

Supporting Information

Designing NHC-Copper(I) Dipyriddyamine Complexes for Blue Light-Emitting Electrochemical Cells

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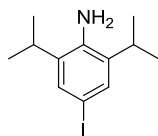
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General Considerations. All reactions were carried out using standard Schlenk technique under an atmosphere of dry Argon. Solvents were purchased from Carlo Erba and degassed prior to use by bubbling argon gas directly in the solvent. Solvents for NMR spectroscopy were dried over molecular sieves. NMR spectra were recorded on 400 MHz and 500 MHz Bruker spectrometers. Proton (^1H) NMR information is given in the following format: multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; sex, sextet; sept, septet; m, multiplet), coupling constant(s) (J) in Hertz (Hz), number of protons. The prefix *app* is occasionally applied when the true signal multiplicity was unresolved and br indicates the signal in question is broadened. Carbon (^{13}C) NMR spectra are reported in ppm (δ) relative to residual CHCl_3 (δ 77.0) unless noted otherwise. HRMS were performed by LCMT analytical services. NMR solvent was passed through a pad of basic alumina before uses. Ligand **L1** (2,2'-dipyridylamine) was purchased from Sigma-Aldrich and used without prior purification.

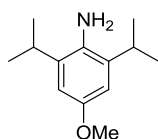
Part 1: Synthesis of diimines **S1-S6** and imidazolium salts **S7-S11** for NHC ligands.

4-iodo-2,6-di-*iso*-propylaniline (S1)



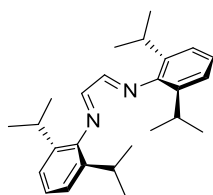
In a round bottom flask 2,6-di-*iso*-propylaniline (17.1 mL, 91 mmol) and sodium bicarbonate (22.9 g, 273 mmol) were introduced in MeOH (200 mL). A ICl solution 1M in DCM (100 mL) was added dropwise and the reaction mixture was stirred at room temperature for 5 days. Then, the solids were filtered off the mixture and rinsed with Et₂O. The filtrate was concentrated under vacuum leading to a dark orange oil. A saturated solution of sodium thiosulfate was added to this oil and the reaction mixture was stirred for 10 minutes. After an extraction with Et₂O, the combined organic layers were dried over MgSO₄ and concentrated under vacuum. The pure product was obtained as brown oil (26.8 g, 97% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.24 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.85 (sept, *J* = 6.8 Hz, 2H, CH(CH₃)₂), 7.28 (s, 2H, CH aromatic) ppm (NH₂ not observed). (in good agreement with the literature).¹

4-methoxy-2,6-di-*iso*-propylaniline (S2)



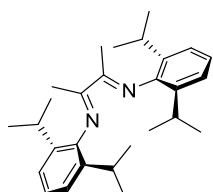
In a Schlenk tube under argon atmosphere, 4-iodo-2,6-di-*iso*-propylaniline (**S1**) (294 mg, 0.97 mmol) was introduced in degassed dry toluene (60 mL). CuI (9.2 mg, 0.05 mmol), tetramethylphenanthroline (23 mg, 0.10 mmol) and CsOH (948 mg, 2.91 mmol) were added. The reaction mixture was stirred 1 hour at 80 °C and freshly distilled MeOH (3.2 mL) was added. The reaction mixture was stirred for 24 h at 80 °C. After returning to room temperature, the reaction mixture was filtered through a pad of silica, the cake was washed with EtOAc and the filtrate was concentrated to dryness under vacuum. The product was obtained as a brown oil (198 mg, 98% yield) (purification by flash chromatography on silica gel could be used to purify if necessary, eluent pentane/EtOAc 99:1). ¹H-NMR (CDCl₃, 400 MHz): δ 1.27 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.98 (sept, *J* = 6.8 Hz, 2H, CH(CH₃)₂), 3.78 (s, 3H, OCH₃), 6.55 (s, 2H, CH aromatic) ppm (NH₂ not observed). (in good agreement with the literature).¹

1,4-di(-2,6-di-*iso*-propylphenyl)-1,4-diaza-1,3-butadiene (S3)



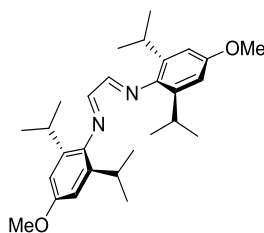
In a round bottom flask, 2,6-di-*iso*-propylaniline (7.15 mL, 37.9 mmol) and glyoxal 40% w/w in water (2.0 mL, 17.2 mmol) were introduced in MeOH (40 mL). The reaction mixture was stirred at room temperature overnight. The precipitate was collected on a frit, washed with MeOH and dried under vacuum. The product was obtained as a yellow powder (5.12 g, 79% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.21 (d, *J* = 6.9 Hz, 24H, CH(CH₃)₂), 2.94 (sept, *J* = 6.9 Hz, 4H, CH(CH₃)₂), 7.11-7.23 (m, 6H, *CH*_{aromatic}), 8.11 (s, 2H, CH=N) ppm. (in good agreement with the literature).^{2,3}

1,4-di(-2,6-di-*iso*-propylphenyl) -2,3-dimethyl -1,4-diaza-1,3-butadiene (S4)



In a round bottom flask, 2,6-di-*iso*-propylaniline (5.32 mL, 28.2 mmol), 2,3-butandione (1.24 mL, 14.1 mmol) and formic acid (99 drops) were introduced in absolute EtOH (20 mL). The reaction mixture was stirred at room temperature overnight. Then, the flask was cooled down in an ice-water bath for 30 minutes to obtain a precipitate which was collected on a frit, washed with cold MeOH and dried under vacuum. The pure product was obtained as a yellow powder (3.95 g, 69% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.18 (d, *J* = 7.0 Hz, 12H, CH(CH₃)₂), 1.20 (d, *J* = 7.0 Hz, 12H, CH(CH₃)₂), 2.10 (s, 6H, CH₃CH=N), 2.72 (sept, *J* = 7.0 Hz, 4H, CH(CH₃)₂), 7.09-7.13 (m, 2H, *CH*_{aromatic}), 7.14-7.20 (m, 4H, *CH*_{aromatic}) ppm. (in good agreement with the literature).⁴

