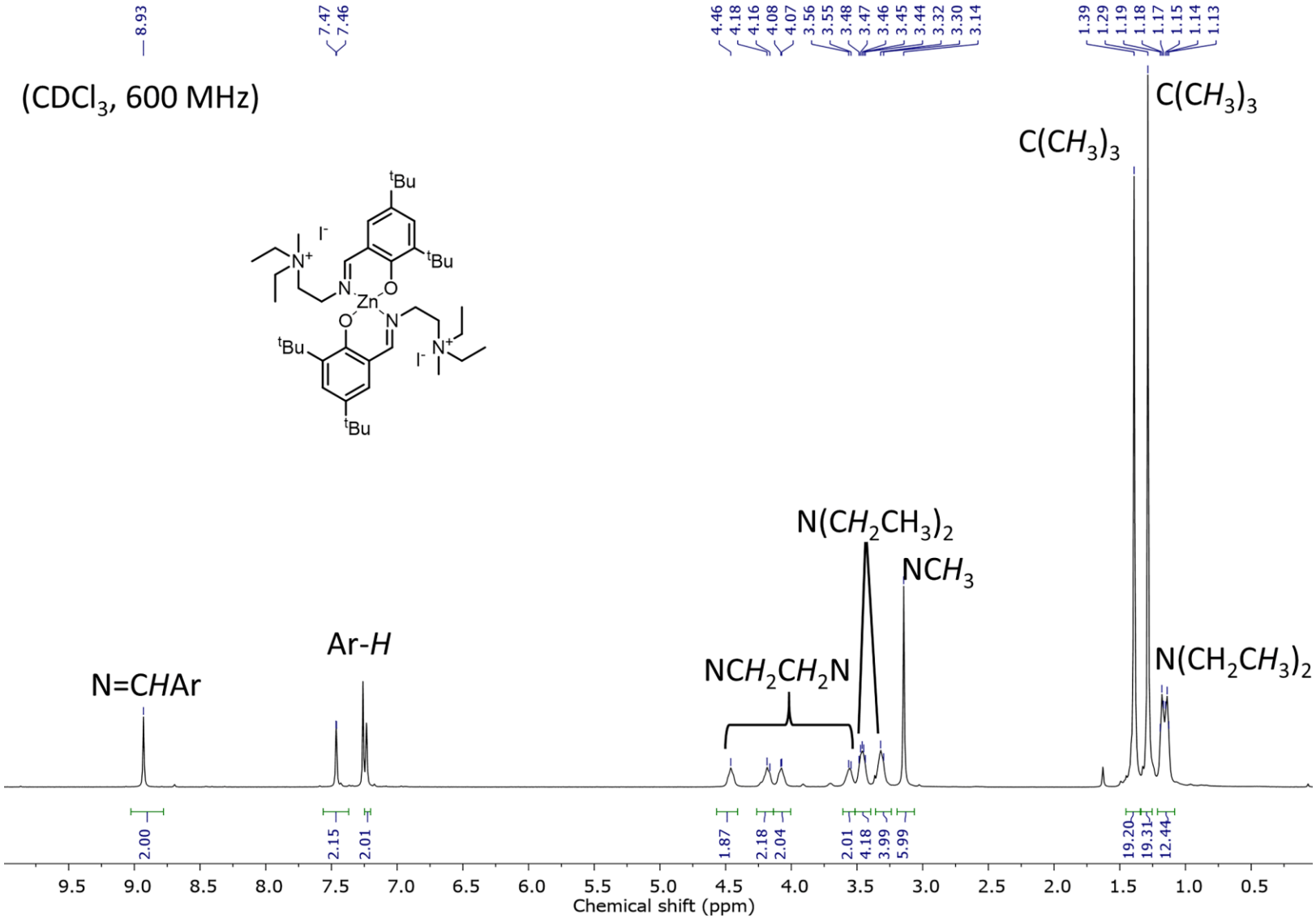


Figure. S15 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of complex **1Me-I**.

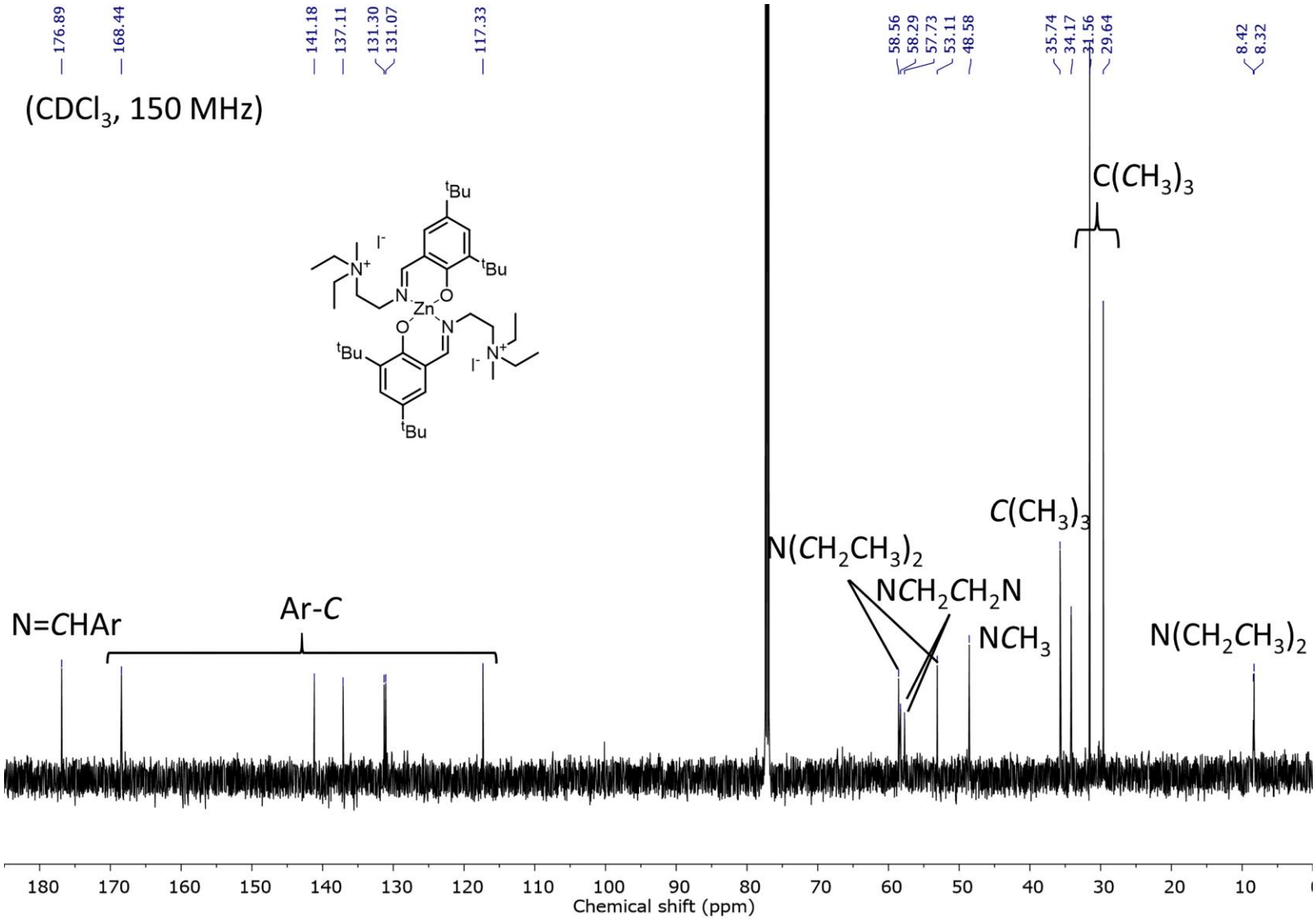


Figure. S16 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of complex **1Me-I.**

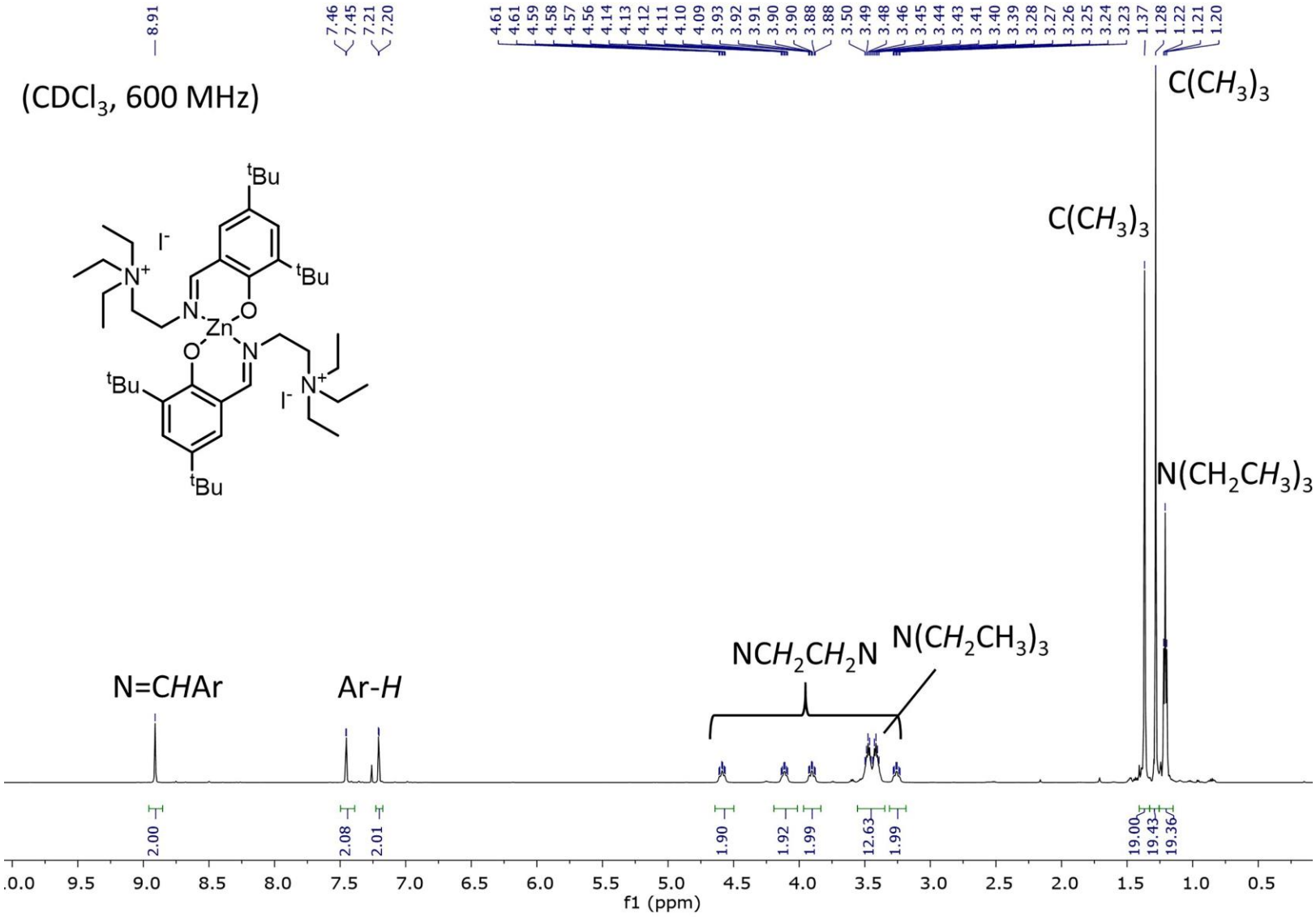


Figure. S17 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of complex **1Et-I**.

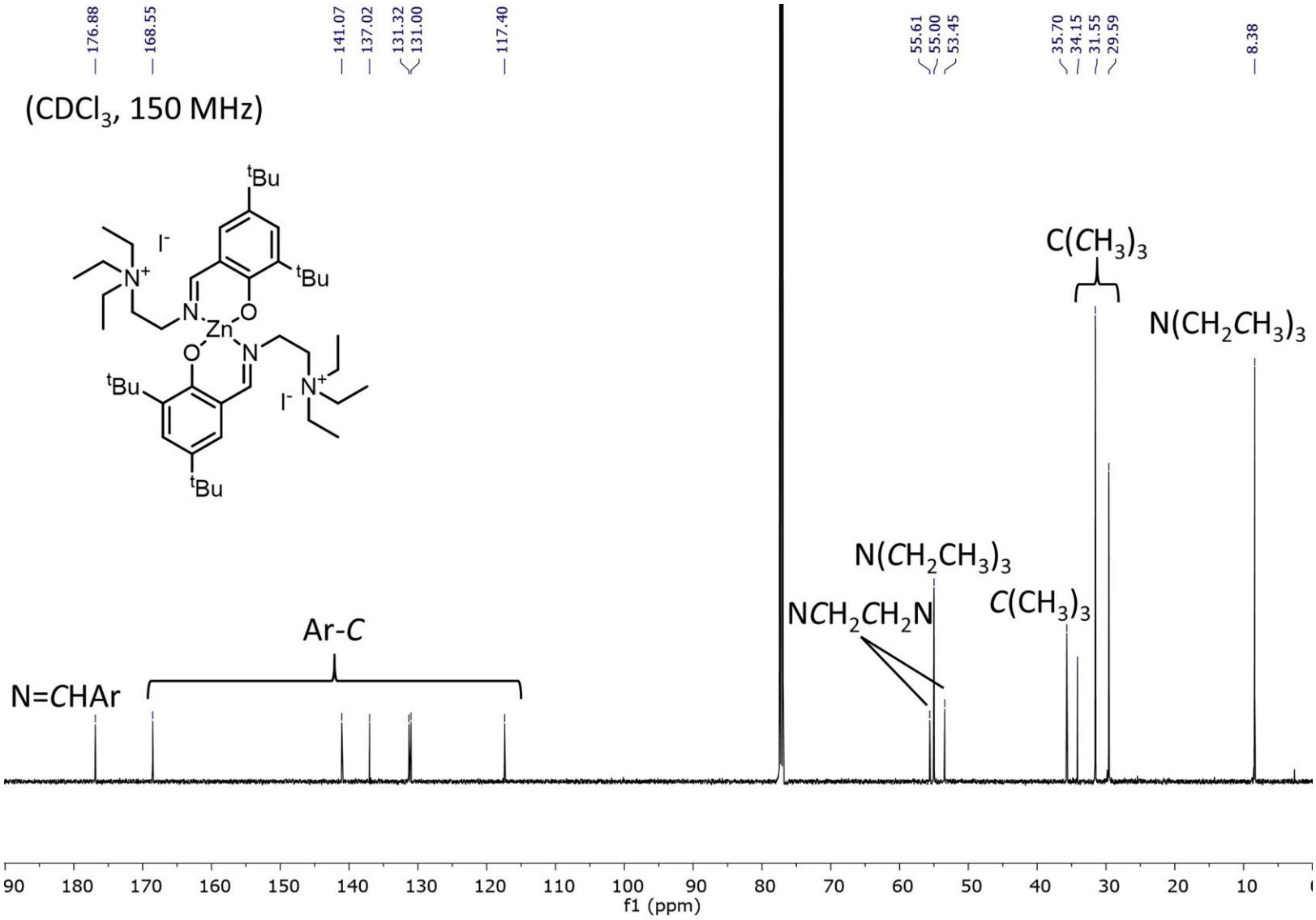


Figure. S18 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of complex **1Et-I**.

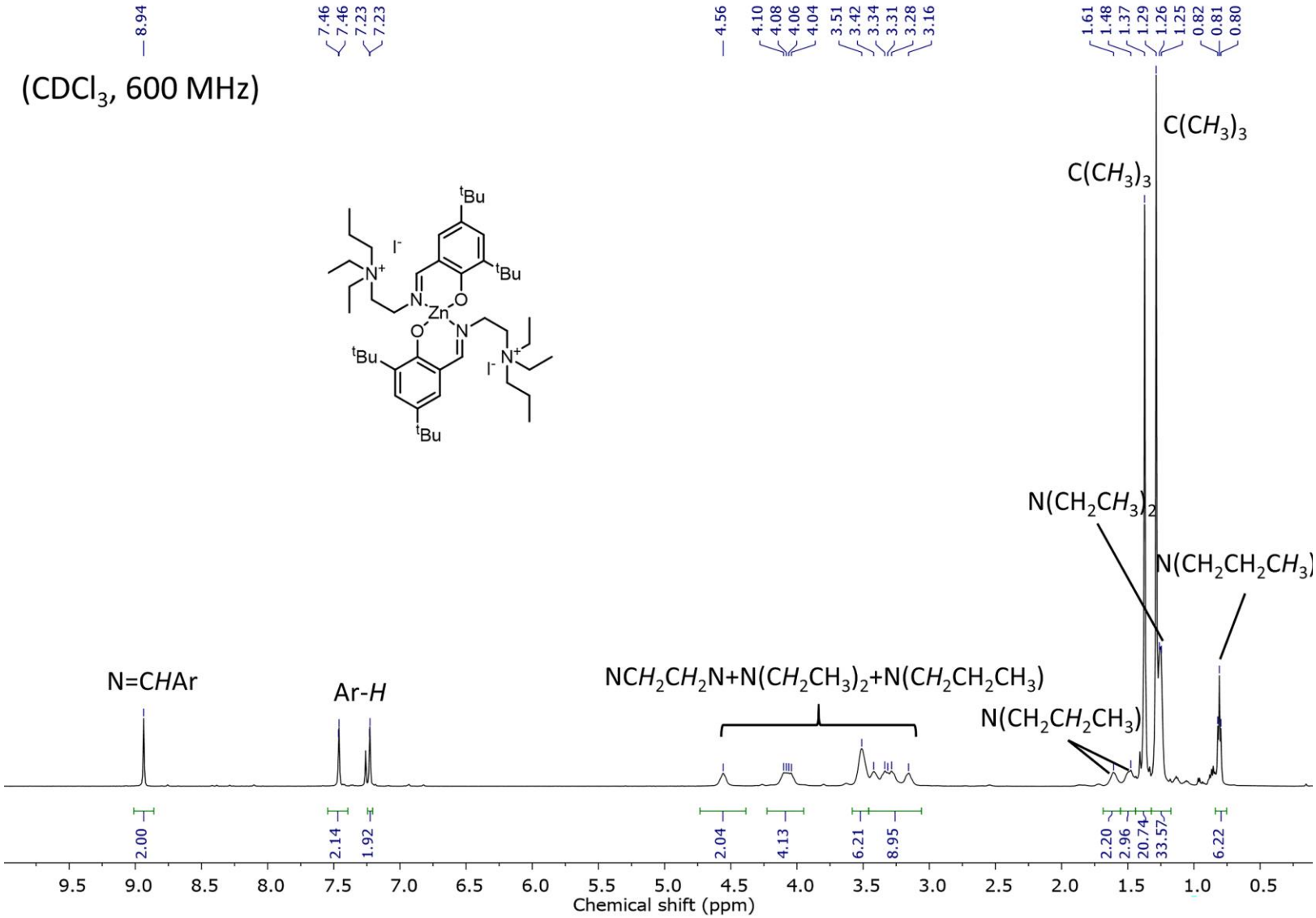


Figure. S19 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of complex **1Pr-I.**