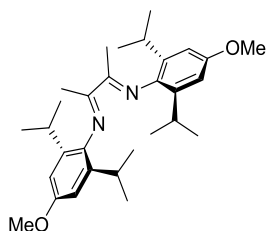
1,4-di(-4-methoxy-2,6-di-*iso*-propylphenyl)-1,4-diaza-1,3-butadiene (S5)



In a Schlenk tube, 4-methoxy-2,6-di-*iso*-propylaniline (S2) (2.0 g, 9.65 mmol) and glyoxal 40% w/w in water (0.55 mL, 4.82 mmol) were introduced in MeOH (20 mL). The reaction mixture was stirred at

room temperature overnight. The mixture was concentrated under vacuum and the residue was recrystallized from methanol and filtered. The product was obtained as a yellow powder (1.39 g, 66%). ¹H-NMR (CDCl₃, 400 MHz): δ 1.20 (d, *J* = 6.8 Hz, 24H, CH(CH₃)₂), 2.98 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 3.84 (s, 6H, OCH₃), 6.74 (s, 4H, *CHaromatic*), 8.08 (s, 2H, CH=N) ppm.(in good agreement with the literature).⁵

1,4-di(-4-methoxy-2,6-di-*iso*-propylphenyl)-2,3-dimethyl-1,4-diaza-1,3-butadiene (S6)

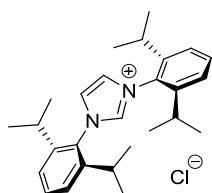


In a Schlenk tube under argon, 4-methoxy-2,6-di-*iso*-propylaniline (**S2**) (386 mg, 1.86 mmol), 2,3-butandione (66 μL, 0.75 mmol) and formic acid (99 drops) were introduced in methanol (12 mL). Reaction mixture was heated at 60°C for 3 days. After cooling down the reaction mixture to room temperature, solvent was removed under vacuum. Adding fresh methanol resulted into formation of a precipitate which was collected on a frit and washed with cold methanol. Recrystallization in methanol yielded into pure diimine **S6** as a yellow solid (672 mg, 60%). ¹H-NMR (CDCl₃, 400 MHz): δ 1.16 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.18 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.06 (s, 6H, CH₃C=N), 2.71 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 3.83 (s, 6H, OCH₃), 6.73 (s, 4H, *CHaromatic*) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 16.5 (2xCH₃, CH₃C=N), 22.6 (4xCH₃, CH(CH₃)₂), 22.9 (4xCH₃, CH(CH₃)₂), 28.7 (4xCH, CH(CH₃)₂), 55.3 (2xCH₃, OCH₃), 108.6 (4xCH, CH aromatic), 136.6 (4xC, *Caromatic*CH(CH₃)₂), 139.7 (2xC, CH₃C=N), 156.3 (2xC, *Caromatic*OCH₃), 169.2 (2xC, *Caromatic*-N). HRMS (ESI): *m/z* calcd for C₃₀H₄₅N₂O₂ [M+H]⁺: 465.3481; found: 465.3489. IR (neat) ν 2964, 2870, 1634, 1603, 1579, 1195, 1117, 1035, 854 cm⁻¹.

General Procedure A for the Synthesis of imidazolium salts.⁶

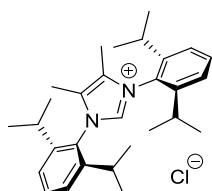
In a dry flamed Schlenk tube under argon atmosphere, the diimine (1 equiv.) was introduced in freshly distilled EtOAc (2.5 mL per mmol) and cooled down to 0 °C. In a test tube, paraformaldehyde (1.3 equiv.) was stirred in a 4 M dioxane solution of HCl (1.6 equiv.) for 10 minutes and added to the diimine solution at 0 °C. The reaction mixture was stirred at room temperature overnight. The precipitate was collected on a frit and washed with EtOAc. Then, the residue was dissolved in MeOH and anhydrous NaHCO₃ (2.5 equiv.) was added. The resulting mixture was stirred at room temperature for 1 hour. Diethyl ether was added affording a precipitate which was collected on a frit and dried under vacuum leading to the pure imidazolium salt.

1,3-bis(-2,6-di-*iso*-propylphenyl)imidazolium chloride (S7)



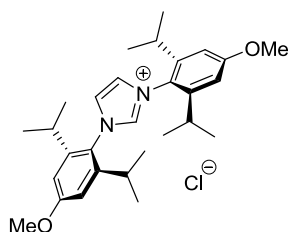
Using diimine **S3** (30.0 g, 79.7 mmol) and following the general procedure **A**, pure product **S7** was obtained as a white powder (19.0 g, 58% yield). ¹H-NMR (d₄-MeOD, 400 MHz): δ 1.27 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.35 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.50 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 7.53 (d, *J* = 7.8 Hz, 4H, CH_{aromatic}), 7.69 (t, *J* = 7.8 Hz, 2H, CH_{aromatic}), 8.29 (s, 2H, CH_{imidazolium}) 9.98 (s, 1H, NCHN) ppm. (in good agreement with the literature).⁶

1,3-bis(-2,6-di-*iso*-propylphenyl)-4,5-dimethylimidazolium chloride (S8)



Using diimine **S4** (3.15 g, 7.78 mmol) and following the general procedure **A**, pure product **S8** was obtained as a white powder (2.73 mg, 77% yield). ¹H-NMR (d₄-MeOD, 400 MHz): δ 1.20 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.32 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.15 (s, 6H, CH_{3imidazolium}), 2.39 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 7.52 (d, *J* = 7.8 Hz, 4H, CH_{aromatic}), 7.67 (t, *J* = 7.8 Hz, 2H, CH_{aromatic}), 9.78 (s, 1H, NCHN) ppm. ¹³C-NMR (d₄-MeOD, 100 MHz): δ 9.78 (2xCH₃, CH_{3imidazolium}), 24.1 (4xCH₃, CH(CH₃)₂), 26.3 (4xCH₃, CH(CH₃)₂), 31.1 (4xCH, CH(CH₃)₂), 127.1 (4xCH, CH_{aromatic}), 130.3 (2xC, NCH_{imidazolium}N), 131.8 (2xC, CH_{aromatic}N), 134.4 (2xCH, CH_{aromatic}), 147.8 (4xC, CH_{aromatic}CH(CH₃)₂) (CH of NHC not observed) ppm. (in good agreement with the literature).⁷

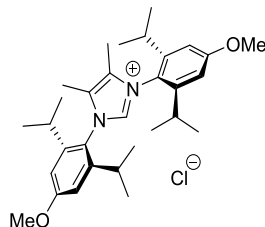
1,3-bis(-4-methoxy-2,6-di-*iso*-propylphenyl)imidazolium chloride (S9)



Using diimine **S5** (1.33 g, 3.05 mmol) and following the general procedure **A**, pure product **S9** was obtained as a white powder (956 mg, 65% yield). ¹H-NMR (d₄-MeOD, 400 MHz): δ 1.26 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.33 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.45 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂),

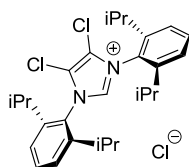
3.92 (s, 6H, OCH₃), 7.00 (s, 4H, CH_{aromatic}), 8.19 (s, 2H, CH_{imidazolium}), 9.89 (s, 1H, NCHN_{imidazolium}) ppm. (in good agreement with the literature).^{5,8}

1,3-bis(-4-methoxy-2,6-di-*iso*-propylphenyl)-4,5-dimethylimidazolium chloride (S10)



Using diimine **S6** (2.65 g, 5.70 mmol) and following the general procedure **A**, pure product **S10** was obtained as a white powder (1.68 g, 58% yield). ¹H-NMR (d₄-MeOD, 400 MHz): δ 1.23 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 1.33 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 2.17 (s, 6H, CH_{3imidazolium}), 2.37 (sept, *J* = 6.7 Hz, 4H, CH(CH₃)₂), 3.92 (s, 6H, OCH₃), 7.02 (s, 4H, CH_{aromatic}), 9.72 (s, 1H, CH_{imidazolium}) ppm. ¹³C-NMR (d₄-MeOD, 100 MHz): δ 8.9 (2xCH₃, CH_{3imidazolium}), 23.2 (4xCH₃, CH(CH₃)₂), 25.3 (4xCH₃, CH(CH₃)₂), 30.4 (4xCH, CH(CH₃)₂), 56.2 (2xCH₃, OCH₃), 111.4 (4xCH, CH aromatic), 122.0 (2xC, CaromaticN), 131.1 (2xC, NCCH_{3imidazolium}), 139.1 (CH, CH_{imidazolium}), 148.6 (4xC, CaromaticCH(CH₃)₂), 163.8 (2xC, CaromaticOCH₃) ppm. IR (neat) ν 2963, 2870, 1603, 1590, 1537, 1470, 1338, 1229, 1191, 1028, 850 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₁H₄₅N₂O₂ [M]⁺: 477.3481; found: 477.3486.

1,3-bis(-2,6-di-*iso*-propylphenyl)-4,5-dichloroimidazolium chloride (S11)



In a flamed dry Schlenk tube under argon atmosphere, to a suspension of NaH (96 mg, 4.0 mmol) and KO^tBu (a spatula) in dry and degassed THF (10 mL), IPr·HCl **S7** (850 mg, 2.0 mmol) was added by portions. The reaction mixture was stirred overnight at room temperature. The resulting mixture was then filtered on a frit under argon atmosphere by Schlenk technique. To the resulting clear solution of free carbene IPr, CCl₄ (386 μL, 4.0 mmol) was added and the reaction mixture was stirred for an additional 3 hours at room temperature. Then, a 4 M dioxane solution of HCl (1.0 mL) was added dropwise at room temperature affording a white precipitate. After a vigorous stirring for an additional 30 min at room temperature, the precipitate was collected on a frit, washed with Et₂O (3x 10 mL) and dried under vacuum. The pure product **S11** was obtained as a white powder (661 mg, 67% yield). ¹H-NMR (d₄-MeOD, 400 MHz): δ 1.27 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.38 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.49 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 7.60 (d, *J* = 7.8 Hz, 4H, CH_{aromatic}), 7.77 (t, *J* =

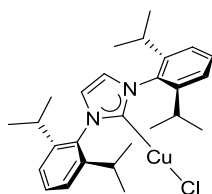
7.8 Hz, 2H, *CHaromatic*) ppm. (in good agreement with the literature).^{9,10}

Part 2: Synthesis of [CuX(NHC)] precursors **1-5** and **16**.

General Procedure B for the Synthesis of [CuCl(NHC)] complexes.^{11,12}

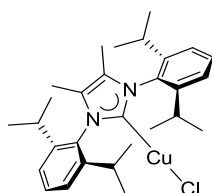
In a dry flamed Schlenk tube under argon atmosphere, imidazolium chloride salt (1 eq.) and copper oxide (0.65 eq.) were introduced in dry and degassed toluene. The reaction mixture was heated under reflux for 12 h. After cooling down to room temperature, the mixture was dissolved in dichloromethane and filtered through a pad of silica. The filtrate was evaporated to dryness and the product was obtained as a white powder without any further purification.