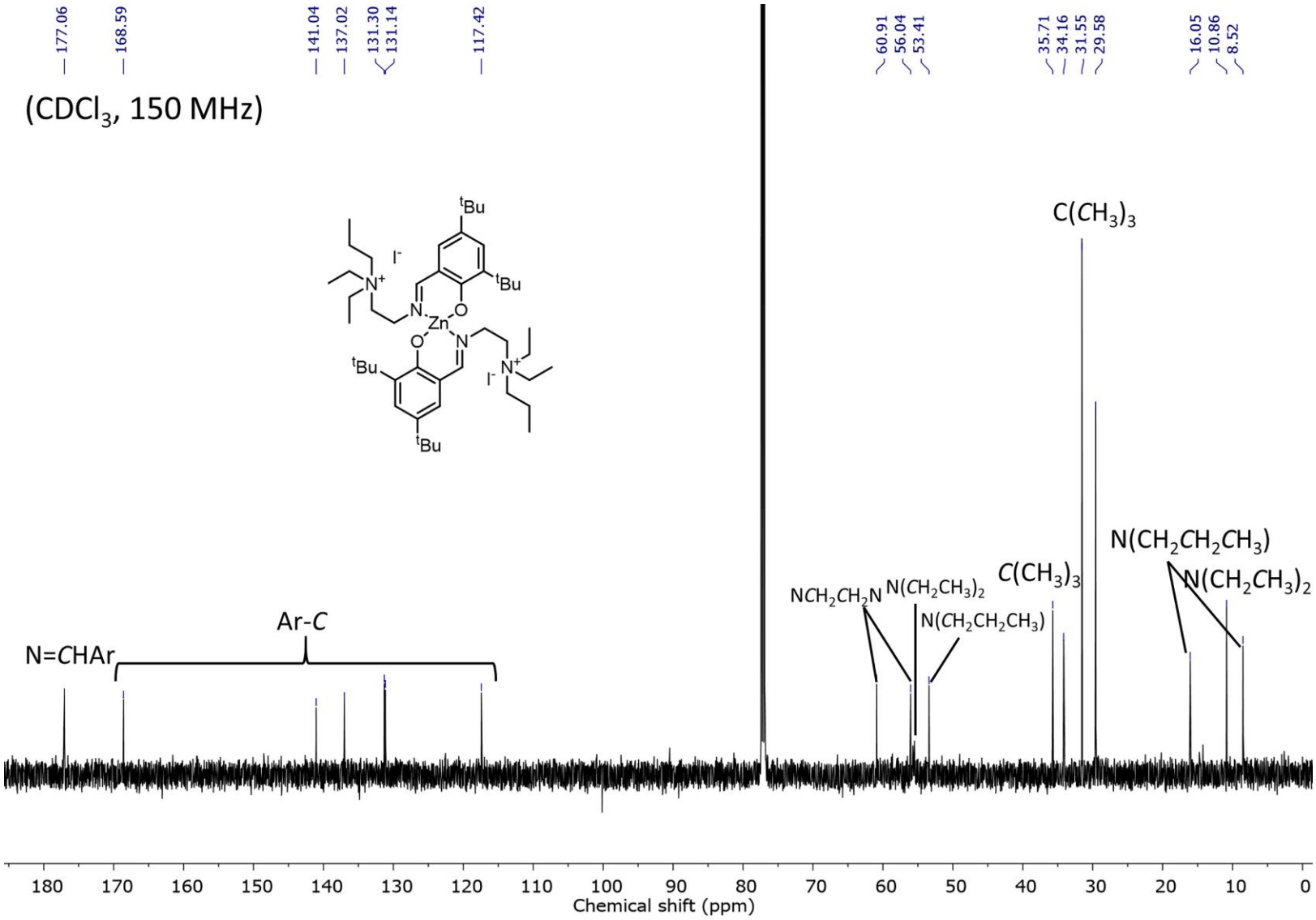


Figure. S20 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of complex **1Pr-I.**

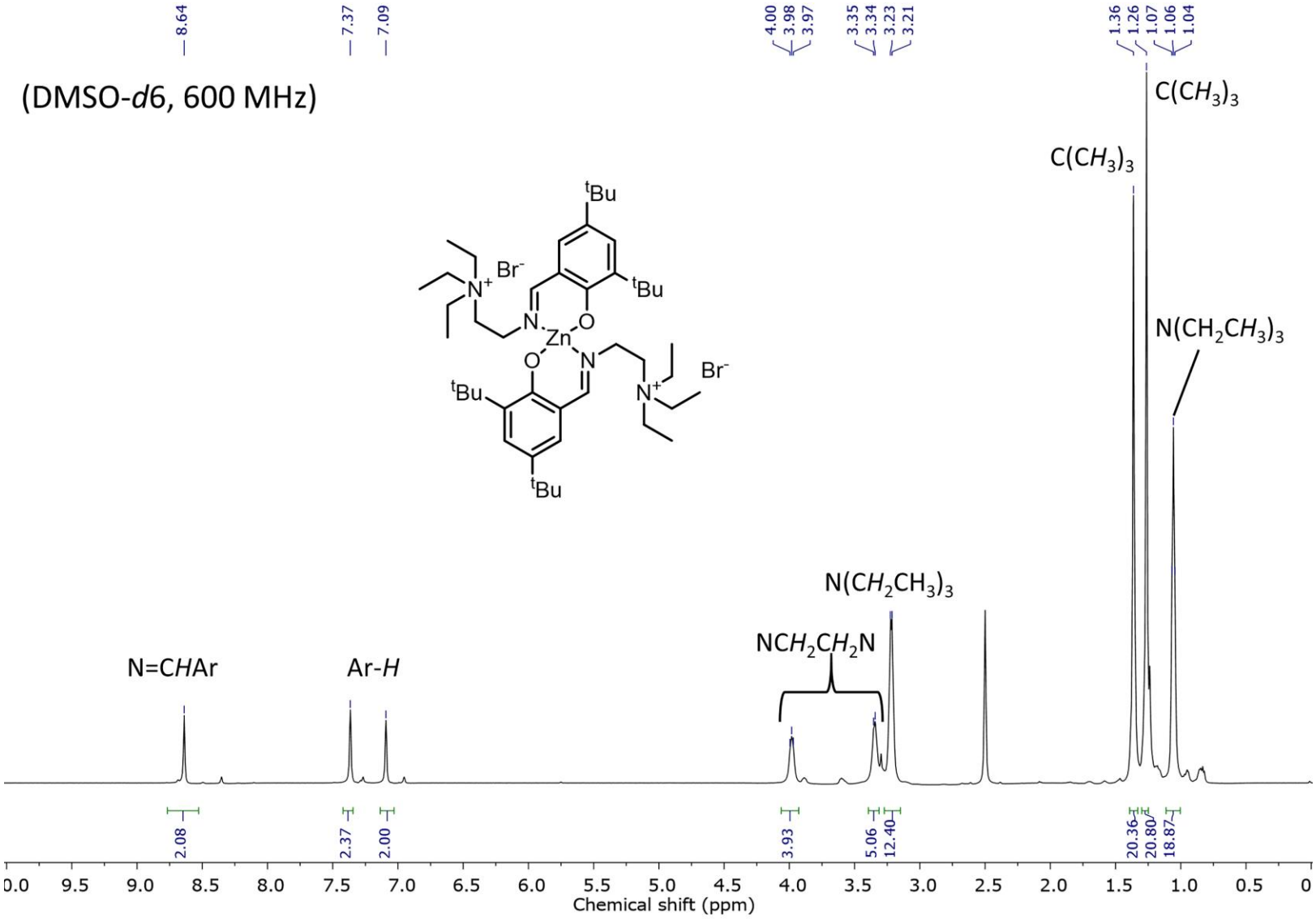


Figure. S21 ^{1}H NMR spectrum (DMSO-*d*6, 600 MHz, 30 °C) of complex **1Et-Br.**

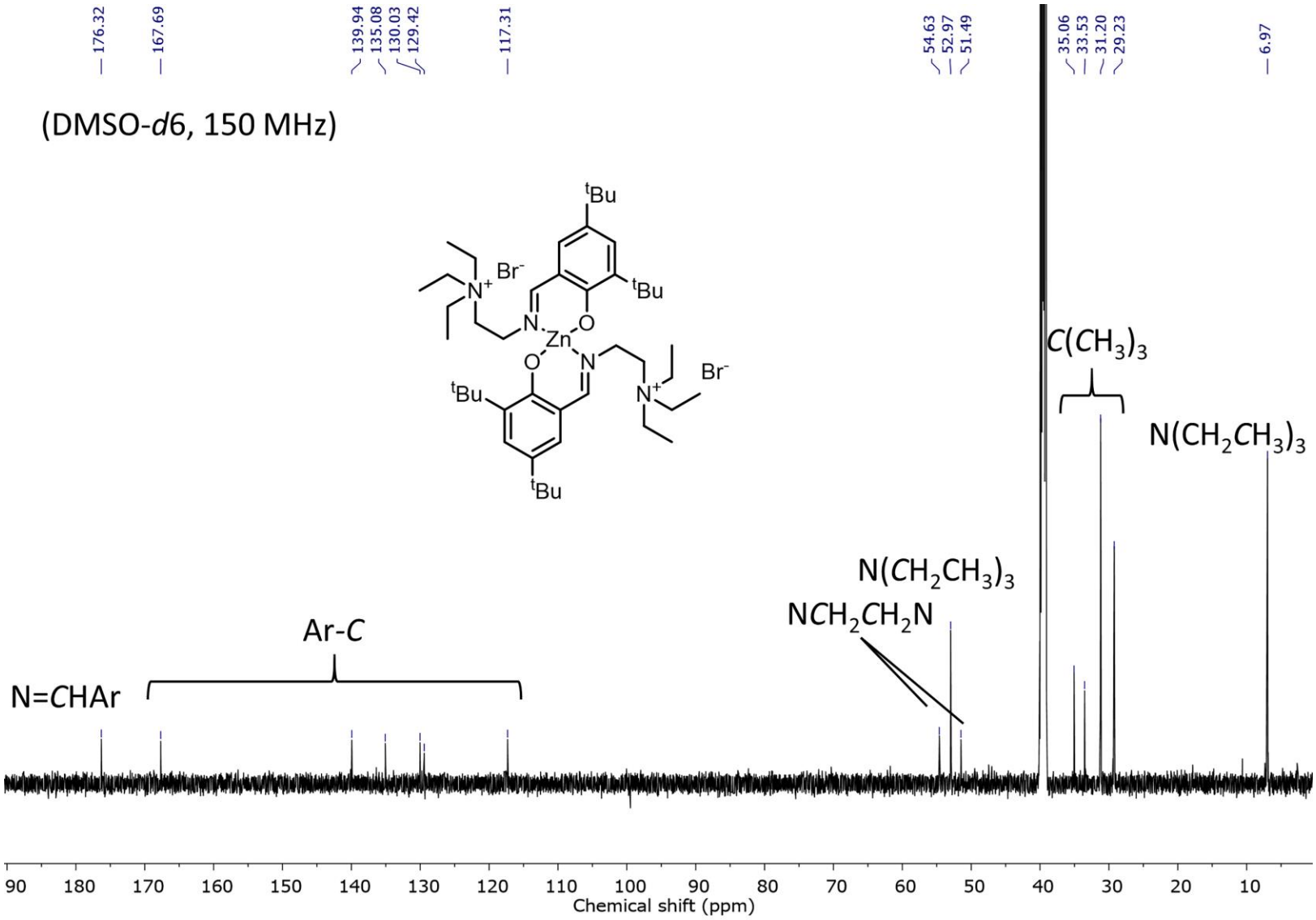


Figure. S22 ^{13}C NMR spectrum (DMSO-*d*6, 150 MHz, 30 °C) of complex **1Et-Br.**