[CuCl(**IPr**)] (1,3-bis(2,6-di-*iso*-propylphenyl)imidazol-2-ylidene) copper chloride (**1**)



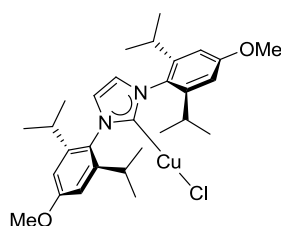
Using imidazolium salt **S7** (5.0 g, 11.75 mmol) and following the general procedure **B**, the copper complex **1** was obtained as a white powder (4.61 g, 80% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.22 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.30 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.56 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 7.13 (s, 2H, CHimidazolylidene), 7.29 (d, *J* = 7.8 Hz, 4H, CHaromatic), 7.49 (t, *J* = 7.8 Hz, 2H, CHaromatic) ppm. (in good agreement with the literature).^{11,12}

[CuCl(^{Me}**IPr**)] (1,3-bis(2,6-di-*iso*-propylphenyl)-4,5-dimethylimidazol-2-ylidene) copper chloride (**2**)



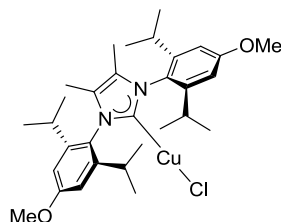
Using imidazolium salt **S8** (453 mg, 1.0 mmol) and following the general procedure **B**, the copper complex **2** was obtained as a white powder (485 mg, 94% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.23 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 1.28 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 1.92 (s, 6H, CH₃Cimidazolylidene), 2.45 (sept, *J* = 6.9 Hz, 4H, CH(CH₃)₂), 7.29 (d, *J* = 7.8 Hz, 4H, CHaromatic), 7.48 (t, *J* = 7.48 Hz, 2H, CHaromatic) ppm. (in good agreement with the literature).¹³

[CuCl(IPr^{MeO})] (1,3-bis(4-methoxy-2,6-di-*iso*-propylphenyl)imidazol-2-ylidene) copper chloride (**3**)



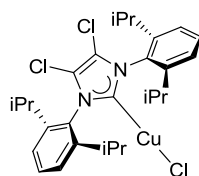
Using imidazolium salt **S9** (485 mg, 1.0 mmol) and following the general procedure **B**, the copper complex **3** was obtained as a white powder (447 mg, 82% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.20 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 1.28 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 2.51 (sept, *J* = 6.7 Hz, 4H, CH(CH₃)₂), 3.88 (s, 6H, OCH₃), 6.77 (s, 4H, CH_{aromatic}), 7.07 (s, 2H, CH_{imidazolylidene}) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 22.9 (4xCH₃, CH(CH₃)₂), 23.9 (4xCH₃, CH(CH₃)₂), 28.00 (4xCH, CH(CH₃)₂), 54.5 (2xCH₃, OCH₃), 108.6 (4xCH, CH_{aromatic}), 122.6 (2xCH, CH_{imidazolylidene}), 126.6 (2xC, CH_{aromatic}N), 146.2 (4xC, CH_{aromatic}CH(CH₃)₂), 169.9 (2xC, CH_{aromatic}OCH₃), 180.5 (C, Cu_{imidazolylidene}) ppm. IR (neat) ν 2962, 2869, 1601, 1590, 1335, 1226, 1036, 876 cm⁻¹. HRMS (ESI): *m/z* calcd for C₂₉H₄₀N₂O₂NaClCu [M+Na]⁺: 569.1972; found: 569.1978.

[CuCl(MeIPr^{MeO})] (1,3-bis(4-methoxy-2,6-di-*iso*-propylphenyl)-4,5-dimethylimidazol-2-ylidene) copper chloride (**4**)



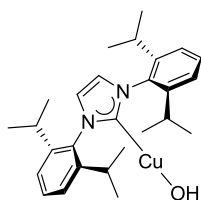
Using imidazolium salt **S10** (513 mg, 1.0 mmol) and following the general procedure **B**, the copper complex **4** was obtained as a white powder (405 mg, 70% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.19 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 1.25 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 1.88 (s, 6H, CH_{3imidazolylidene}), 2.40 (sept, *J* = 6.7 Hz, 4H, CH(CH₃)₂), 3.86 (s, 6H, OCH₃), 6.76 (s, 4H, CH_{aromatic}) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 9.5 (2xCH₃, CH_{3imidazolylidene}), 23.2 (4xCH₃, CH(CH₃)₂), 25.4 (4xCH₃, CH(CH₃)₂), 28.8 (4xCH, CH(CH₃)₂), 55.3 (2xCH₃, OCH₃), 109.6 (4xCH, CH_{aromatic}), 125.9 (2xC, CH_{aromatic}N), 126.2 (2xC, CH_{3imidazolylidene}), 147.36 (4xC, CH_{aromatic}CH(CH₃)₂), 160.6 (2xC, CH_{aromatic}OCH₃), 177.7 (C, Cu_{imidazolylidene}) ppm. IR (neat) ν 2961, 2926, 1602, 1589, 1471, 1335, 1293, 1031, 847 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₁H₄₄N₂O₂NaClCu [M+Na]⁺: 597.2285; found: 597.2306.

[CuCl(^{Cl}IPr)] (1,3-bis(2,6-di-*iso*-propylphenyl)-4,5-dichloroimidazol-2-ylidene) copper chloride (**5**).