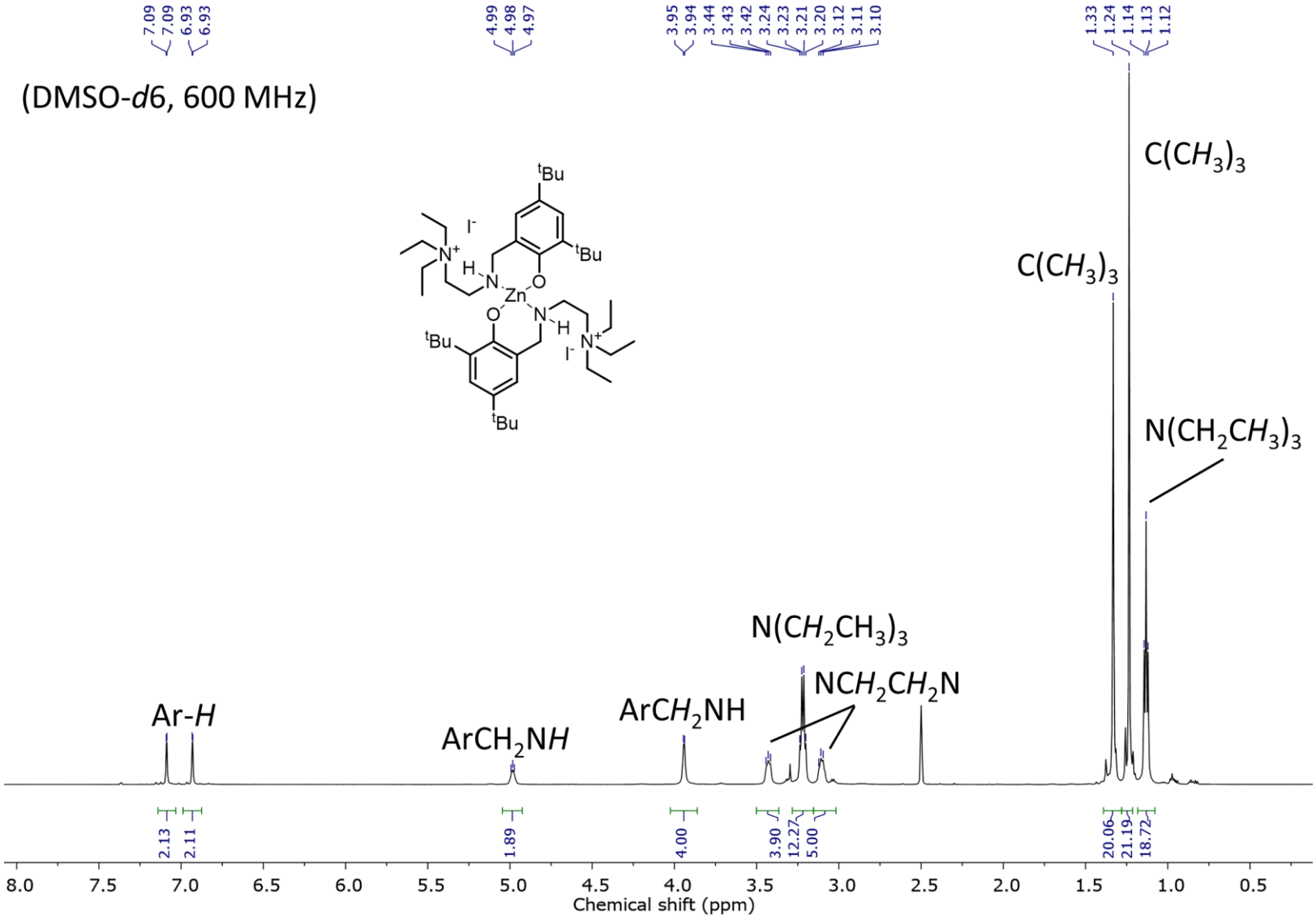


Figure. S23 ^{1}H NMR spectrum (DMSO-*d*6, 600 MHz, 30 °C) of complex **2.**

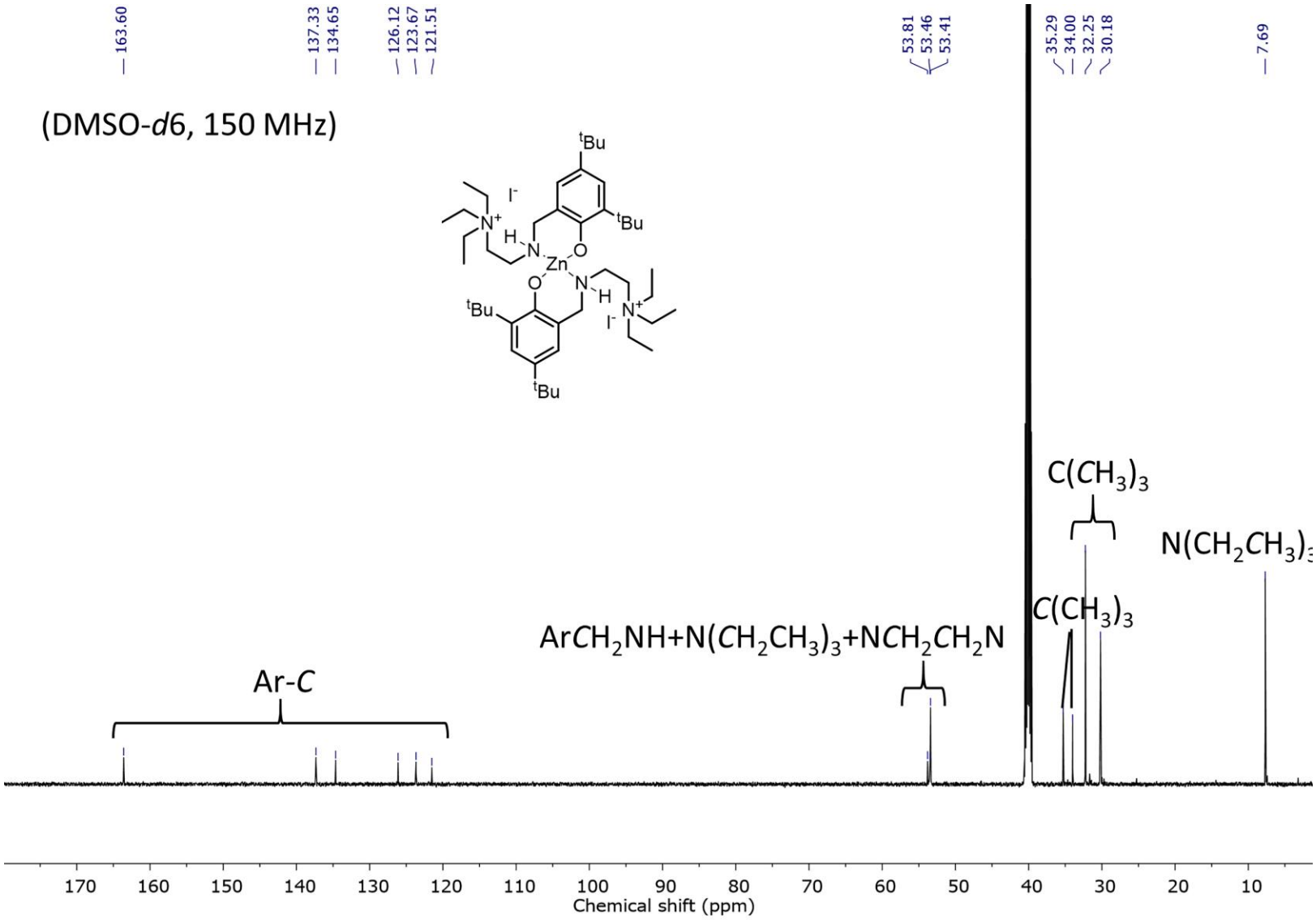


Figure. S24 ^{13}C NMR spectrum (DMSO-*d*6, 150 MHz, 30 °C) of complex **2.**

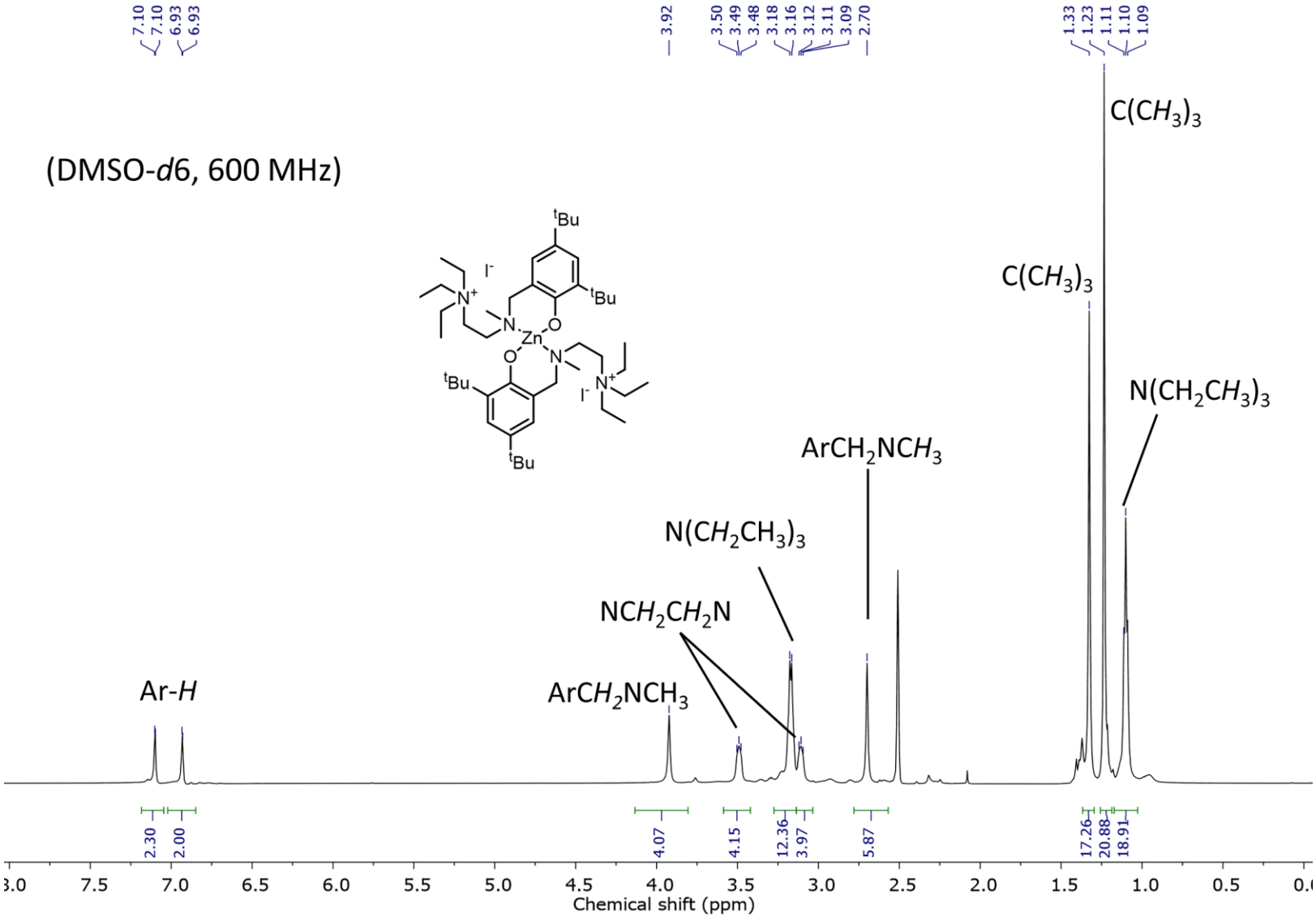


Figure. S25 ^{1}H NMR spectrum (DMSO-*d*6, 600 MHz, 30 °C) of complex **3.**

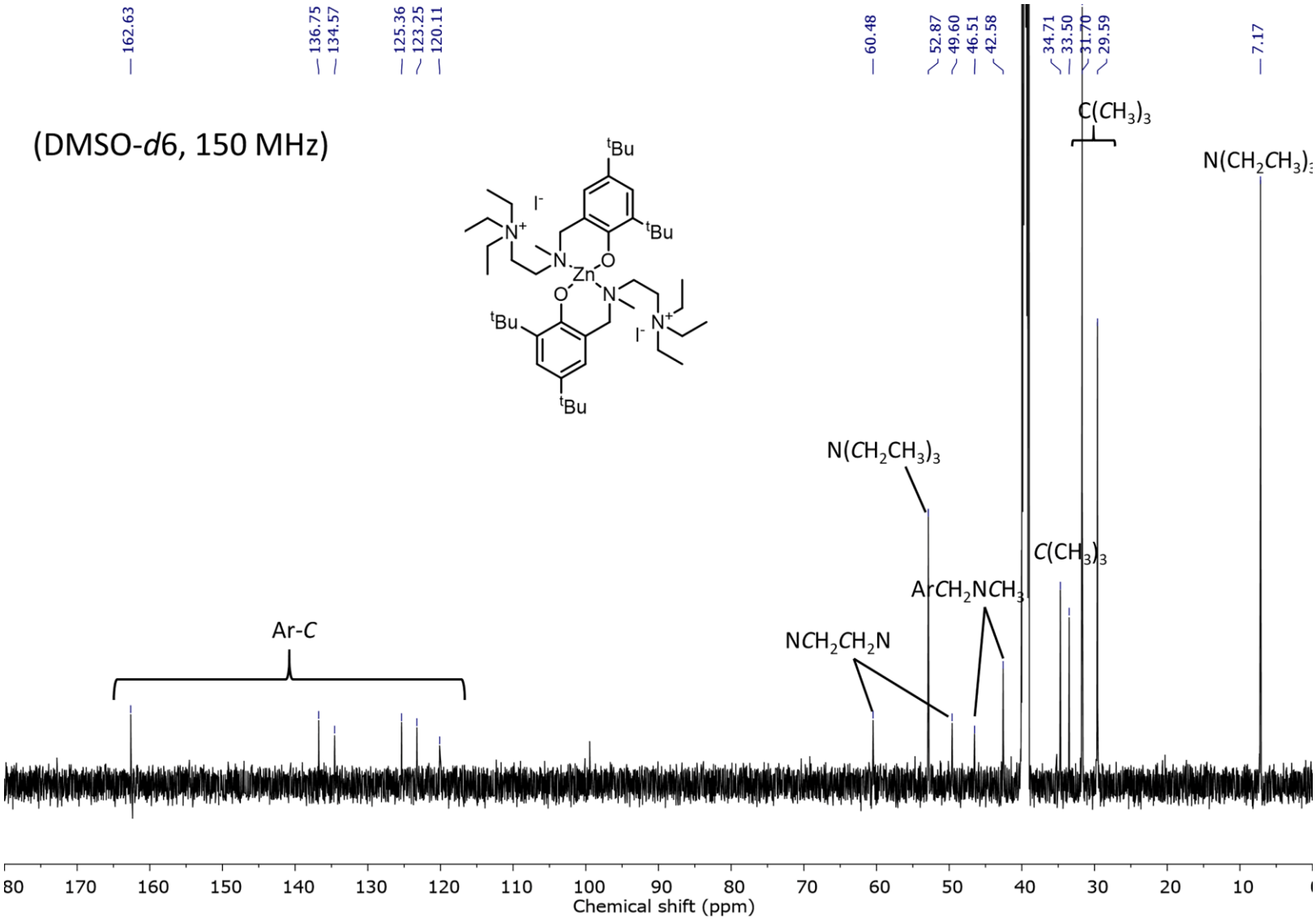


Figure. S26 ^{13}C NMR spectrum (DMSO-*d*6, 150 MHz, 30 °C) of complex **3.**

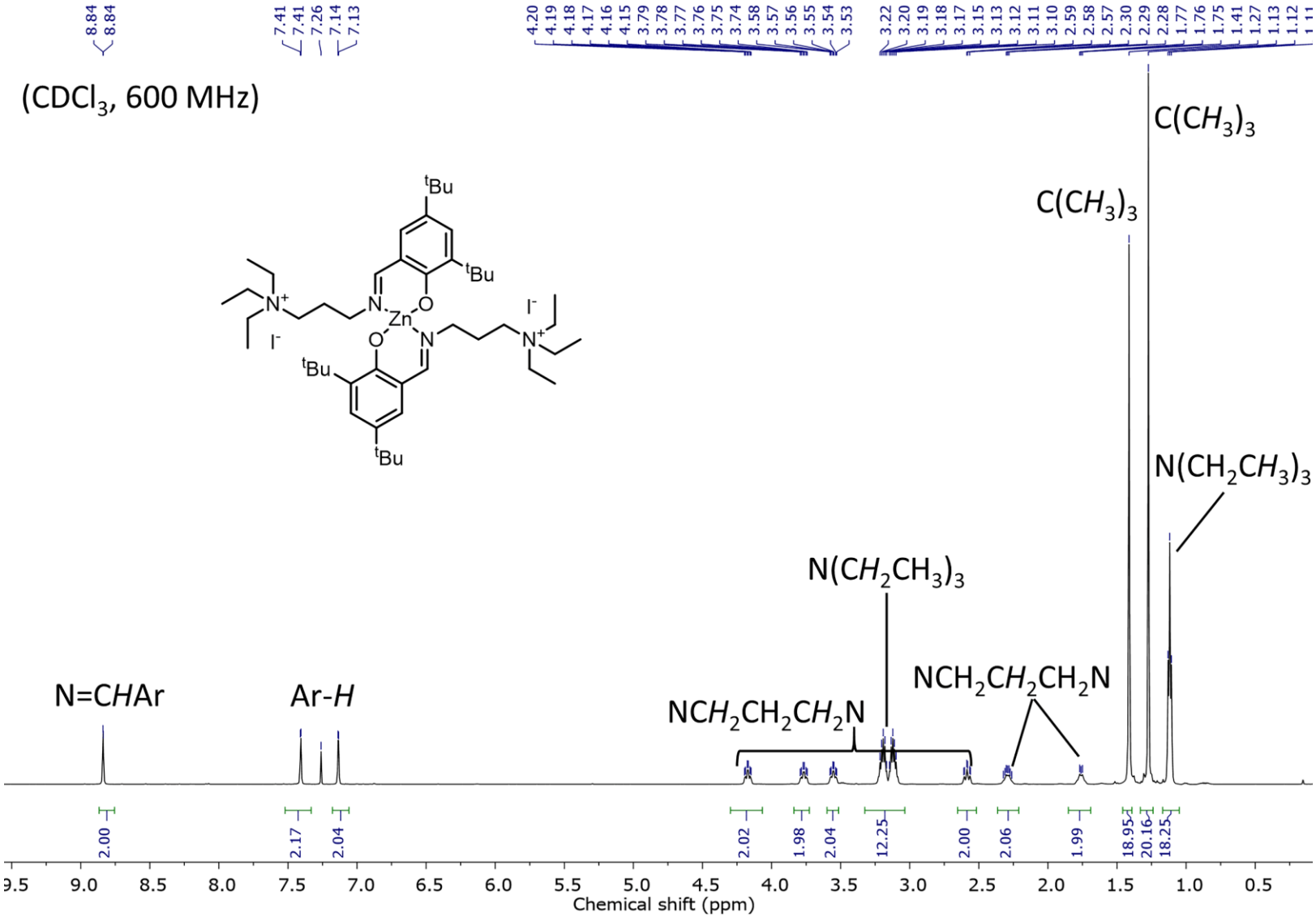


Figure. S27 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of complex **4.**

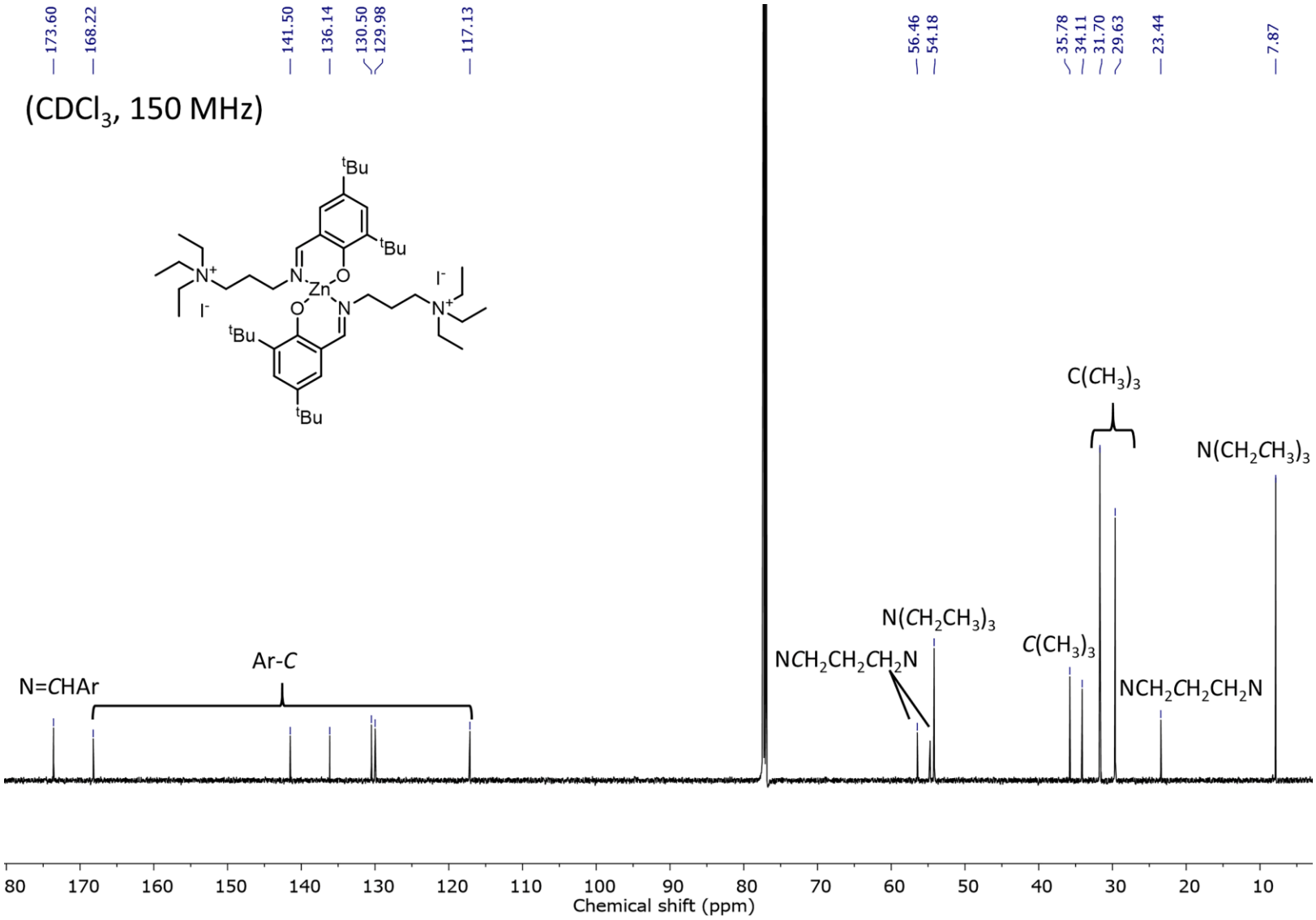


Figure. S28 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of complex **4.**

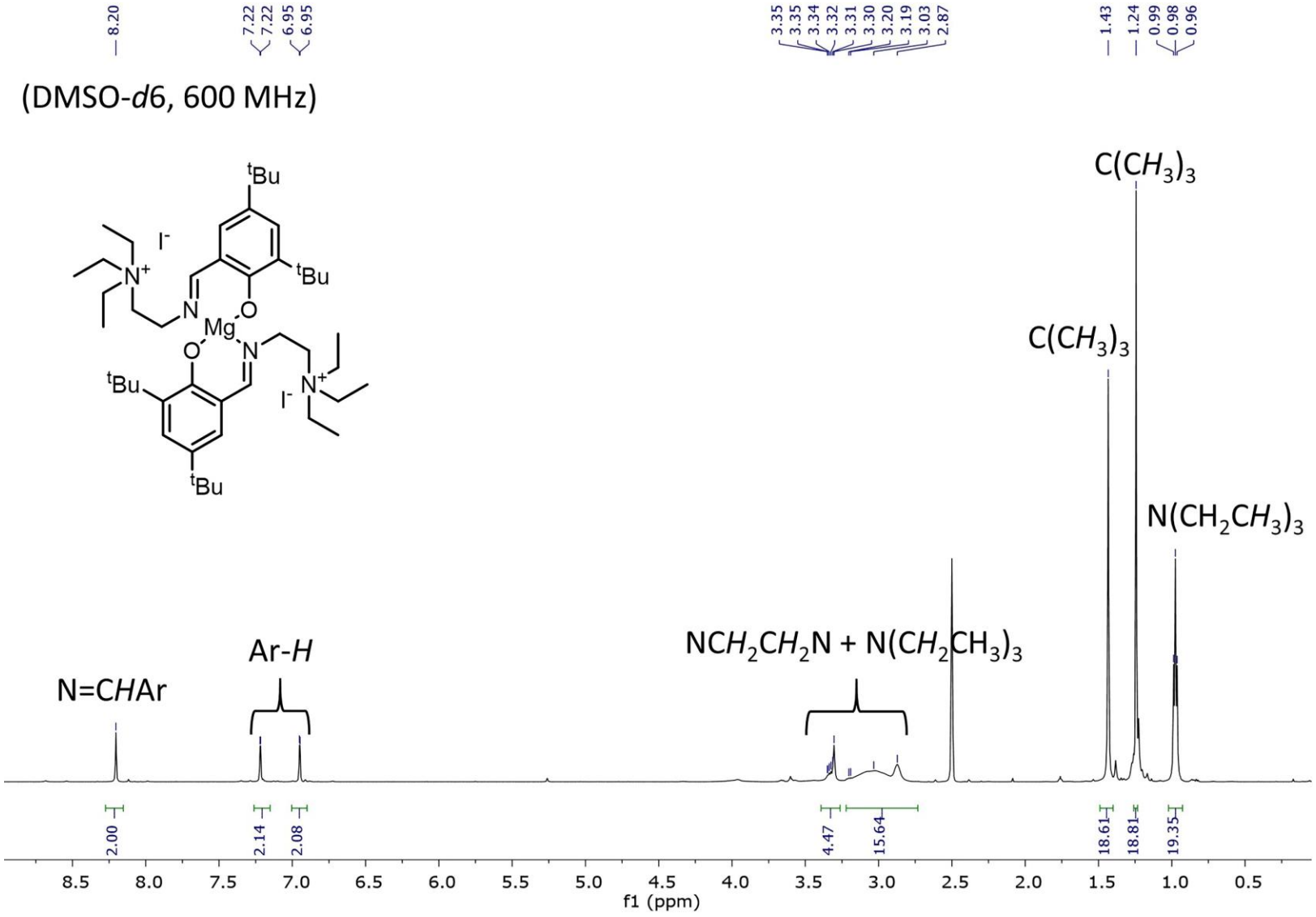


Figure. S29 ^{1}H NMR spectrum (DMSO-*d*6, 600 MHz, 30 °C) of complex **5**.

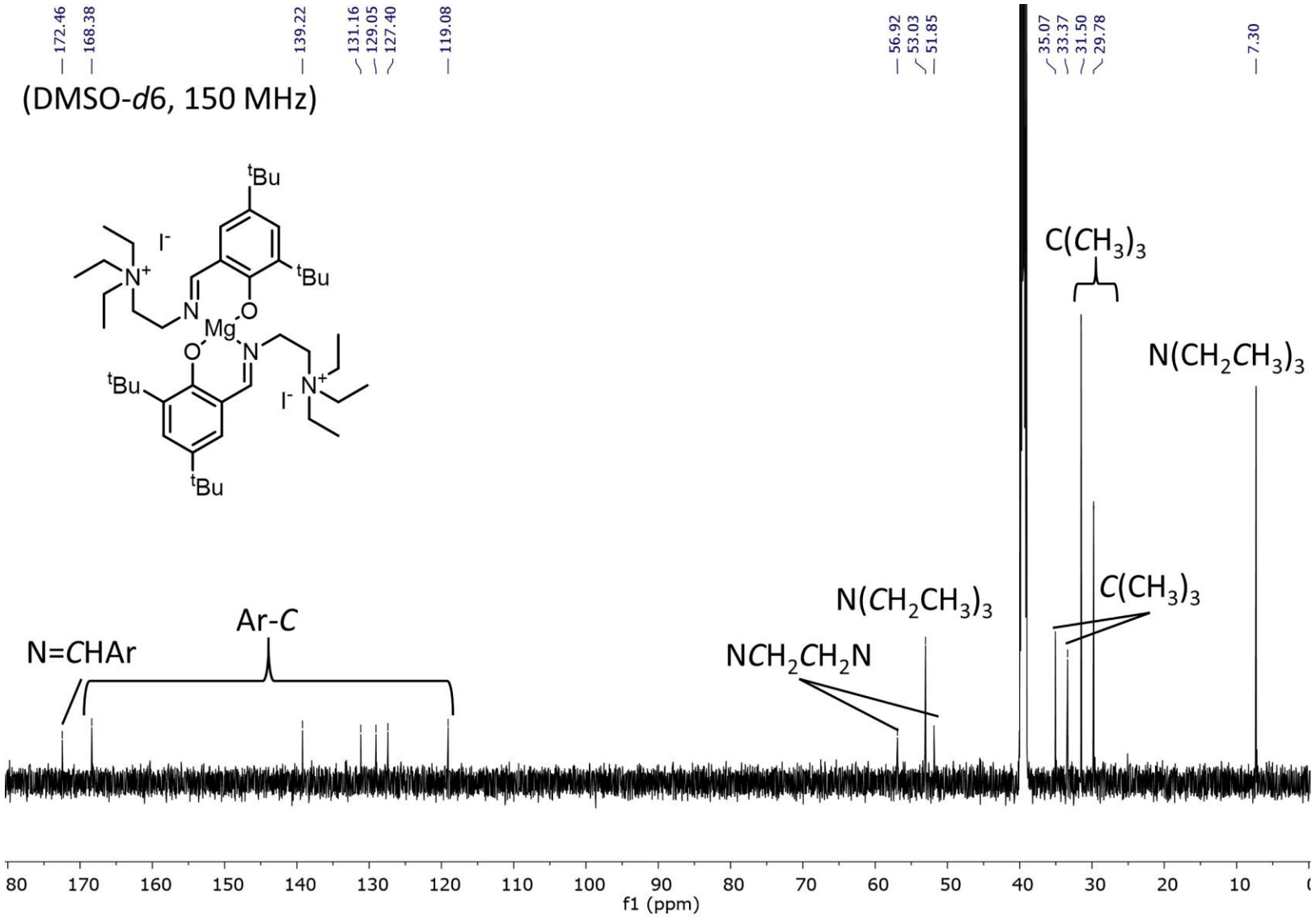


Figure. S30 ^{13}C NMR spectrum (DMSO-*d*6, 150 MHz, 30 °C) of complex **5**.