Using imidazolium salt **S11** (342 mg, 0.7 mmol) and following the general procedure **B**, the copper complex **5** was obtained as a white powder (155 mg, 40% yield). ¹H-NMR (CDCl₃ – 400 MHz): δ 1.27 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 1.29 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 2.46 (sept, *J* = 6.9 Hz, 4H, CH(CH₃)₂), 7.33 (d, *J* = 7.8 Hz, 4H, CH_{aromatic}), 7.55 (t, *J* = 7.8 Hz, 2H, CH_{aromatic}) ppm. (in good agreement with the literature).^{13, 14}

[CuOH(IPr)] (1,3-bis(2,6-di-*iso*-propylphenyl)imidazol-2-ylidene) copper hydroxide (**16**)¹⁵



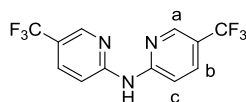
In a flamed-dried Schlenk tube under argon atmosphere, [CuCl(IPr)] (**1**) (1.00 g, 2.05 mmol) and CsOH·H₂O (691 mg, 4.10 mmol) were introduced in dry and degassed THF (20 mL). The reaction mixture was stirred at room temperature for 20 hours. Then, the reaction mixture was filtered through a pad of Celite®, the cake was washed with THF. The filtrate was concentrated to get a 5 mL solution and pentane was added, affording a white precipitate which was collected on a frit, washed with pentane and dried under vacuum. The pure complex **16** was obtained as a white powder (687 mg, 71% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.21 (d, *J* = 6.6 Hz, 12H, CH(CH₃)₂), 1.29 (d, *J* = 6.6 Hz, 12H, CH(CH₃)₂), 2.55 (sept, *J* = 6.6 Hz, 4H, CH(CH₃)₂), 7.09 (s, 2H, CH_{imidazolylidene}), 7.28 (d, *J* = 7.6 Hz, 4H, CH_{aromatic}), 7.47 (t, *J* = 7.6 Hz, 2H, CH_{aromatic}) ppm. (in good agreement with the literature)¹⁵

Part 3: Synthesis of ligands L2-L6

*General procedure C for the synthesis of dipyridylamine derivatives.*¹⁶

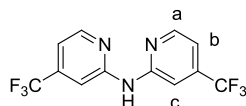
In a dry flamed Schlenk tube under argon atmosphere, Pd(dba)₂ (0.02 equiv.) and dppp (0.04 equiv.) were dissolved in dry and degassed toluene (25 ml). The 2-bromopyridine derivative (1 equiv.) was added, successively followed by the 2-aminopyridine derivative (1.2 equiv.) and KO^tBu (1.4 equiv.). The reaction mixture was heated at 110 °C overnight. After cooling to room temperature, the solution was filtered through a pad of Celite®. The cake was washed with ethyl acetate. The filtrate was concentrated under vacuum, leading to a brownish solid. The crude product was purified by flash chromatography on silica gel.

5,5'-di(trifluoromethyl)-2,2'-dipyridylamine (L2)



Using 2-bromo-5-trifluoromethylpyridine (1.47 g, 6.50 mmol) and 2-amino-5-trifluoromethylpyridine (1.26 g, 7.80 mmol) and following the general procedure C, the dpa derivative L2 (eluent pentane/EtOAc: 95/5) was obtained as a beige powder (1.18 g, 59% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 7.72 (d, *J* = 8.8 Hz, 2H, Hc), 7.86 (dd, *J* = 8.8, 2.3 Hz, 2H, Hb), 8.34 (*br s*, 1H, NH), 8.56 (s, 2H, Ha) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 111.7 (s, 2xCH, Cc), 120.1 (q, ²*J*_{13C-19F} = 33.3 Hz, 2xC, C-CF₃), 123.9 (q, ¹*J*_{13C-19F} = 271 Hz, 2xCF₃), 135.3 (q, ³*J*_{13C-19F} = 3.2 Hz, 2xCH, Cb), 145.4 (q, ³*J*_{13C-19F} = 4.2 Hz, 2xCH, Ca), 155.5 (s, 2xC, C-NH) ppm. ¹⁹F-NMR (CDCl₃, 376 MHz): δ -61.7 ppm. IR (neat) ν 1608, 1531, 1408, 1315, 1117, 1078, 835 cm⁻¹. HRMS (ESI): *m/z* calcd for C₁₂H₈N₃F₆ [M+H]⁺: 308.0622; found: 308.0634.

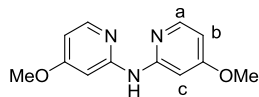
4,4'-di(trifluoromethyl)-2,2'-dipyridylamine (L3)



Using 2-bromo-4-trifluoromethylpyridine (737 mg, 3.26 mmol) and 2-amino-4-trifluoromethylpyridine (348 μL, 3.92 mmol) and following the general procedure C, the dpa derivative L3 (eluent pentane/EtOAc: 70/30) was obtained as a beige powder (996 mg, 99% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 7.12 (d, *J* = 4.9 Hz, 2H, Hb), 7.86 (s, 2H, Hc), 8.15 (s, 1H, NH), 8.46 (d, *J* = 4.9 Hz, 2H, Ha) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 108.0 (q, ³*J*_{13C-19F} = 4.0 Hz, 2xCH, Cb), 112.5 (q, ³*J*_{13C-19F} = 3.3 Hz, 2xCH, Cc), 122.8 (q, ¹*J*_{13C-19F} = 273 Hz, 2xCF₃), 140.2 (q, ²*J*_{13C-19F} = 33.8 Hz, 2xC, C-CF₃), 149.0 (s, 2xCH, Ca), 154.1 (s, 2xC, C-NH) ppm. ¹⁹F-NMR (CDCl₃, 376 MHz): δ -

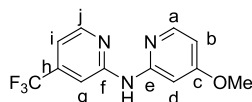
65.0 ppm. IR (neat) ν 1614, 1547, 1429, 1318, 1165, 1134, 1085, 832 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_8\text{N}_3\text{F}_6$ $[\text{M}+\text{H}]^+$: 308.0622; found 308.0610.

4,4'-dimethoxy-2,2'-dipyridylamine (L4)



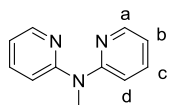
Using 2-bromo-4-methoxypyridine (1.06 mL, 8.65 mmol) and 2-amino-4-methoxypyridine (1.29 g, 10.4 mmol) and following the general procedure **C**, the dpa derivative **L4** (eluent pentane/EtOAc: 30/70) was obtained as a white yellowish powder (628 mg, 31% yield). $^1\text{H-NMR}$ (CDCl_3 , 400 MHz): δ 3.85 (s, 6H, OCH_3), 6.44 (dd, $J = 6.0, 2.4$ Hz, 2H, Hb), 7.13 (d, $J = 2.4$ Hz, 2H, Hc), 8.06 (d, $J = 6.0$ Hz, 2H, Ha) ppm. $^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz): δ 55.2 (2x CH_3 , OCH_3), 96.1 (2xCH, Cc), 104.7 (2xCH, Cb), 148.3 (2xCH, Ca), 156.0 (2xC, C-NH), 167.2 (2xC, C- OCH_3) ppm. IR (neat) ν 1593, 1564, 1538, 1434, 1210, 1172, 1042, 800 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{14}\text{N}_3\text{O}_2$ $[\text{M}-\text{H}]^+$: 232.1086; found: 232.1093.