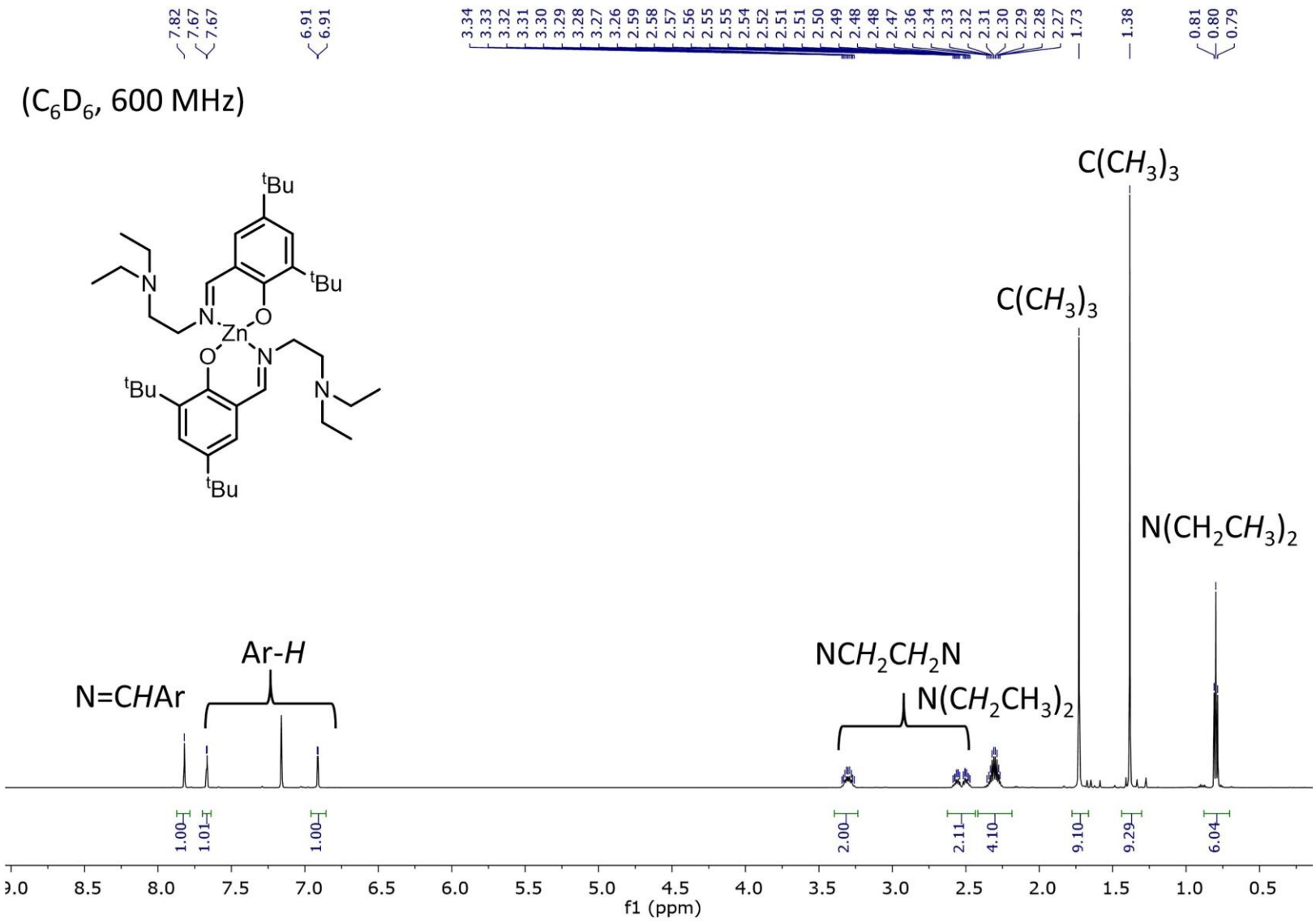


Figure. S31 ^{1}H NMR spectrum (C_6D_6, 600 MHz, 30 °C) of complex **7**.

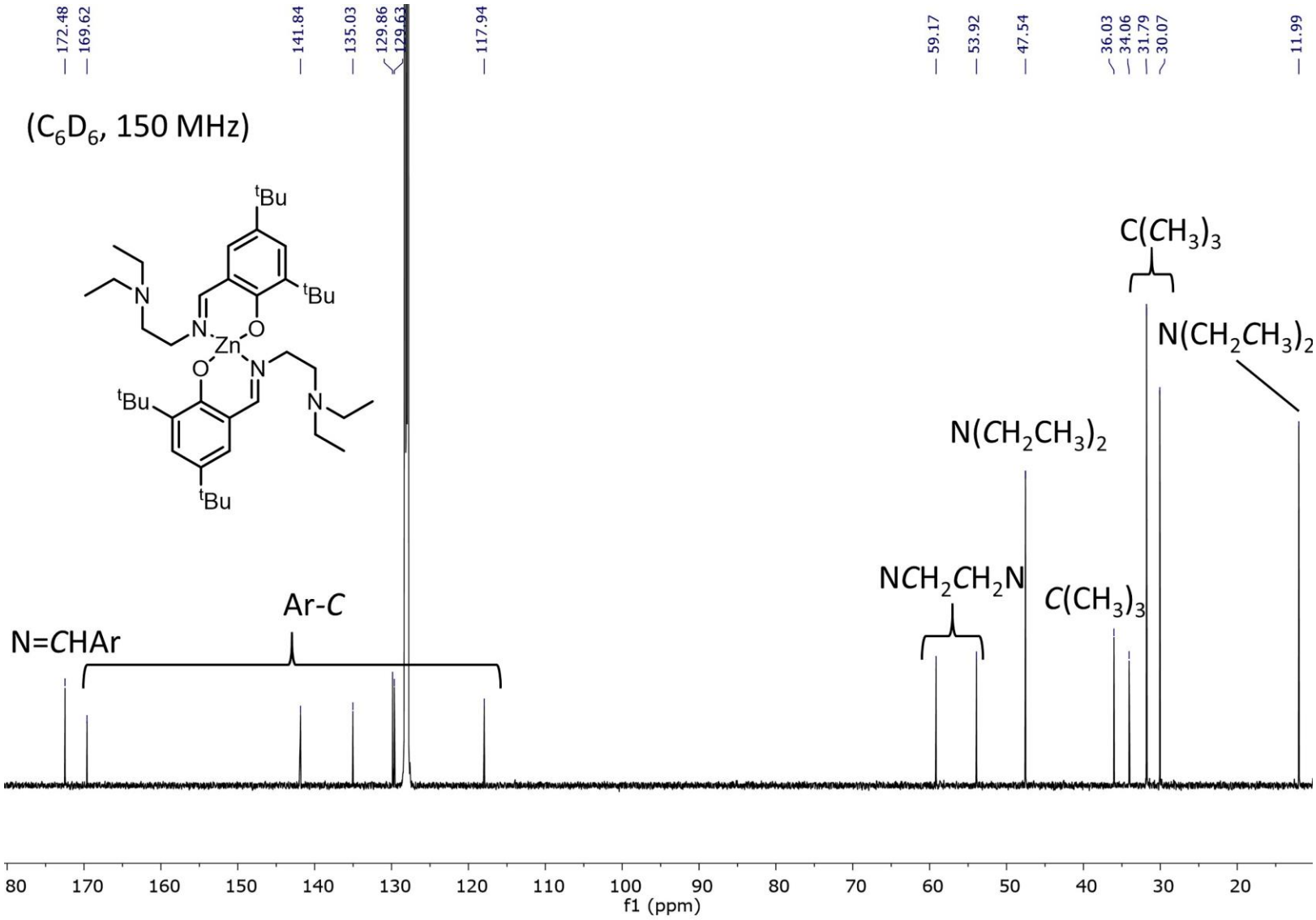


Figure. S32 ^{13}C NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of complex **7**.

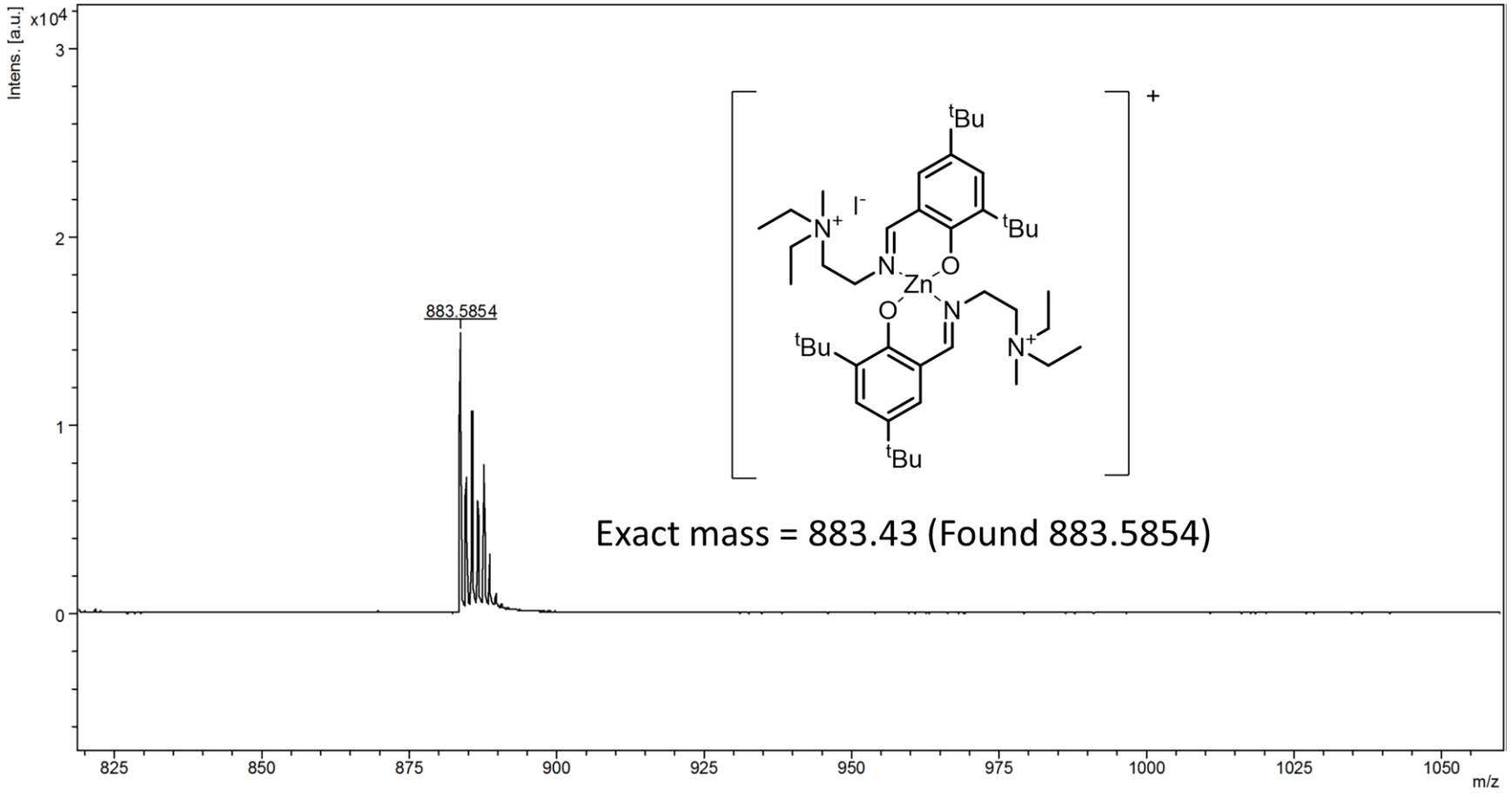


Figure. S33 MALDI-TOF mass spectrum of complex **1Me-I**.

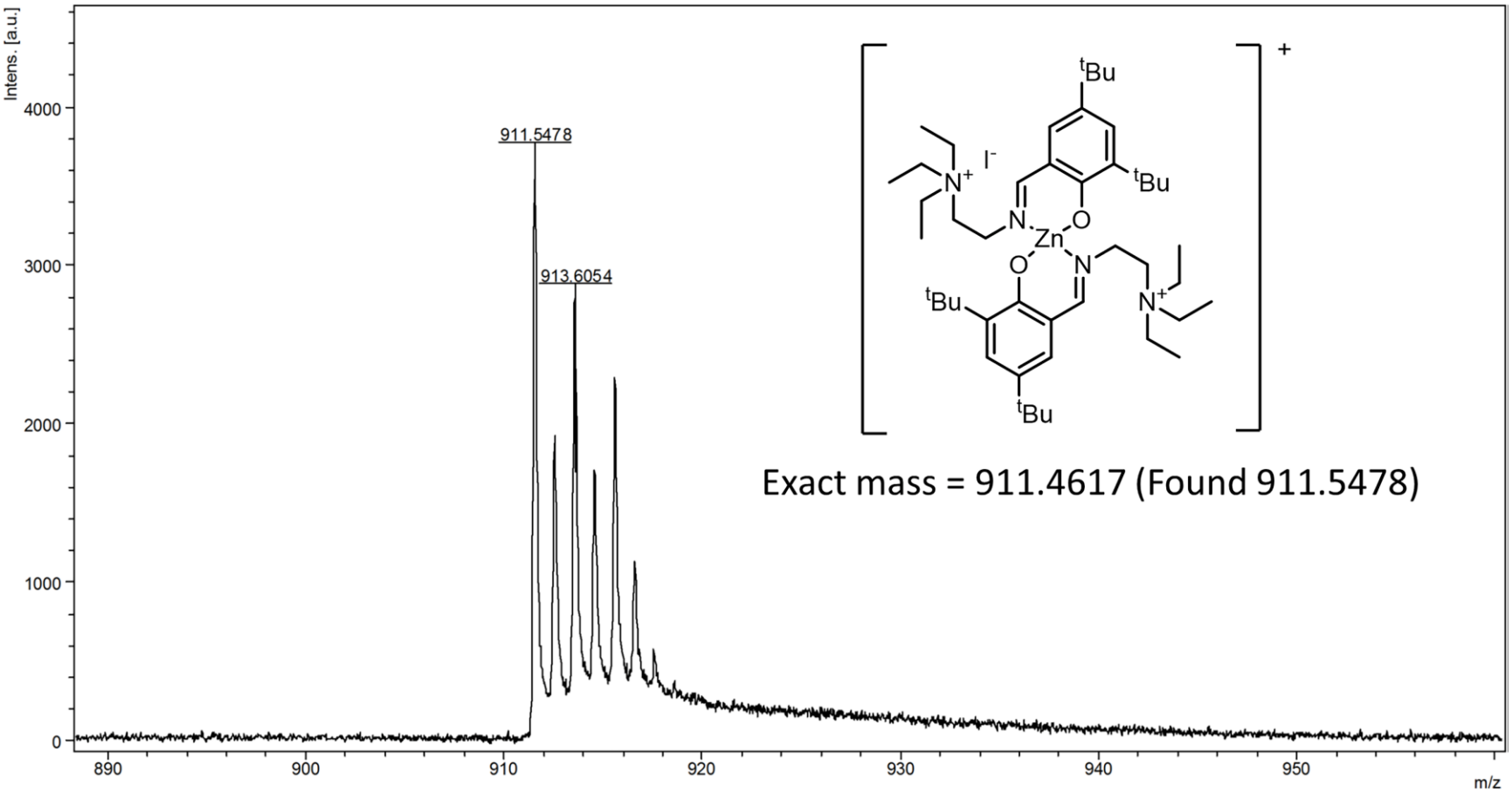


Figure. S34 MALDI-TOF mass spectrum of complex **1Et-I**.

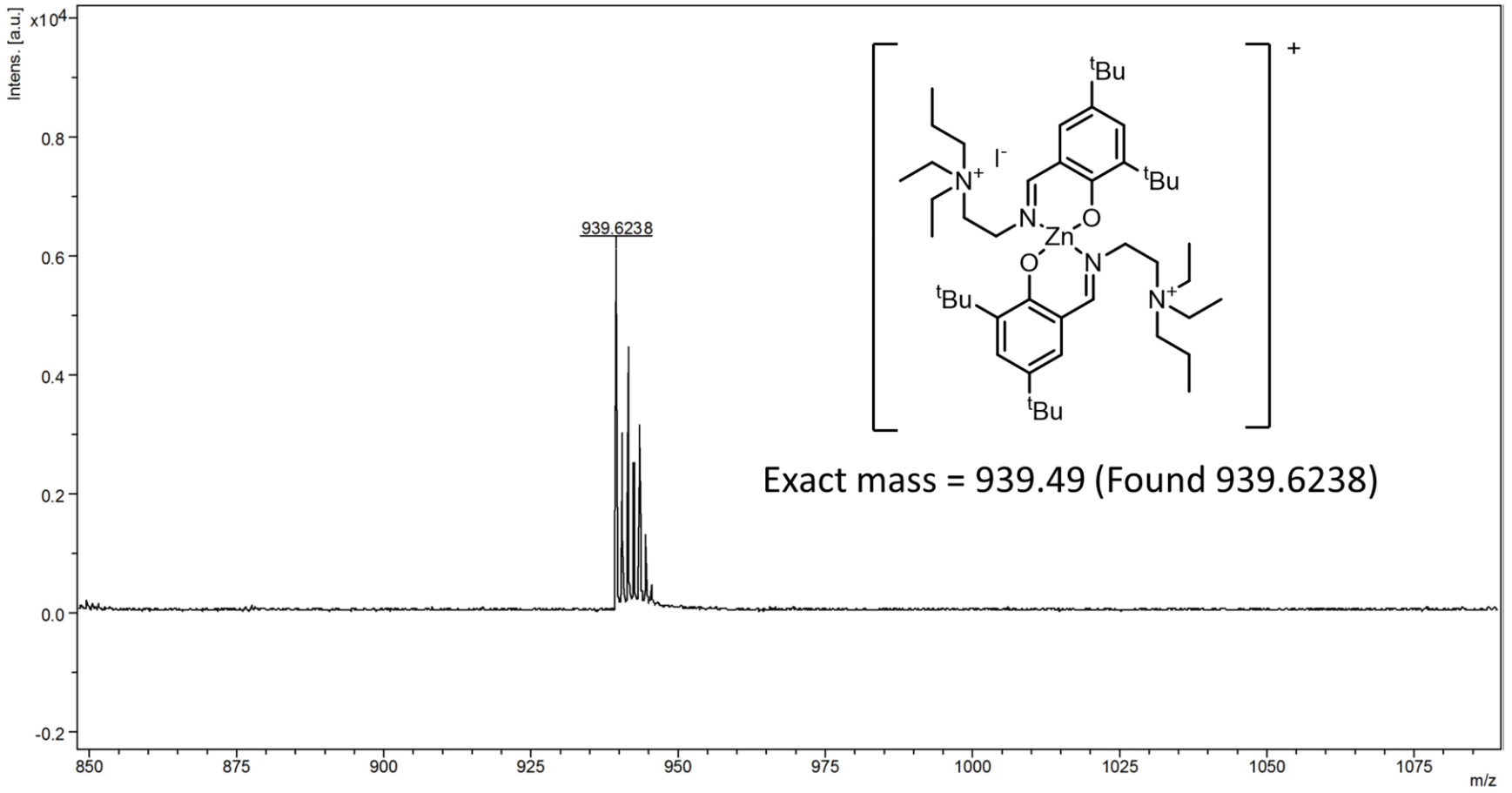


Figure. S35 MALDI-TOF mass spectrum of complex **1Pr-I**

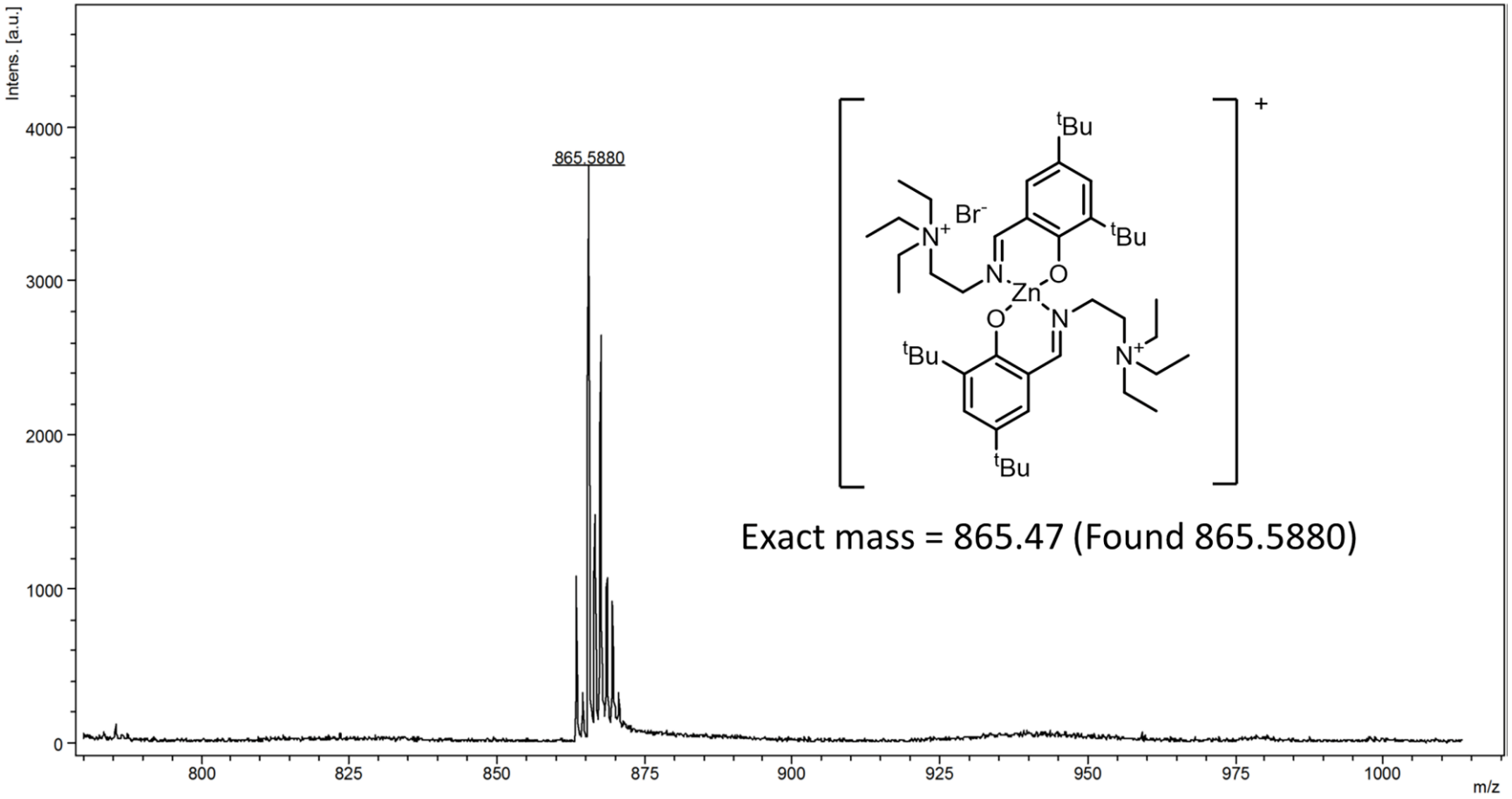


Figure. S36 MALDI-TOF mass spectrum of complex **1Et-Br**

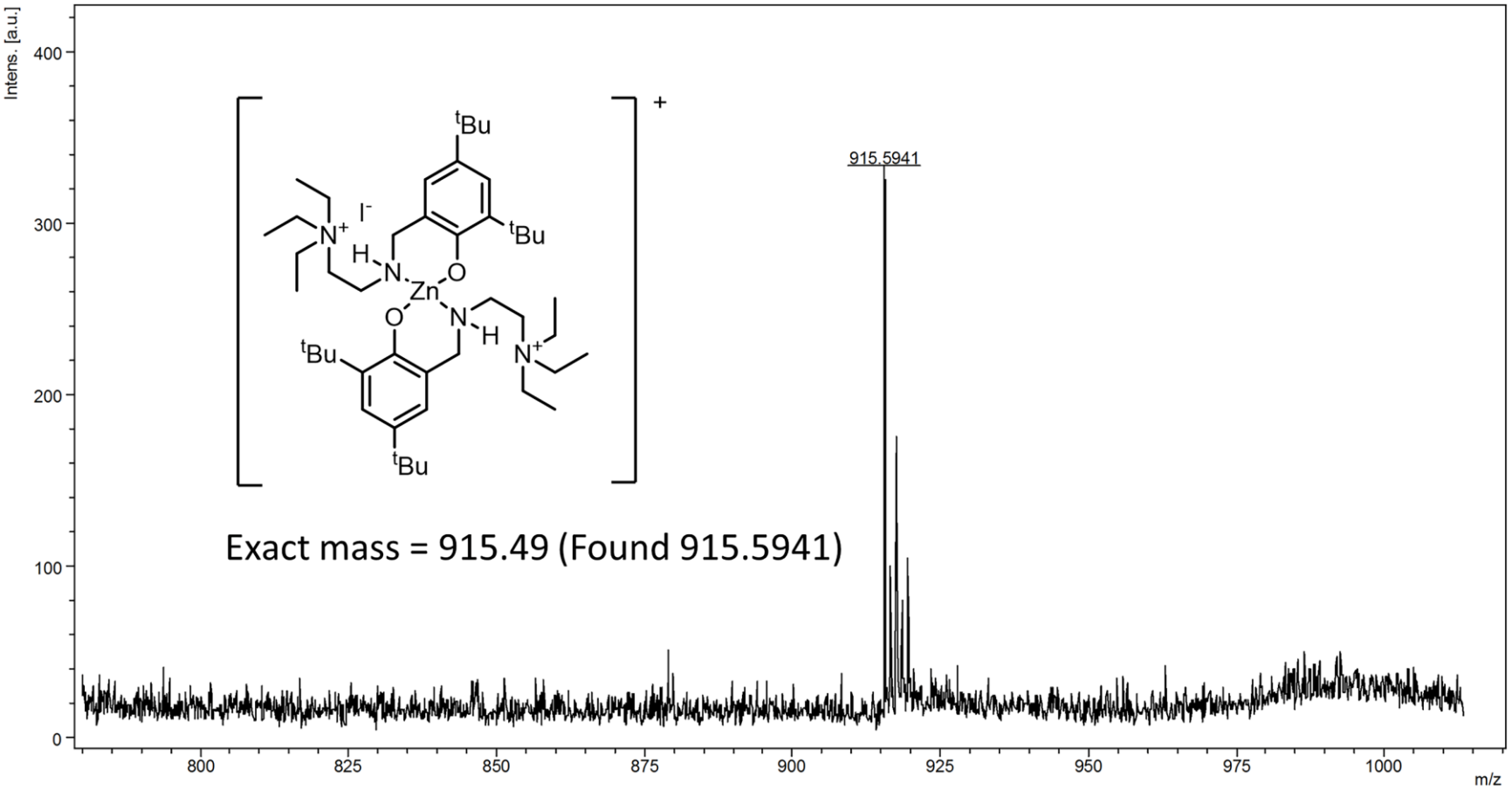


Figure. S37 MALDI-TOF mass spectrum of complex **2.**

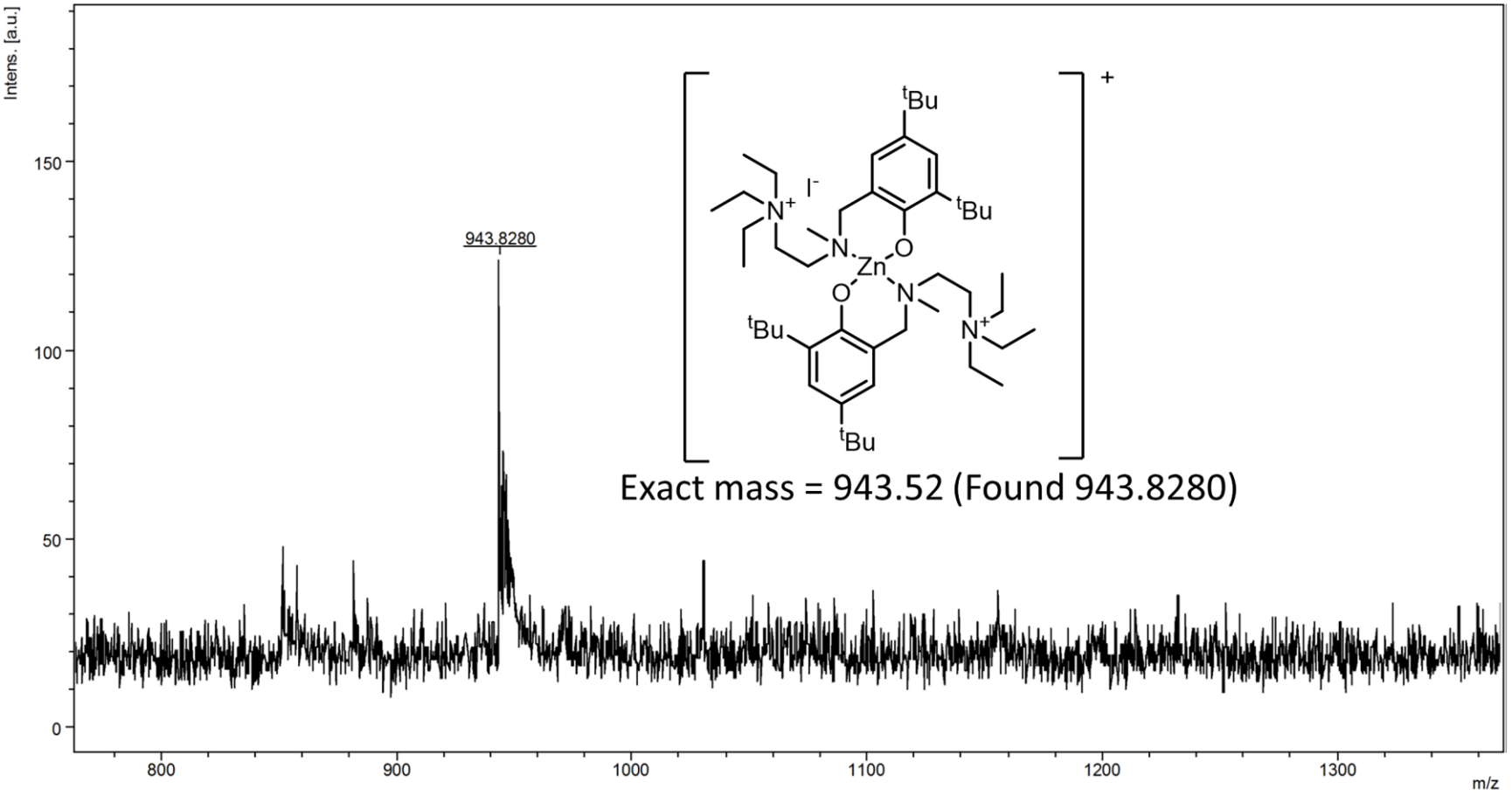


Figure. S38 MALDI-TOF mass spectrum of complex **3.**

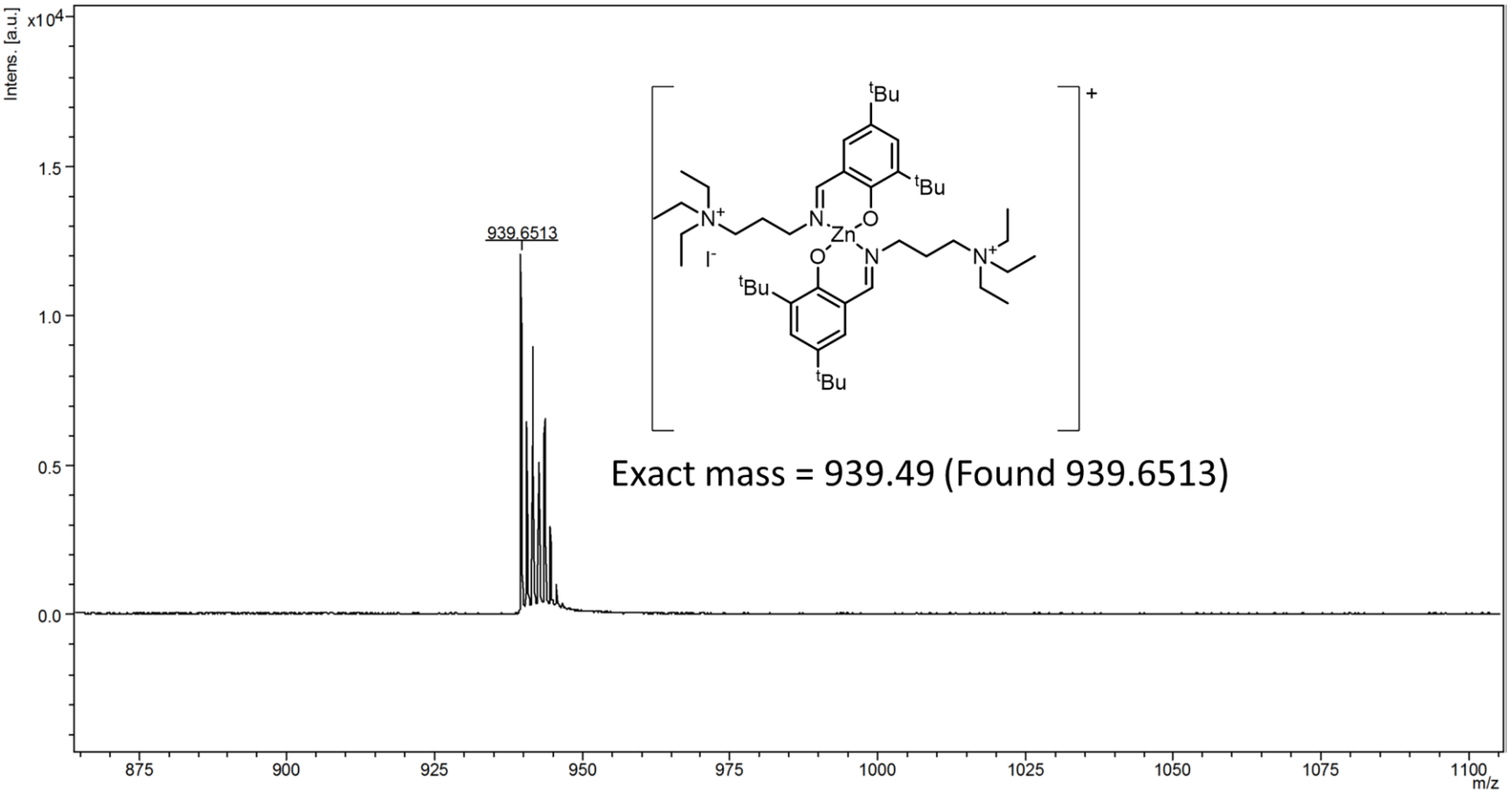


Figure. S39 MALDI-TOF mass spectrum of complex **4.**

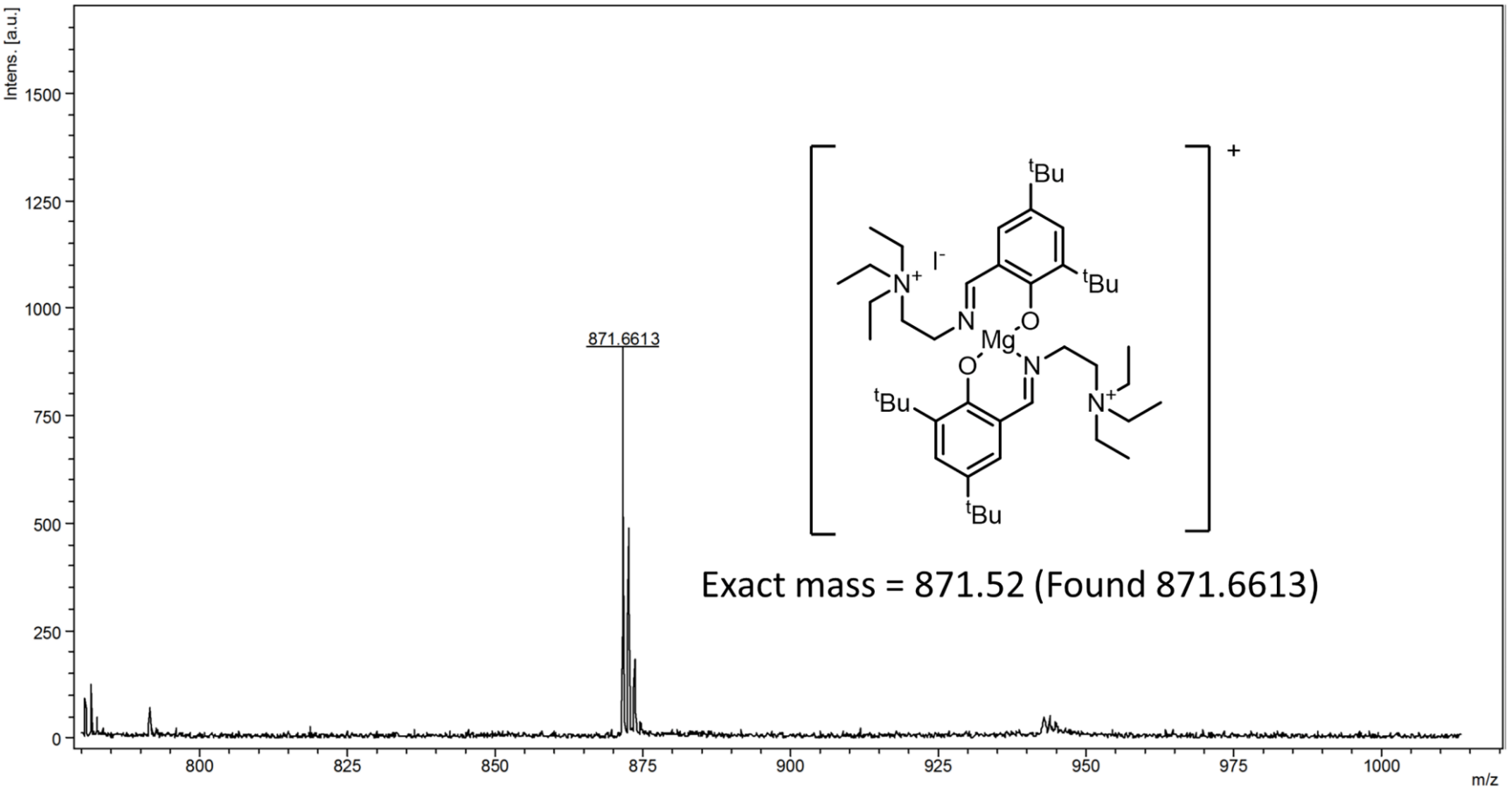


Figure. S40 MALDI-TOF mass spectrum of complex **5.**

Table S1. PO and CO_2 coupling reaction using complex **1Et-I** as catalysts[a]

Entry	Solvent (1 mL)	%conversion[b]	TON[c]	TOF[d] (h^{-1})
1	-	49	980	163
2	DMF	47	940	157
3	Toluene	42	840	140
4	THF	29	580	97
5	DCM	8	160	27

[a] Reaction conditions: PO (2.0 mL), PO:**1Et-I** ratio = 2000:1, CO_2 = 100 psi, T = 75 °C, 6 h. [b] Determined by ^{1}H-NMR spectroscopy by comparison of the integrals of PC (4.8 ppm) and PO (3.8 ppm) of the crude sample. [c] TON = (monomer:catalyst ratio) x %conversion/100 [d] TOF = TON/time(h).

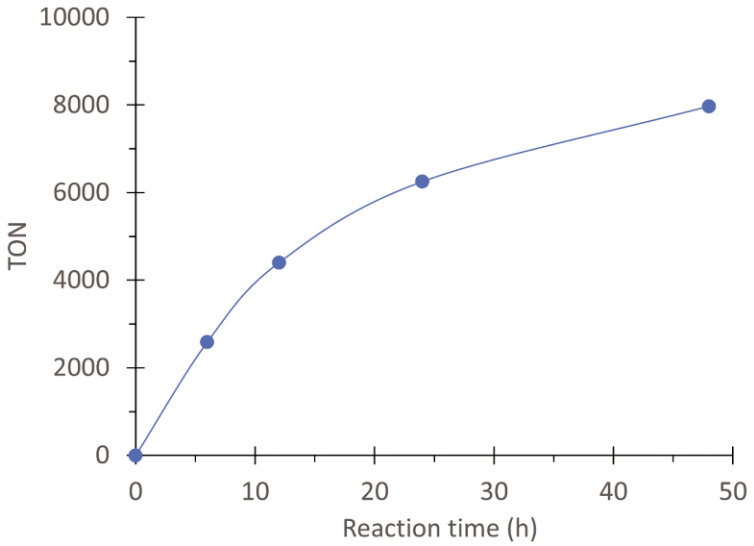


Figure S41 A plot between TON and reaction time. Reaction conditions: PO (2.0 mL), PO:**1Et-I** ratio = 10000:1, CO_2 = 300 psi, T = 100 °C. TON = (PO:**1Et-I** ratio) x %conversion/100.