4-trifluoromethyl-4'-methoxy-2,2'-dipyridylamine (L5)



Using 2-bromo-4-trifluoromethylpyridine (432 μL , 3.50 mmol) and 2-amino-4-methoxypyridine (521 mg, 4.20 mmol) and following the general procedure **C**, the dpa derivative **L5** (eluent pentane/EtOAc: 40/60) was obtained as a white yellowish powder (811 mg, 86% yield). $^1\text{H-NMR}$ (CDCl_3 , 400 MHz): δ 3.88 (s, 3H, OCH_3), 6.52 (dd, $J = 5.9, 2.1$ Hz, 1H, Hb), 7.04 (d, $J = 5.1$ Hz, 1H, Hi), 7.13 (s, 1H, Hd), 7.89 (s, 1H, Hg), 8.11 (d, $J = 5.9$ Hz, 1H, Ha), 8.39 (d, $J = 5.1$ Hz, 1H, Hj) ppm (NH not observed). $^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz): δ 55.2 (s, CH, OCH_3), 96.7 (s, CH, Cd), 105.1 (s, CH, Cb), 107.9 (q, $^3J_{13\text{C}-19\text{F}} = 3.1$ Hz, CH, Cg), 111.5 (q, $^3J_{13\text{C}-19\text{F}} = 3.1$ Hz, CH, Ci), 122.9 (q, $^1J_{13\text{C}-19\text{F}} = 273.3$ Hz, CF_3), 139.9 (q, $^2J_{13\text{C}-19\text{F}} = 33.6$ Hz, C, Ch), 148.5 (s, CH, Cj), 148.8 (s, CH, Ca), 154.9 (s, C, Cf), 155.2 (s, C, Ce), 167.4 (s, C, Cc) ppm. $^{19}\text{F-NMR}$ (CDCl_3 , 376 MHz): δ -65.0 ppm. IR (neat) ν 1598, 1492, 1426, 1394, 1333, 1276, 1165, 1127, 821 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{11}\text{N}_3\text{OF}_3$ $[\text{M}+\text{H}]^+$: 270.0654; found: 270.0845.

N-methyl-2,2'-dipyridylamine (L6)



In a round bottom flask 2,2'-dipyridylamine **L1** (1.20 g, 7.00 mmol) and KOH (1.97 g, 35.0 mmol) were introduced in DMSO (35 mL). The reaction mixture was stirred at room temperature for 30 min. Iodomethane (524 μ L, 8.40 mmol) was added and the reaction mixture was stirred at room temperature for 1 h. Water (50 mL) was added and the aqueous layer was extracted with Et₂O (3x50 mL). The combined organic layers were dried over Na₂SO₄, filtered and concentrated under vacuum. The crude product was purified by flash chromatography on silica gel (pentane/EtOAc: 50/50) to obtain the pure product **L6** as a yellowish oil (1.18 g, 91% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 3.64 (s, 3H, CH₃-N), 6.87 (t, J = 8.4 Hz, 2H, Hb), 7.17 (d, J = 8.4 Hz, 2H, Hd), 7.55 (td, J = 8.4, 4.2 Hz, 2H, Hc), 8.35 (d, J = 4.2 Hz, 2H, Ha) ppm. (in good agreements with the literature).¹⁷

Part 4: Synthesis of copper complexes [Cu(NHC)(N[^]N)][X] 7-15

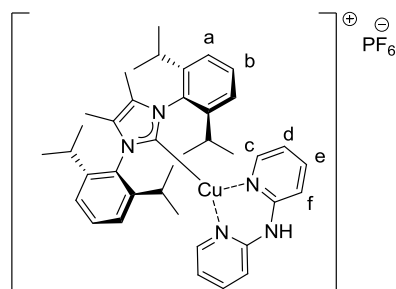
For NMR description and spectra of complexes 17-19, see our previous work (manuscript and ESI).¹⁸

*General procedures D for the synthesis of [Cu(NHC)(N[^]N)][X] complexes.*¹⁸

Procedure D1: In a flame-dried Schlenk tube under argon atmosphere, [CuCl(NHC)] complex (1 equiv.) and dpa ligand (1.05 equiv.) were dissolved in degassed absolute ethanol and heated under reflux for one hour. After cooling the reaction mixture to room temperature, aqueous solution of KPF₆ (2 equiv.) was added affording a white precipitate. The solid was collected on a frit, washed with water and dried under air and then under vacuum.

Procedure D2: In a flame-dried Schlenk tube under argon atmosphere, [CuOH(IPr)] complex 16 (1 equiv.) and dpa ligand (1 equiv.) were dissolved in dry degassed toluene. HBF₄·Et₂O (1 equiv.) was added dropwise and the reaction mixture was stirred overnight at room temperature. Pentane was added, affording a white precipitate which was collected on a frit, washed with pentane and dried under vacuum. Then, in a round bottom flask, the [Cu(IPr)(N[^]N)][BF₄] complex and KPF₆ (5 equiv.) were dissolved in MeOH, the mixture was stirred for 1 hour at room temperature. The mixture was then concentrated to dryness, the crude mixture was dissolved in dichloromethane, filtered through a pad of Celite® and filtrate was concentrated under vacuum, leading to the pure [Cu(IPr)(N[^]N)][PF₆] complex as a powder.