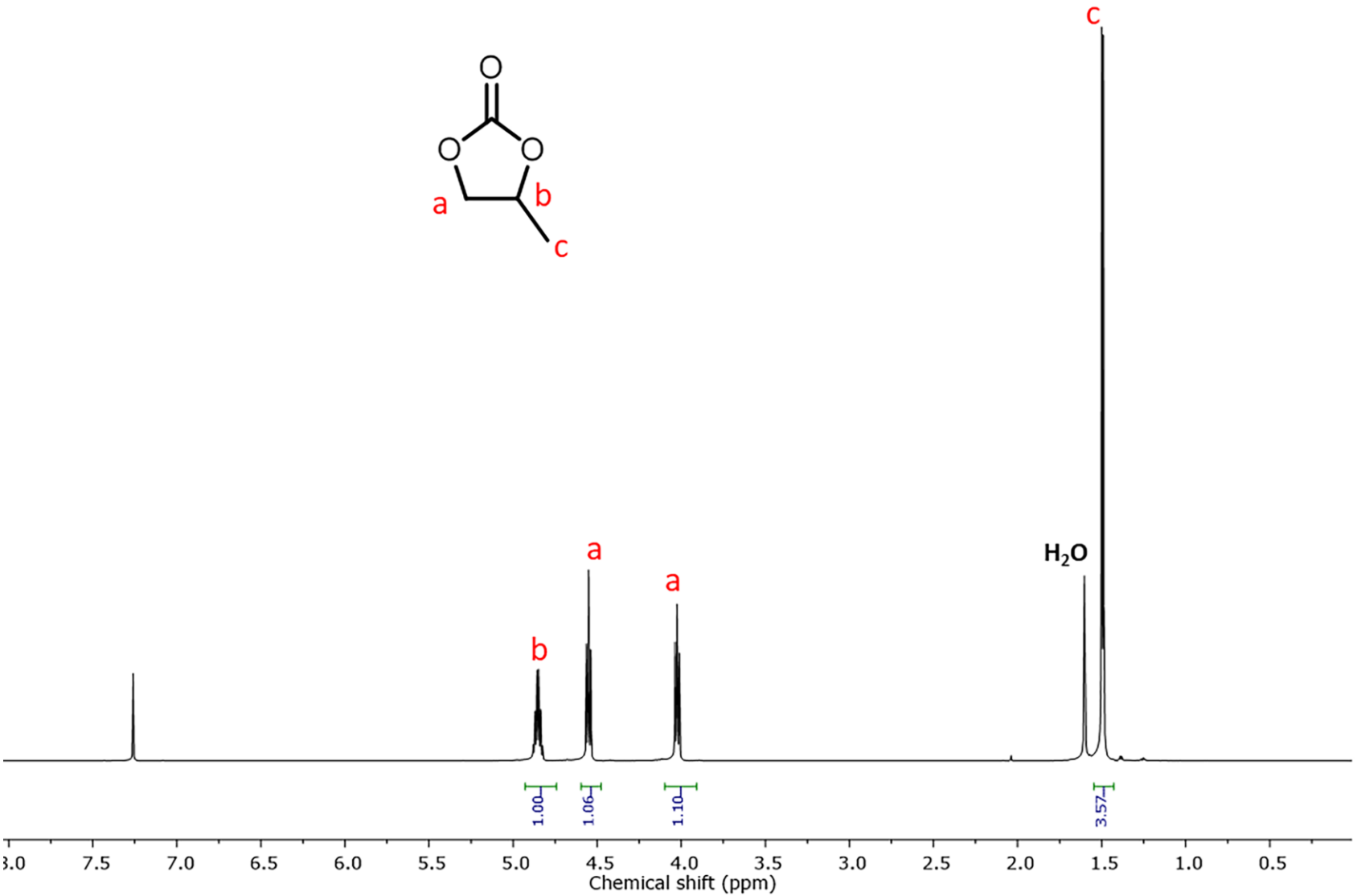


Figure. S42 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of propylene carbonate.

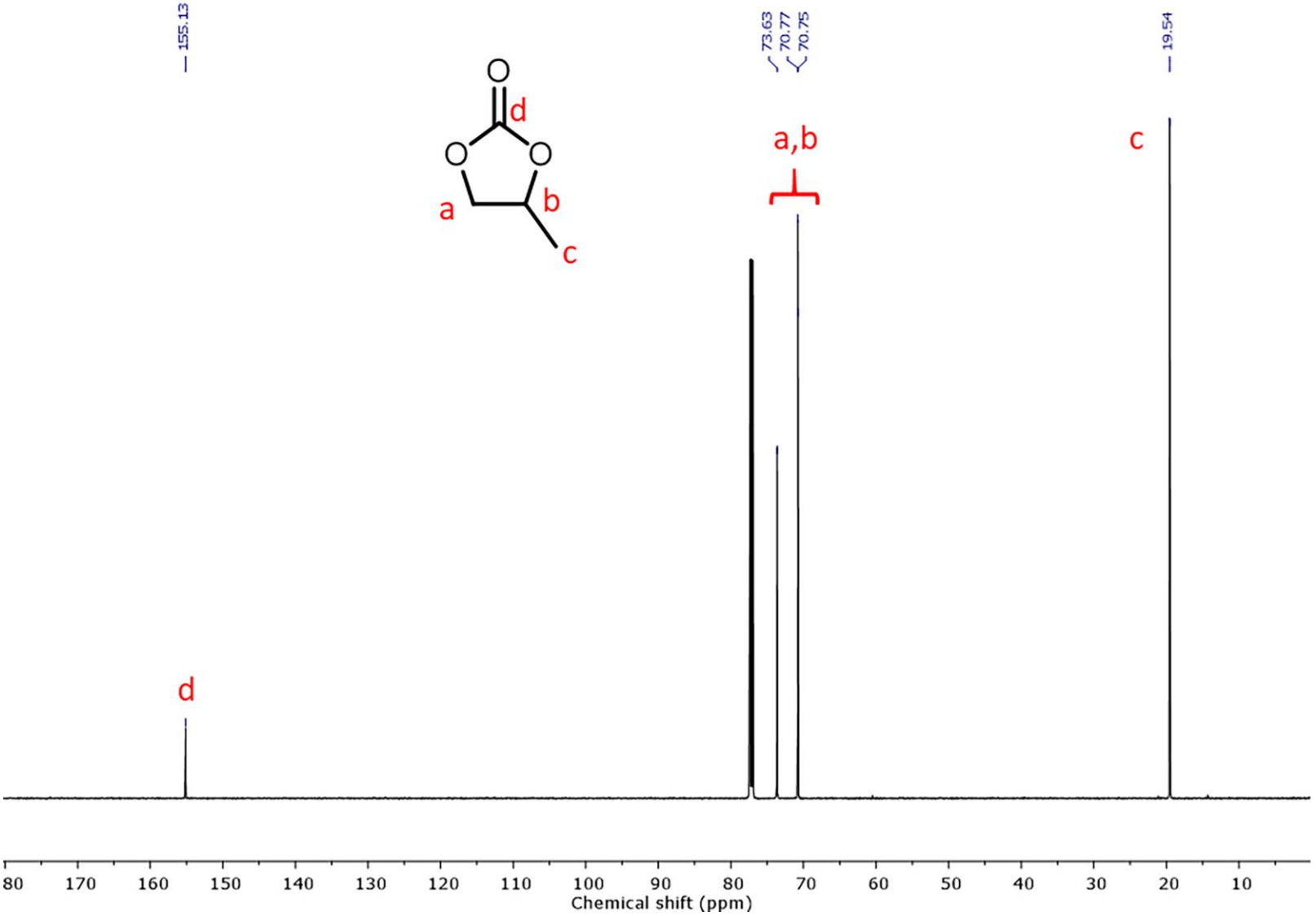


Figure. S43 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of propylene carbonate.

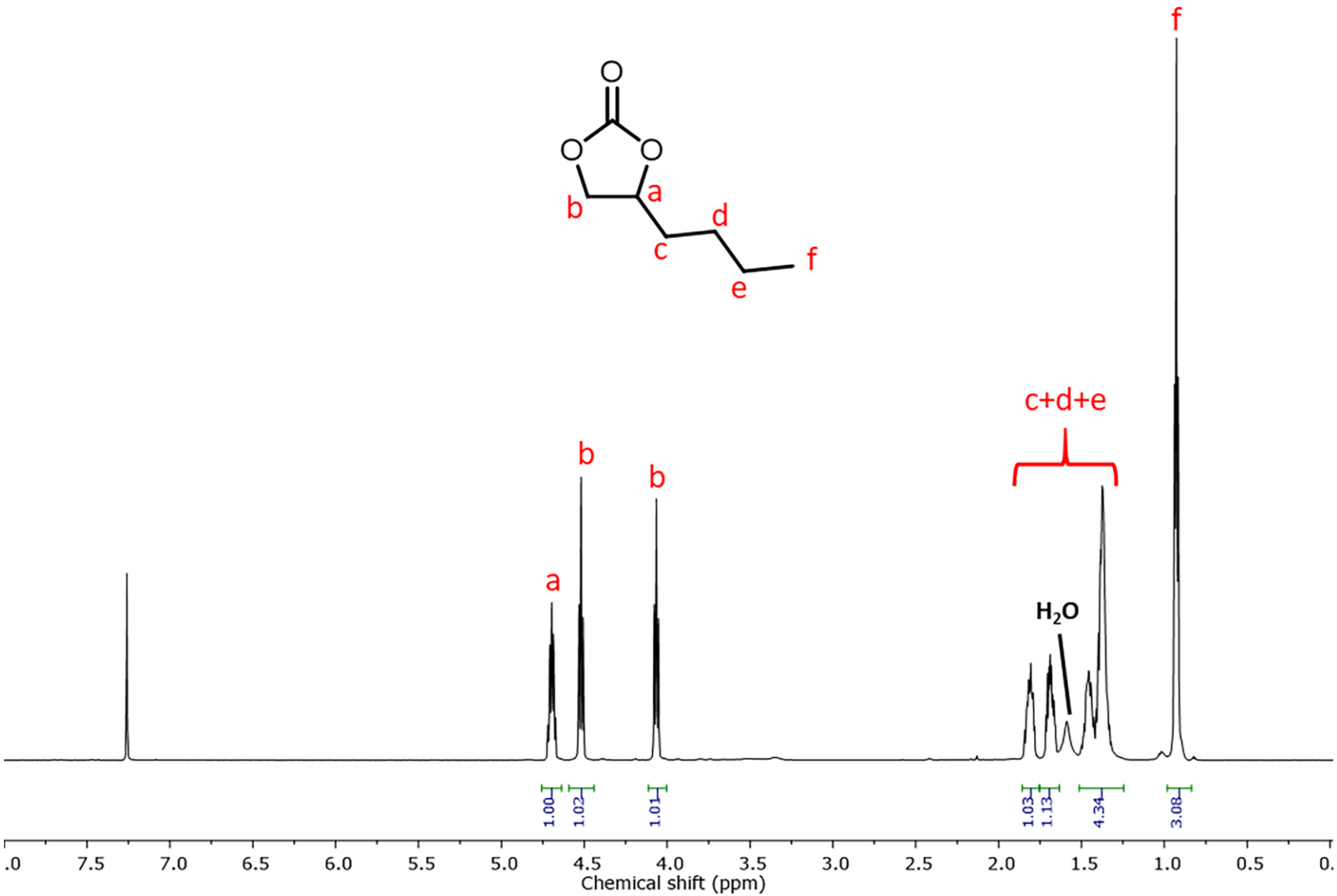


Figure. S44 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of 1,2-hexylene carbonate.

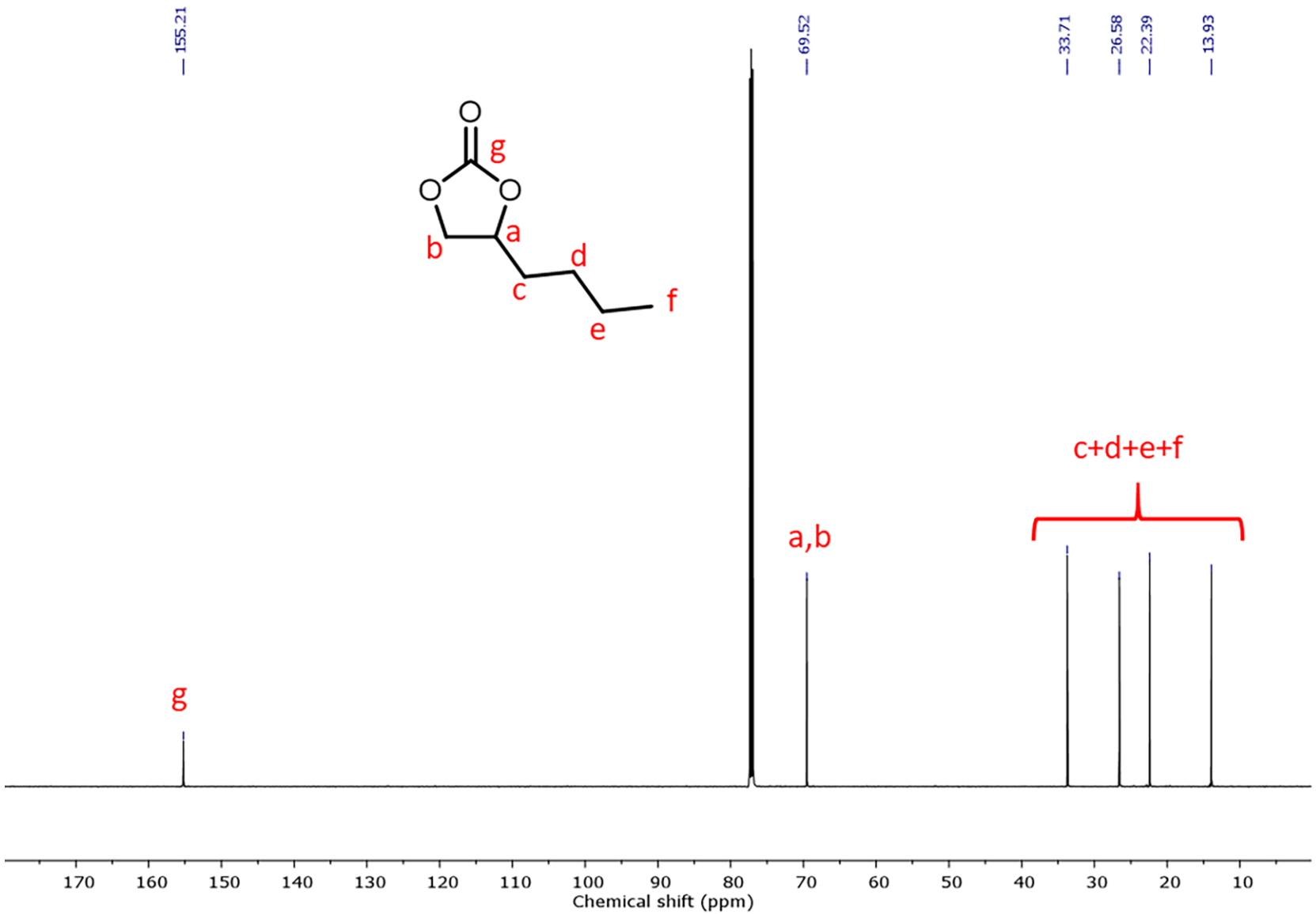


Figure. S45 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of 1,2-hexylene carbonate.

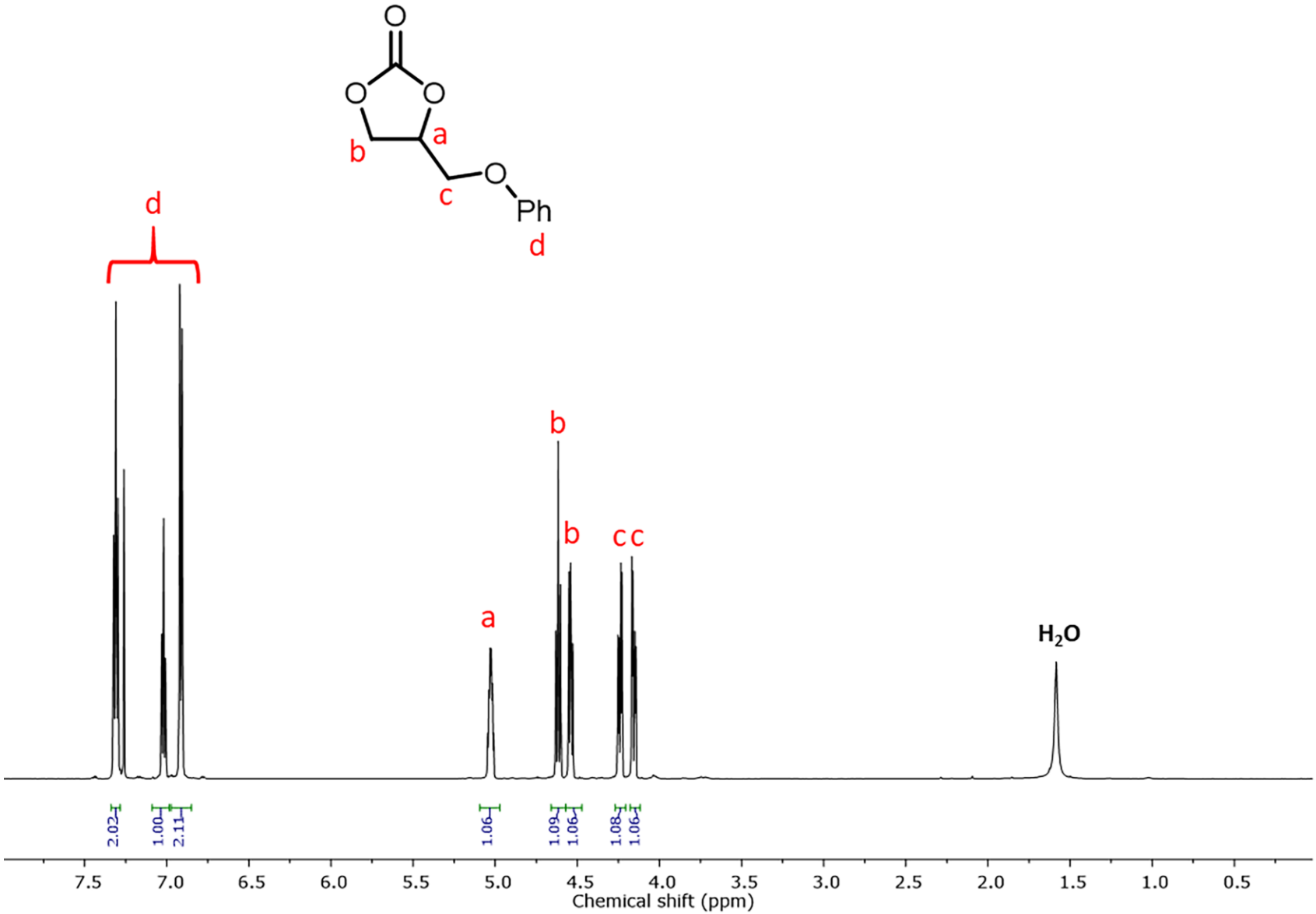


Figure. S46 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of 3-phenoxypropylene carbonate.

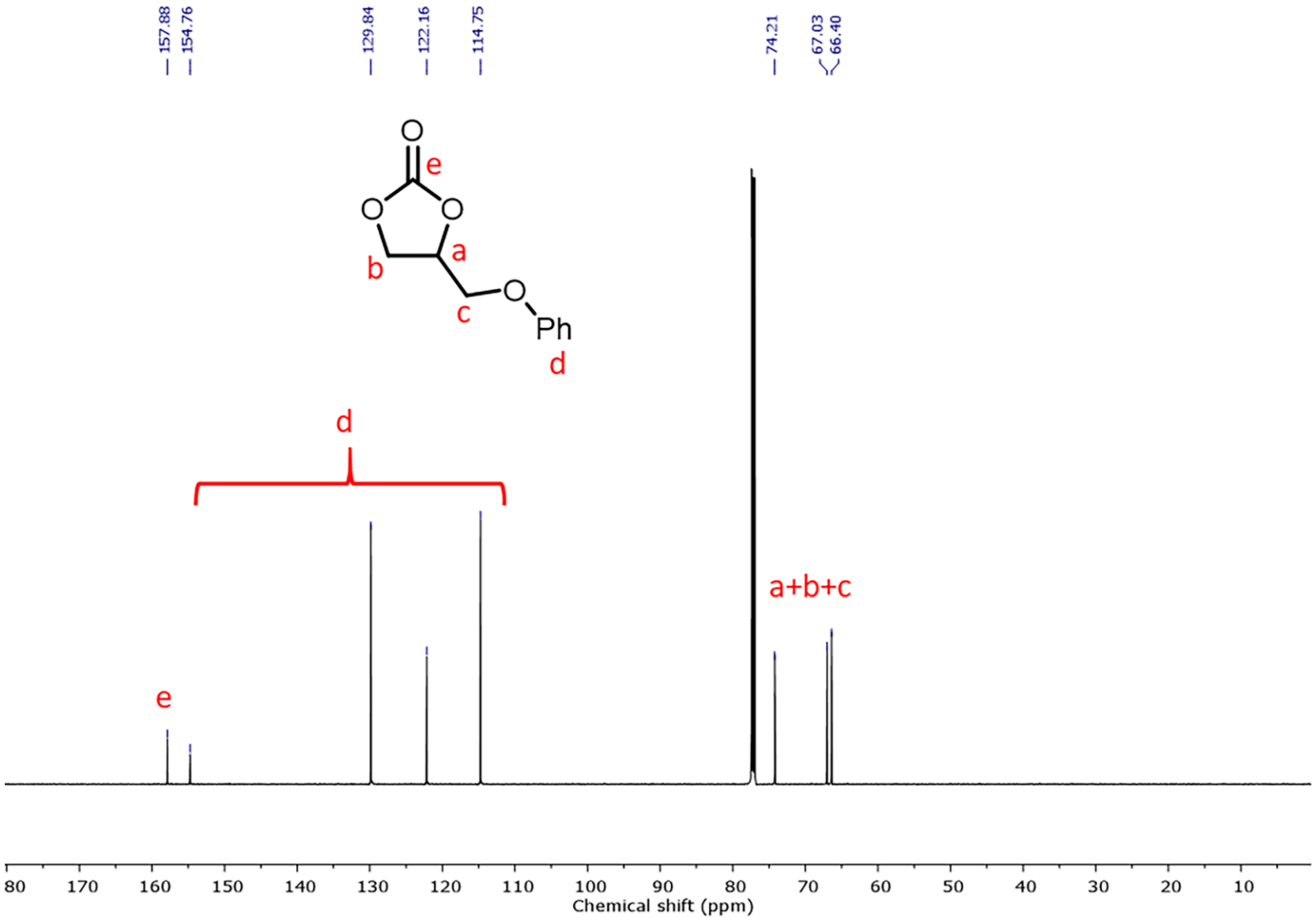


Figure. S47 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of 3-phenoxypropylene carbonate.