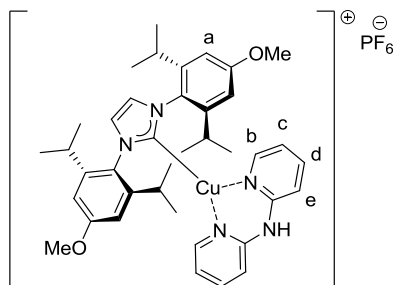
[Cu^{(Me)IPr}(L1)][PF₆] (7)



Using copper complex 2 (110 mg, 0.21 mmol) and ligand L1 (38.4 mg, 0.22 mmol) and following the general procedure D1, the complex 7 was obtained as white solid (151 mg, 90% yield). ¹H-NMR (CDCl₃, 500 MHz): δ 1.03 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.23 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.94 (s, 6H, CH₃imidazolylidene), 2.51 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 6.03 (d, *J* = 4.6 Hz, 2H, Ha), 6.28 (t, *J* = 6.4 Hz, 2H, Hd), 7.12 (d, *J* = 8.4 Hz, 2H, Hf), 7.34 (d, *J* = 7.8 Hz, 4H, Ha), 7.45 (t, *J* = 7.8 Hz, 2H, Hb), 7.58 (t, *J* = 7.8 Hz, 2H, He), 8.04-8.08 (*br s*, 1H, NH) ppm. ¹³C-NMR (CDCl₃, 125 MHz): δ 10.0 (2xCH₃, CH₃imidazolylidene), 23.3 (4xCH₃, CH(CH₃)₂), 24.9 (4xCH₃, CH(CH₃)₂), 28.8 (4xCH, CH(CH₃)₂), 115.2 (2xCH, Cf), 116.4 (2xCH, Cd), 125.0 (4xCH, Ca), 126.2 (2xC, CH₃C-Nimidazolylidene), 130.7 (2xCH, Cb), 134.7 (2xC, Caromatic-Nimidazolylidene), 139.1 (2xCH, Ce), 146.4 (4xC, CaromaticCH(CH₃)₂), 147.4 (2xCH, Cc), 153.1 (2xC, CaromaticNH dpa) 179.4 (C,

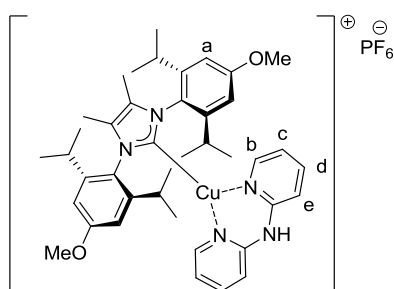
CuCimidazolylidene) ppm. IR (neat) ν 3385, 2966, 1627, 1580, 1472, 1363, 839 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{39}\text{H}_{49}\text{CuN}_5 [\text{M}-\text{PF}_6]^+$: 650.3284; found: 650.3309.

[Cu(IPr^{OMe})(L1)][PF₆] (8)



Using copper complex **3** (181 mg, 0.33 mmol) and ligand **L1** (60.0 mg, 0.35 mmol) and following the general procedure **D1**, the complex **8** was obtained as white solid (234 mg, 86% yield). ¹H-NMR (CDCl_3 , 400 MHz): δ 1.05 (d, $J = 6.7$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.20 (d, $J = 6.7$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 2.61 (sept, $J = 6.7$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 3.92 (s, 6H, OCH_3), 6.30 (d, $J = 4.3$ Hz, 2H, Hb), 6.33 (t, $J = 5.8$ Hz, 2H, Hc), 6.80 (s, 4H, Ha), 7.15 (m, 4H, 2Himidazolylidene + 2H, He), 7.49 (t, $J = 7.2$ Hz, 2H, Hd), 8.09-8.13 (br s, 1H, NH) ppm. ¹³C-NMR (CDCl_3 , 100 MHz): δ 24.0 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 24.2 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 28.9 (4xCH, $\text{CH}(\text{CH}_3)_2$), 55.7 (2x CH_3 , OCH_3), 109.9 (4xCH, Ca), 115.2 (2xCH, Ce), 116.2 (2xCH, Cc), 123.8 (2xCH, CHimidazolylidene), 129.2 (2xC, Caromatic-Nimidazolylidene), 139.2 (2xCH, Nd), 147.7 (4xC, Caromatic $\text{CH}(\text{CH}_3)_2$), 147.8 (2xCH, Cb), 153.1 (2xC, CaromaticNH dpa), 161.0 (2xC, C- OCH_3), 184.3 (C, CuCimidazolylidene) ppm. IR (neat) ν 3386, 2963, 1632, 1583, 1474, 1334, 837 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{39}\text{H}_{49}\text{CuN}_5\text{O}_2 [\text{M}-\text{PF}_6]^+$: 682.3182; found: 682.3199.

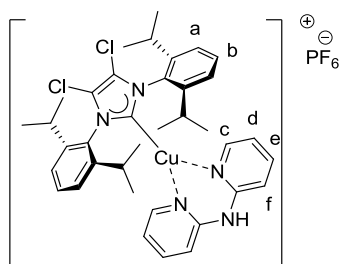
[Cu(^{Me}IPr^{OMe})(L1)][PF₆] (9)



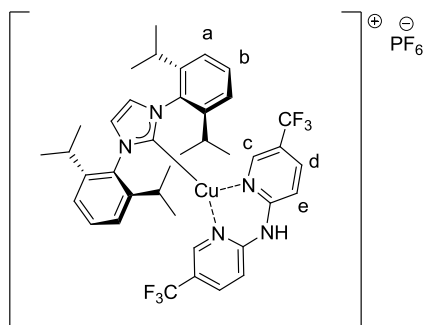
Using copper complex **4** (190 mg, 0.33 mmol) and ligand **L1** (60.0 mg, 0.33 mmol) and following the general procedure **D1** gave a mixture of expected complex **9** and starting materials (**4** and **L1**). After a recrystallization by slow gas diffusion of pentane in a dichloromethane solution of the crude mixture, the pure complex **9** was obtained as white solid (158 mg, 56% yield). ¹H-NMR (CDCl_3 , 500 MHz): δ 1.00 (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.20 (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.94 (s, 6H, CH_3 imidazolylidene), 2.46 (sept, $J = 6.8$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 3.93 (s, 6H, OCH_3), 6.18 (d, $J = 4.5$ Hz,