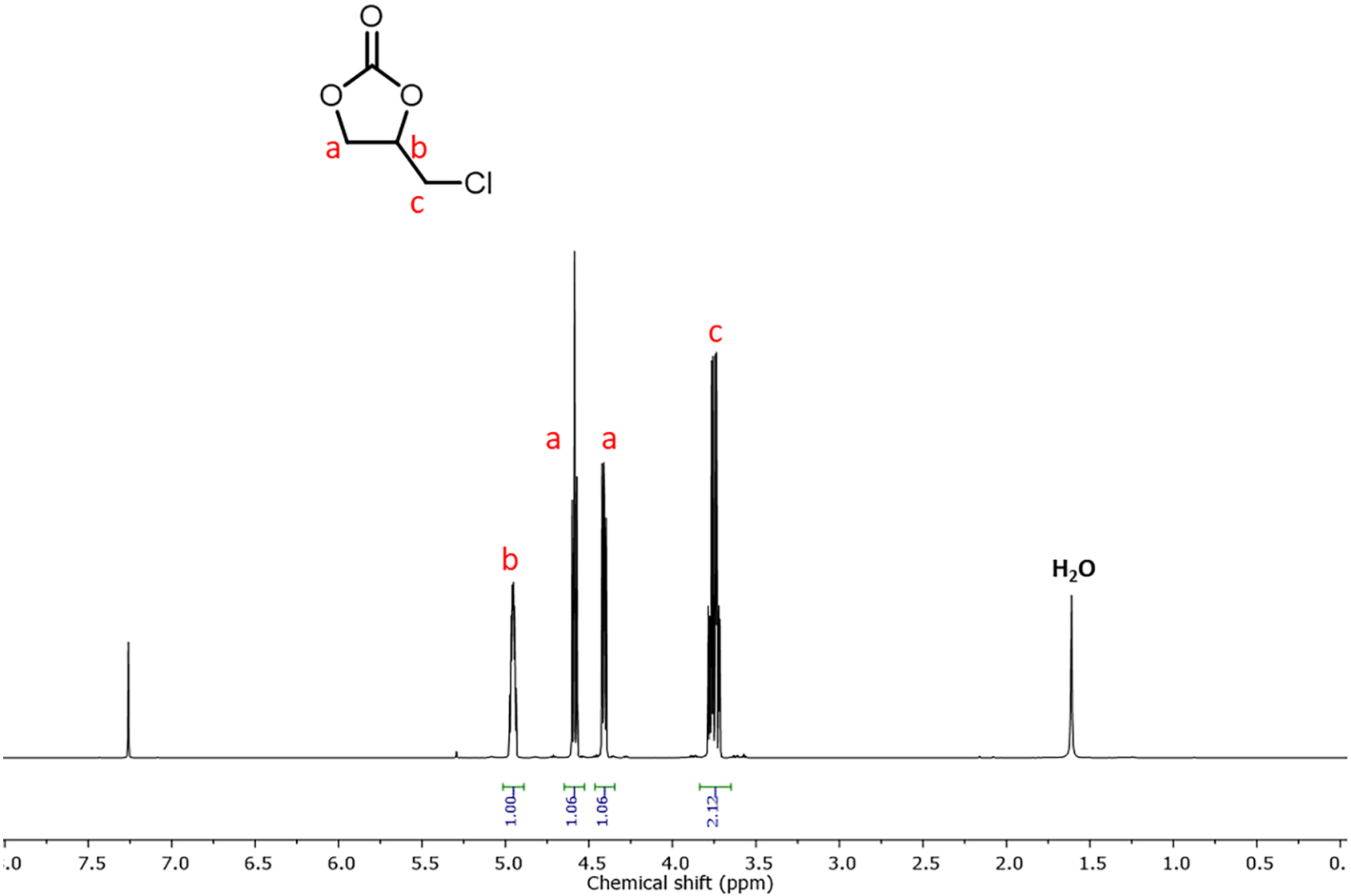


Figure. S48 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of 3-chloropropylene carbonate.

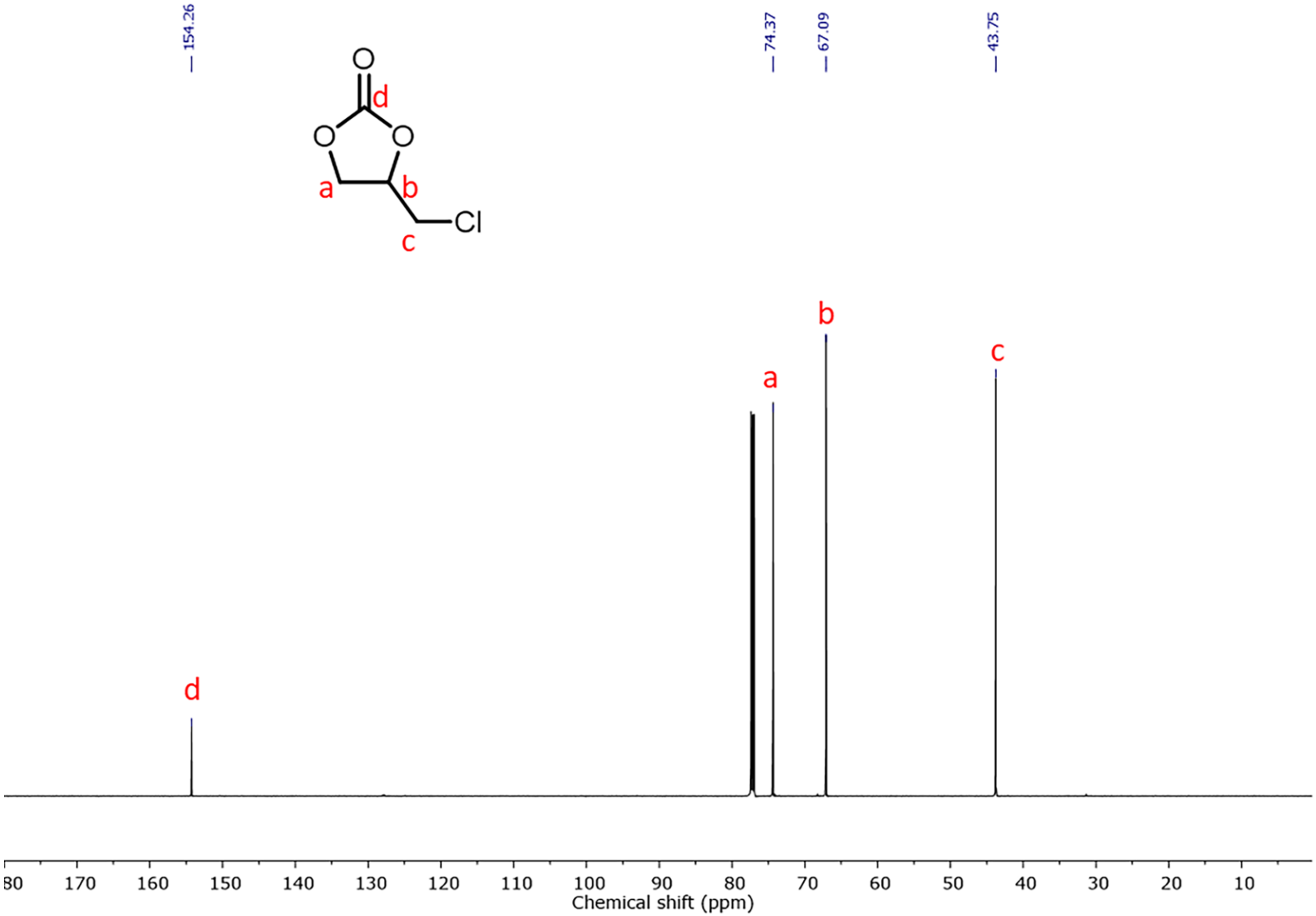


Figure. S49 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of 3-chloropropylene carbonate.

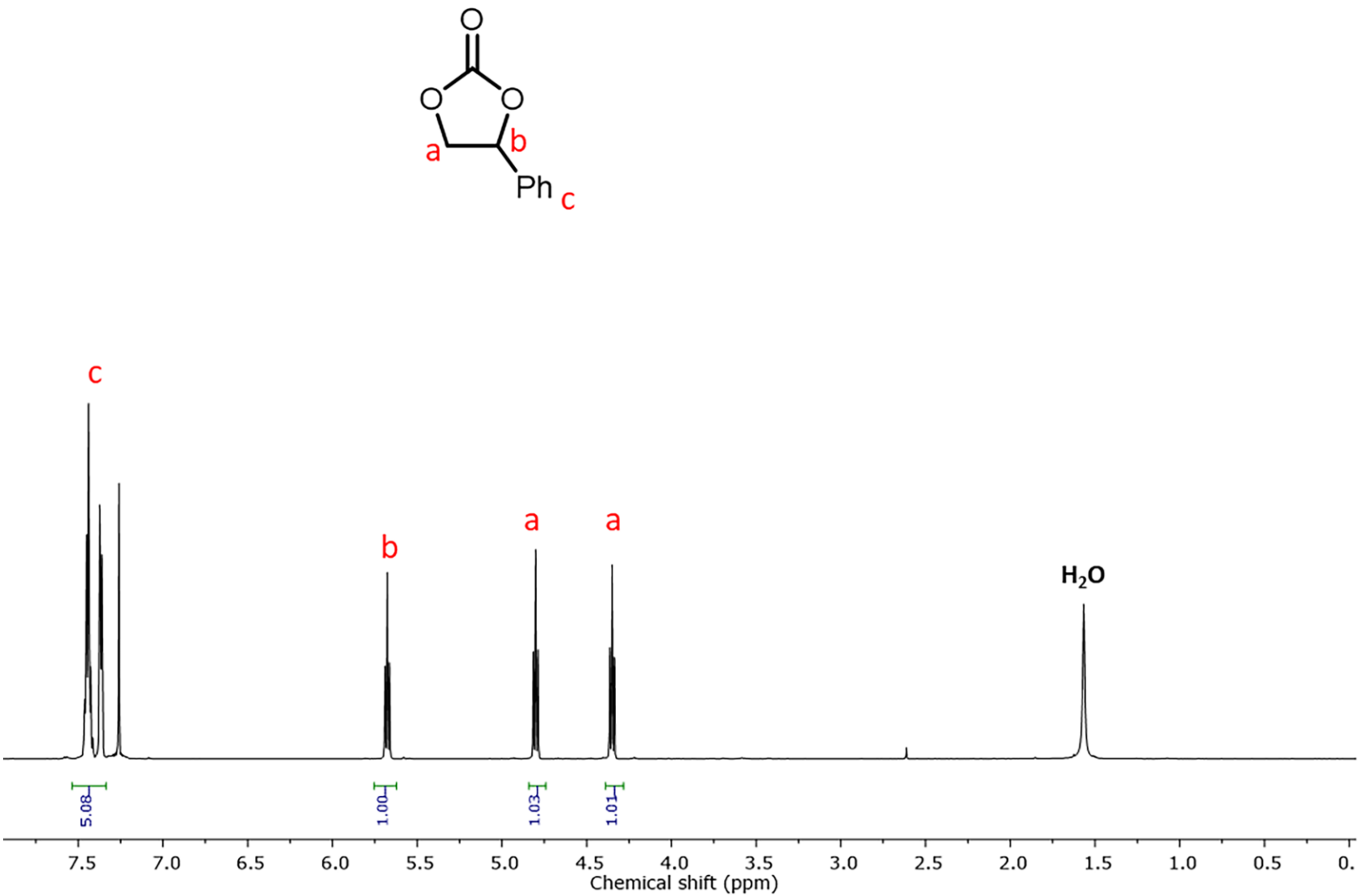


Figure. S50 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of styrene carbonate.

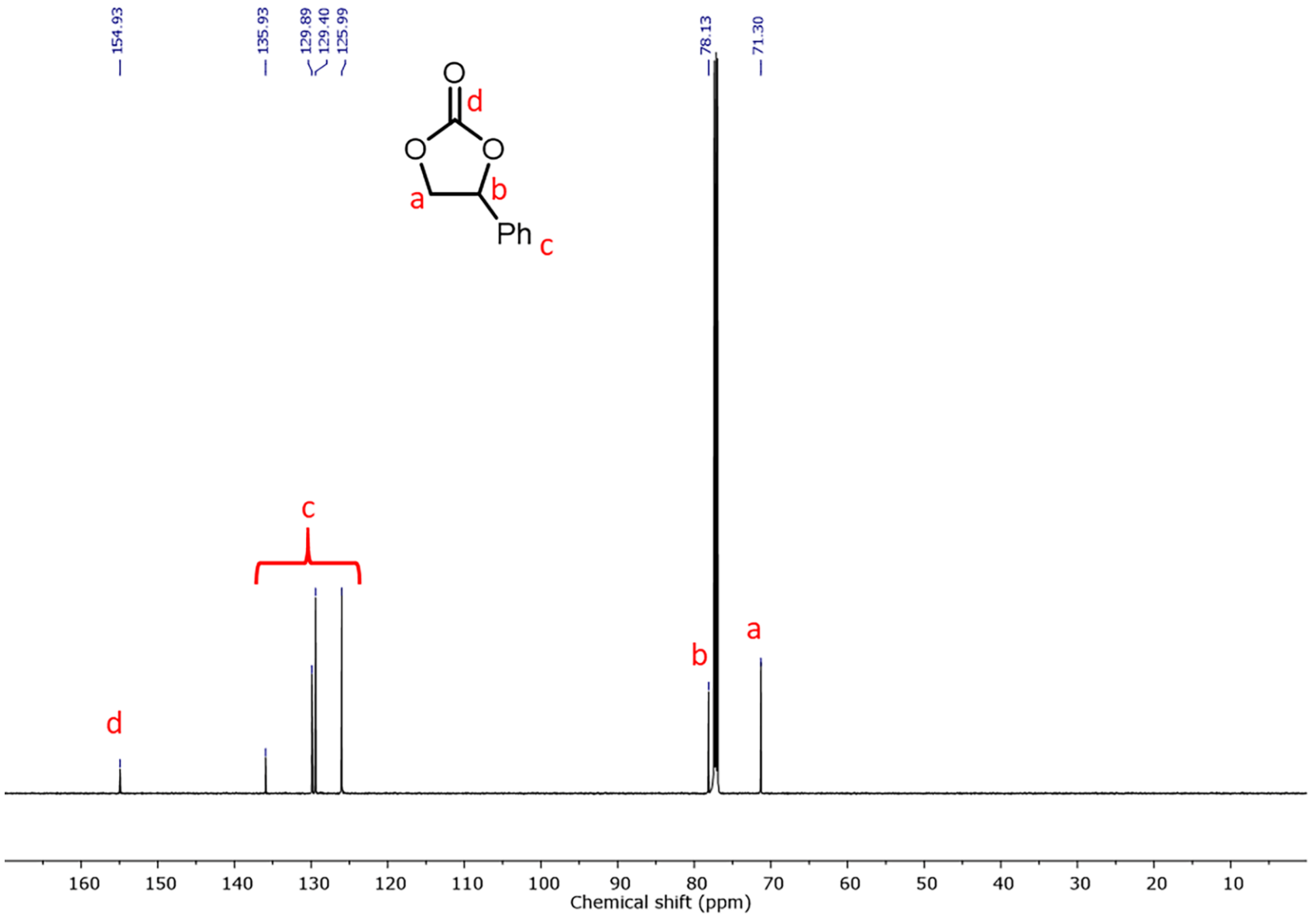


Figure. S51 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of styrene carbonate.

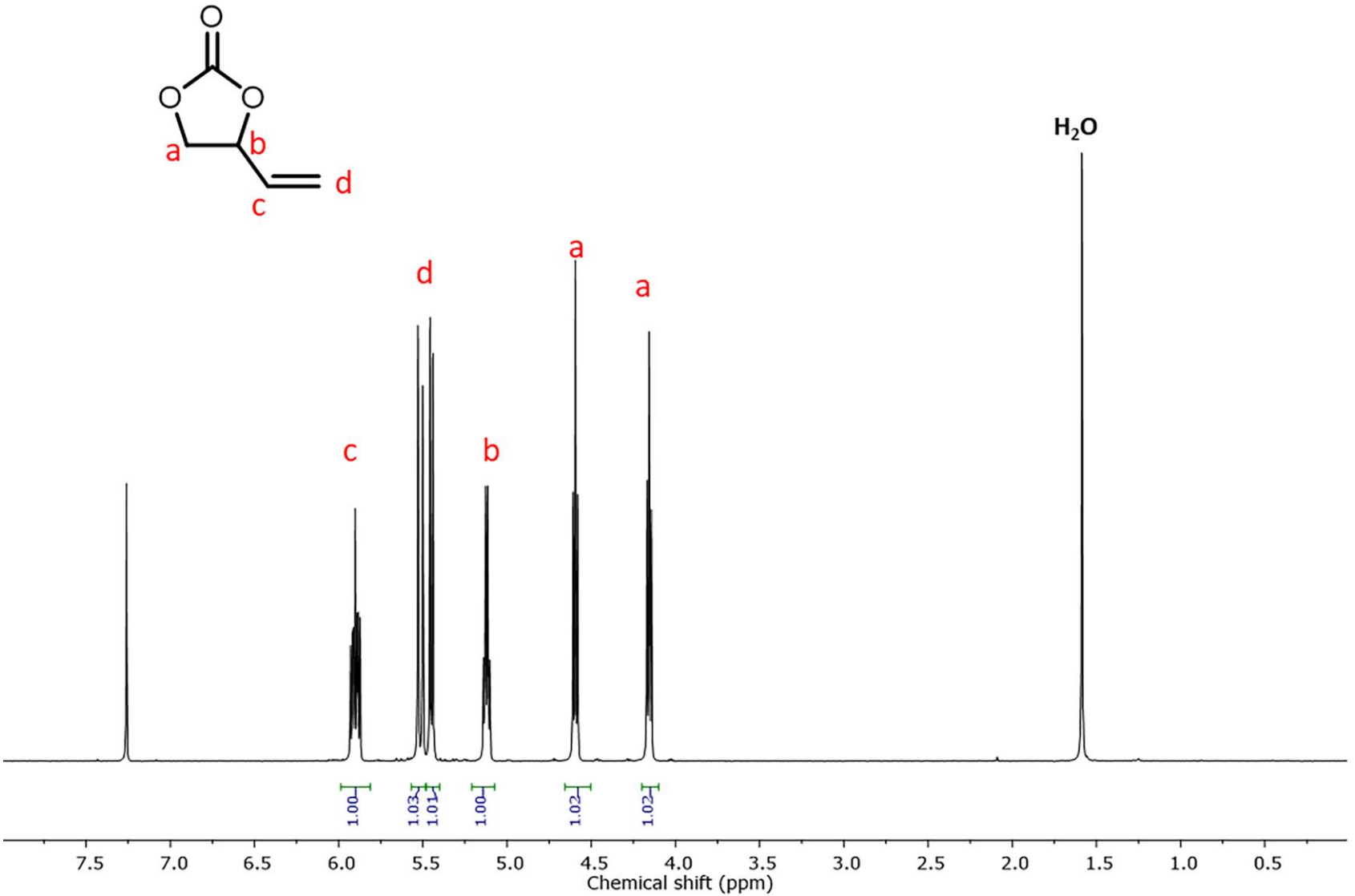


Figure. S52 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of vinyl ethylene carbonate.

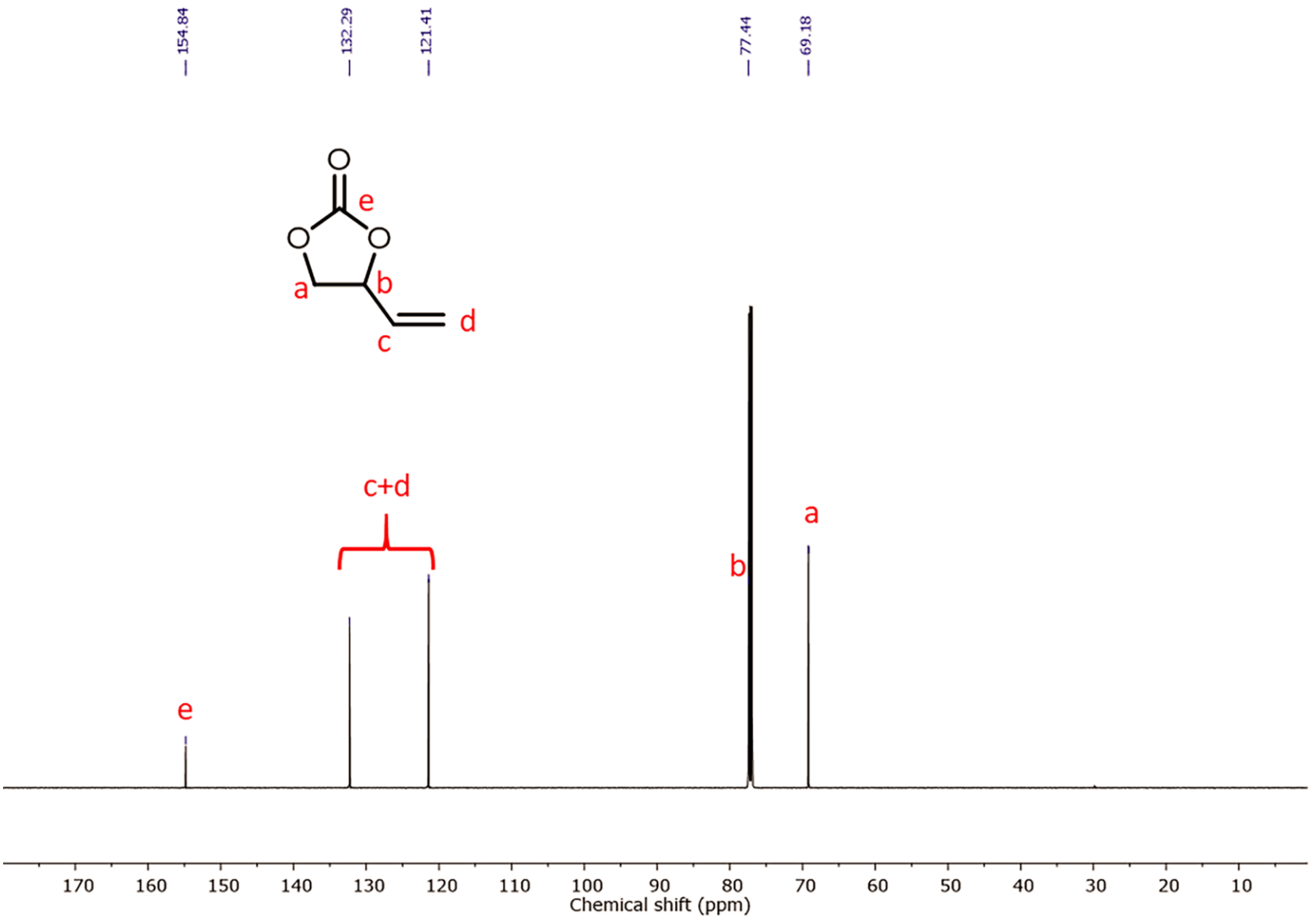


Figure. S53 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of vinyl ethylene carbonate.

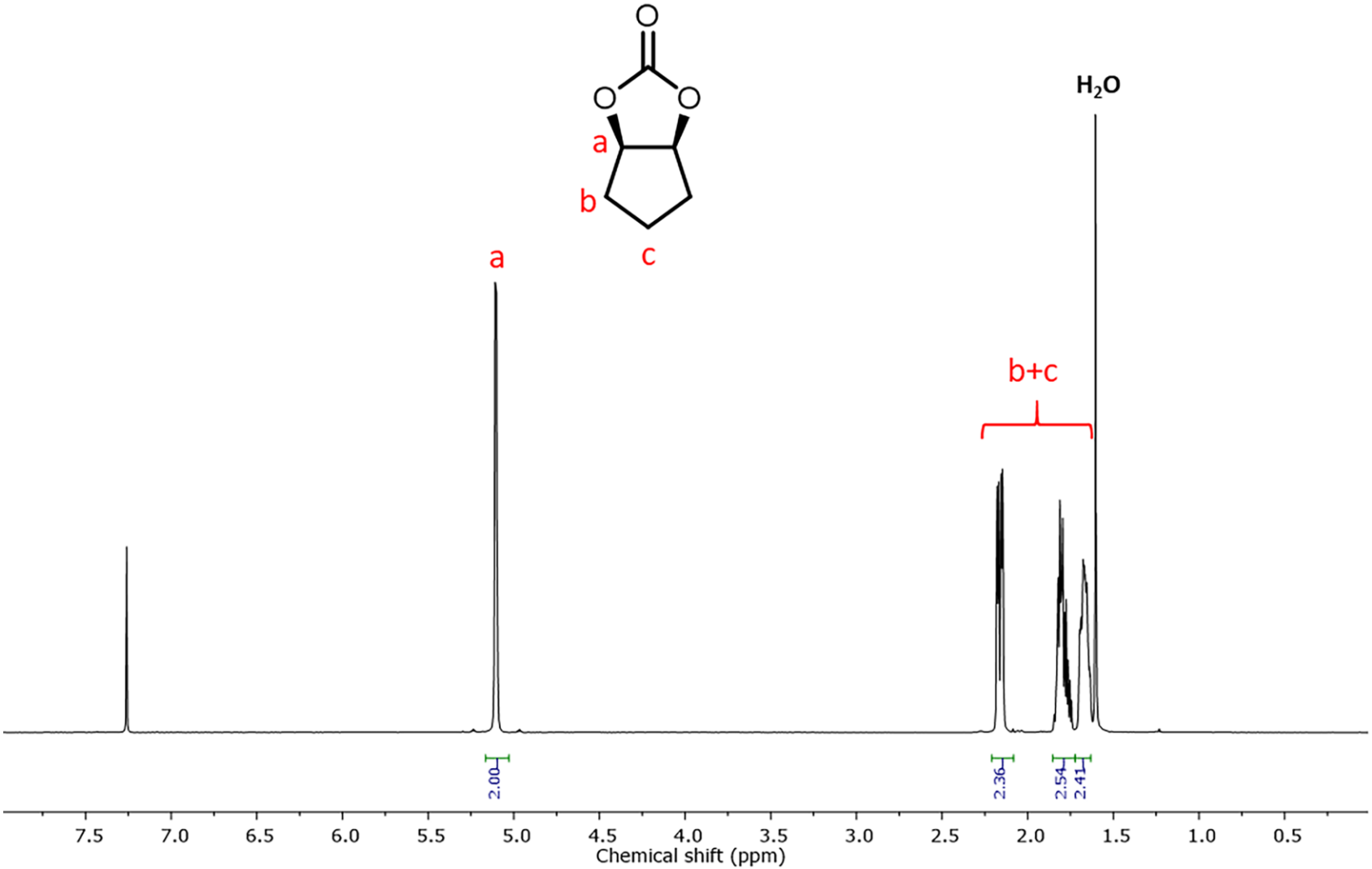


Figure. S54 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of *cis*-cyclopentene carbonate.

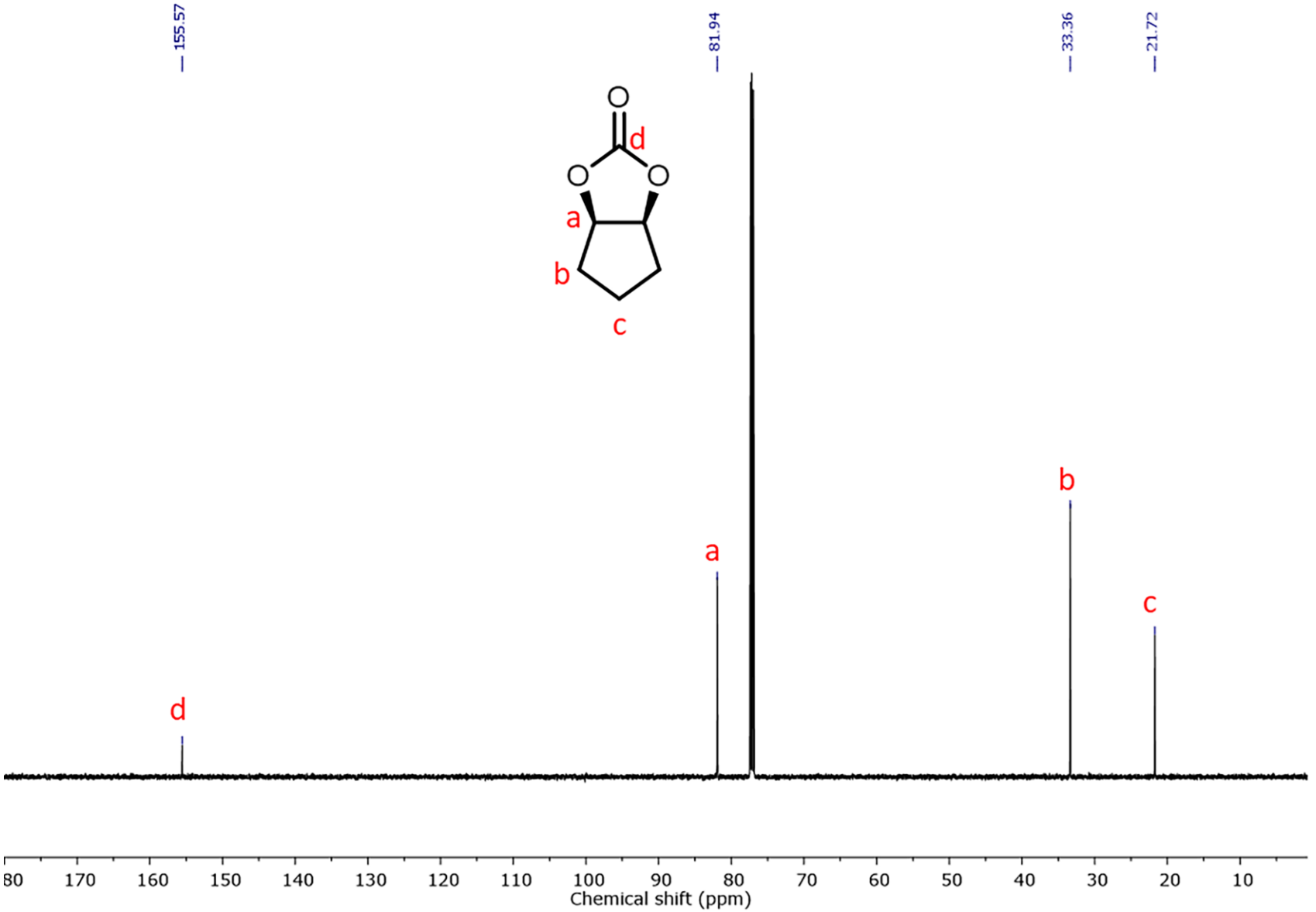


Figure. S55 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of *cis*-cyclopentene carbonate.

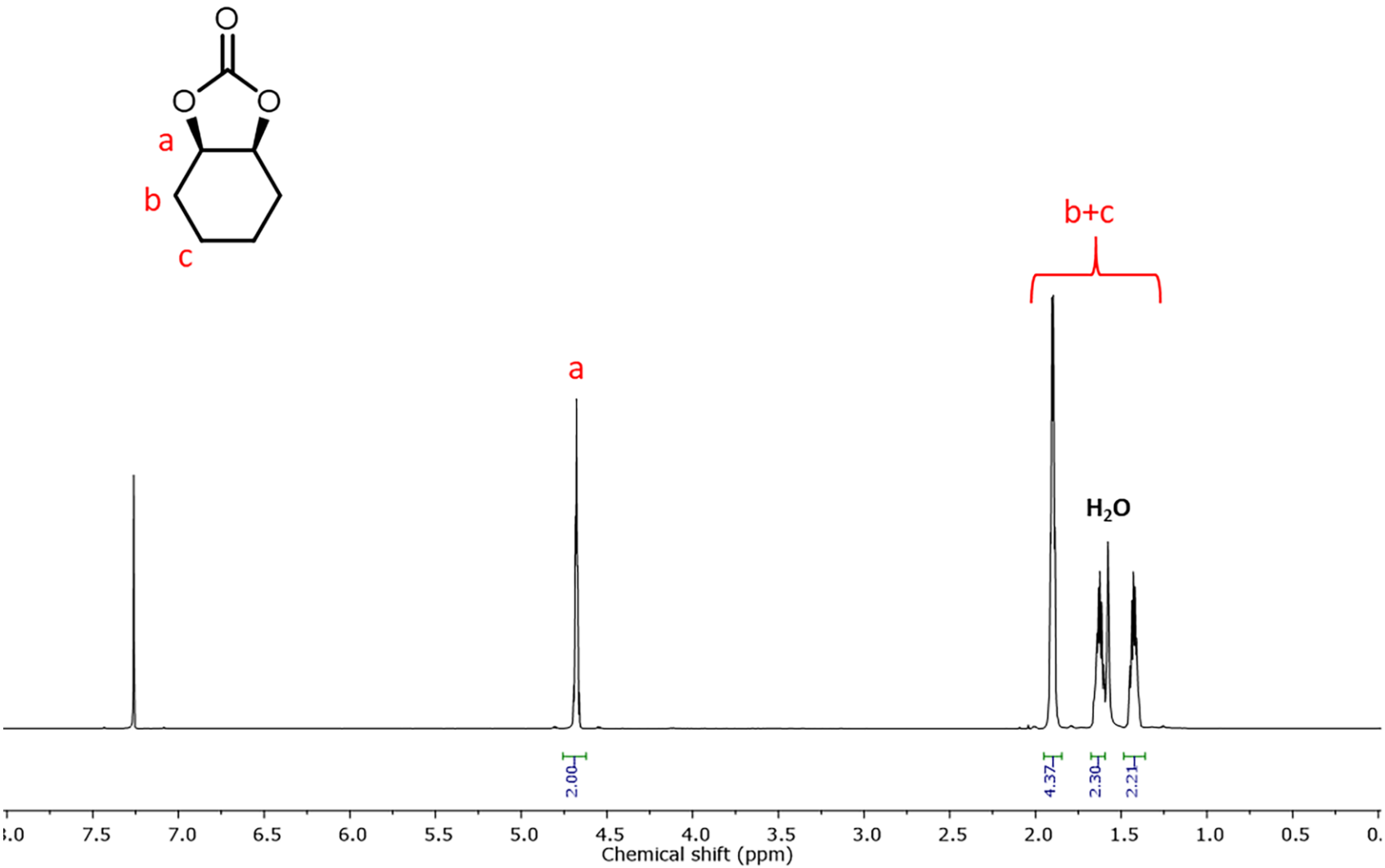


Figure. S56 ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, 30 °C) of *cis*-cyclohexene carbonate.

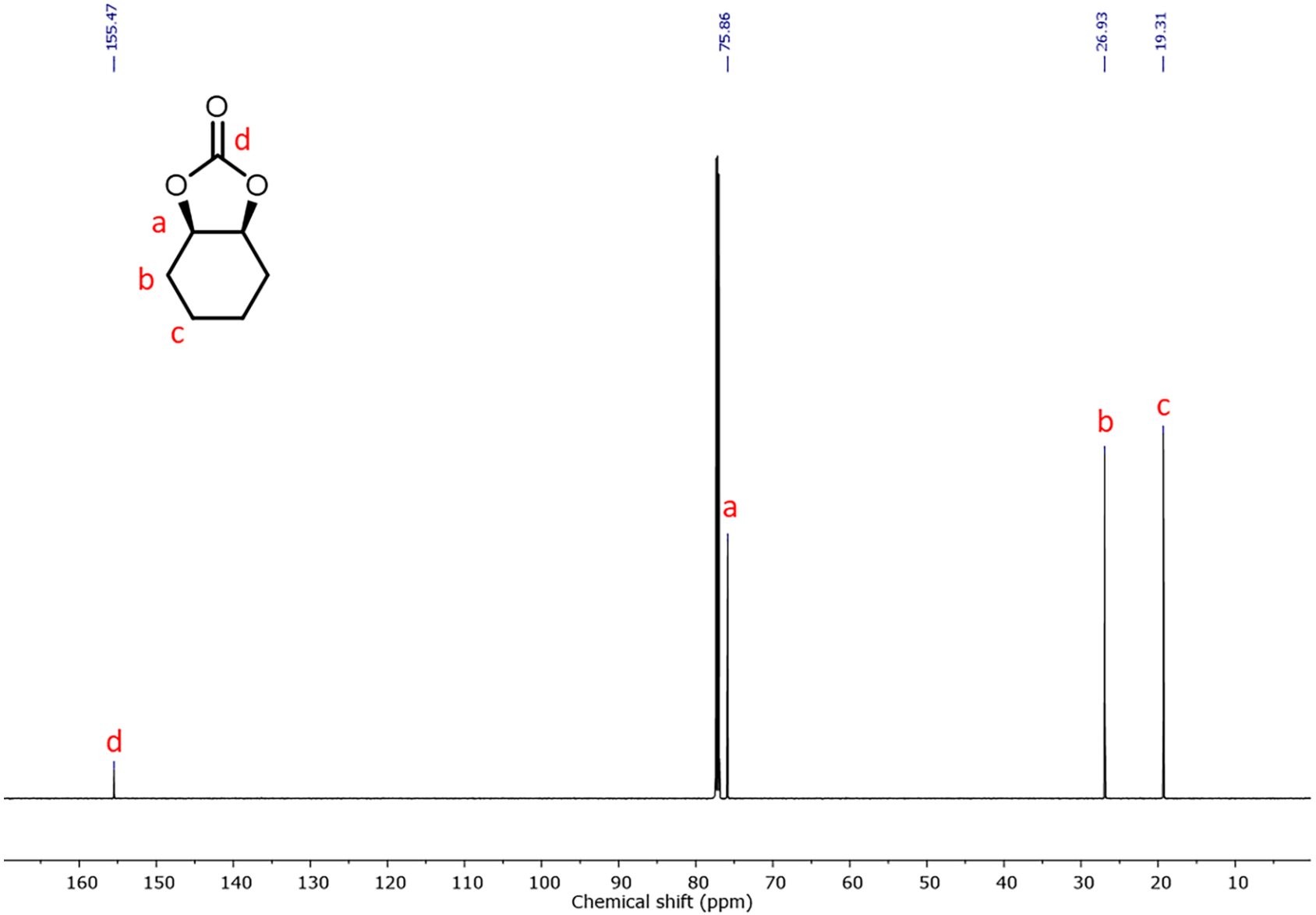


Figure. S57 $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 150 MHz, 30 °C) of *cis*-cyclohexene carbonate.

.**X-ray crystallographic data**

Table S2 Crystal and structure refinement data for compound **6**

Compound	**6**
CCDC	2090817
Elemental formula	$C_{24}H_{42}Cl_{3.85}I_{0.15}N_2OZn$
Formula weight	595.25
Crystal system	Monoclinic
Space group	$P2_1c$
a / Å	13.4677 (7)
b / Å	8.8859 (4)
c / Å	24.3901 (13)
α / ∘	90
β / ∘	92.600 (2)
γ / ∘	90
Cell volume, V / Å^3	2915.8 (3)
No. of formula units/cell, Z	4
$\rho_{calc.}$/Mg m^{-3}	1.356
F(000)	1245
Absorption coefficient, μ / mm^{-1}	1.37
T / K	136
Crystal colour, shape	Colourless, Block
Crystal size / mm	0.22 × 0.18 × 0.18
Total no. of reflections measured (not including absences)	79140
No. of unique reflections, and R_{int} for equivalents	5996, 0.050
No. of 'observed' reflections ($I > 2\sigma_I$)	5211
Data/restraints/parameters	5996/320/34
Goodness-of-fit on F^2, S	1.05
R indices ('observed' data)	R_1 = 0.0307, wR_2 = 0.0661
R indices (all data)	R_1 = 0.0390, wR_2 = 0.0693
Largest diff. peak and hole / eÅ^{-3}	0.85 and -0.71

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