2H, Hb), 6.32 (t, $J = 6.3$ Hz, 2H, Hc), 6.80 (s, 4H, Ha), 7.09 (d, $J = 8.5$ Hz, 2H, He), 7.47 (td, $J = 7.2$, 1.4 Hz, 2H, Hd), 8.00 (s, 1H, NH) ppm. ^{13}C -NMR (CDCl_3 , 125 MHz): δ 9.9 (2x CH_3 , $\text{CH}_3\text{imidazolylidene}$), 23.2 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 24.8 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 28.9 (4x CH , $\text{CH}(\text{CH}_3)_2$), 55.6 (2x CH_3 , OCH_3), 110.0 (4x CH , Ca), 115.0 (2x CH , Ce), 116.1 (2x CH , Cc), 126.5 (2x C , *Caromatic-Nimidazolylidene*), 127.7 (2x C , $\text{CH}_3\text{C-Nimidazolylidene}$), 139.0 (2x CH , Cd), 147.8 (4x C , *CaromaticCH}(\text{CH}_3)_2*), 147.9 (2x CH , Cb), 153.1 (2x C , *CaromaticNH dpa*), 161.1 (2x C , C-OCH_3), 180.3 (C, *CuCimidazolylidene*) ppm. IR (neat) ν 3386, 2961, 1630, 1582, 1471, 1335, 838 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{41}\text{H}_{53}\text{CuN}_5\text{O}_2$ $[\text{M-PF}_6]^+$: 710.3495; found: 710.3517.

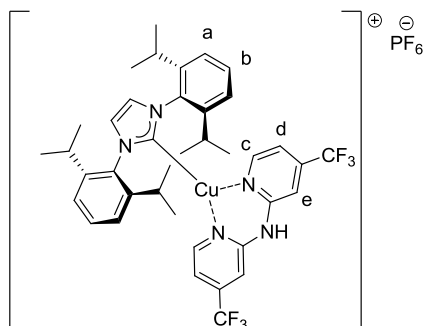
[Cu($^{\text{Cl}}\text{IPr}$)(L1)][PF₆] (10)



Using copper complex **5** (71.6 mg, 0.13 mmol) and ligand **L1** (23.1 mg, 0.14 mmol) and following the general procedure **D1**, the complex **10** was obtained as white solid (89.4 mg, 82% yield). ^1H -NMR (CDCl_3 , 500 MHz): δ 1.06 (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.27 (d, $J = 6.8$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 2.53 (sept, $J = 6.8$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 6.05 (d, $J = 4.1$ Hz, 2H, Hc), 6.31 (t, $J = 6.3$ Hz, 2H, Hd), 7.17 (d, $J = 8.4$ Hz, 2H, Hf), 7.37 (d, $J = 7.8$ Hz, 4H, Ha), 7.49 (dd, $J = 8.4$, 1.7 Hz, 2H, He), 7.65 (t, $J = 7.8$ Hz, 2H, Hb), 8.10-8.14 (*br s*, 1H, NH) ppm. ^{13}C -NMR (CDCl_3 , 125 MHz): δ 23.4 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 24.5 (4x CH_3 , $\text{CH}(\text{CH}_3)_2$), 29.2 (4x CH , $\text{CH}(\text{CH}_3)_2$), 115.5 (2x CH , Cf), 116.7 (2x CH , Cd), 119.1 (2x C , $\text{ClC-Nimidazolylidene}$), 125.2 (4x CH , Ca), 131.7 (2x CH , Cb), 133.0 (2x C , *Caromatic-Nimidazolylidene*), 139.4 (2x CH , Ce), 146.7 (4x C , *Caromatic CH}(\text{CH}_3)_2*), 147.1 (2x CH , Cc), 153.1 (2x C , *CaromaticNdpa*), 182.6 (C, *CuCimidazolylidene*) ppm. IR (neat) ν 3383, 2960, 1627, 1581, 1470, 1363, 837 cm^{-1} . HRMS (ESI): m/z calcd for $\text{C}_{37}\text{H}_{43}\text{N}_5\text{C}_1_2\text{Cu}$ $[\text{M-PF}_6]^+$: 690.2192; found: 690.2174.

[Cu(IPr)(L2)][PF₆] (11)

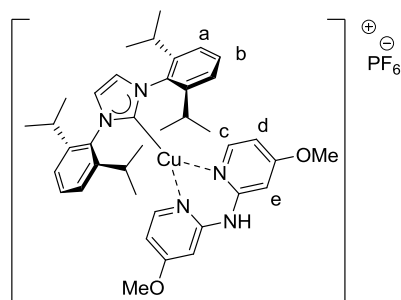
Using copper complex **16** (155 mg, 0.33 mmol), ligand **L2** (101 mg, 0.33 mmol), HBF₄·Et₂O (45 μL, 0.33 mmol) and following the general procedure **D2**, the complex **11** was obtained as an off-white powder (176 mg, 70% yield). ¹H-NMR (CDCl₃, 500 MHz): δ 1.11 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.22 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.70 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 7.02 (s, 2H, Hc), 7.23 (s, 2H), 7.28 (d, *J* = 7.8 Hz, 4H, Ha), 7.44 (d, *J* = 8.5 Hz, 2H, Hd), 7.49 (t, *J* = 7.8 Hz, 2H, Hb), 7.79 (d, *J* = 8.5 Hz, 2H, He) ppm. ¹³C-NMR (CDCl₃, 125 MHz) (signals of the CF₃ substituent were not observed): δ 23.9 (4xCH₃, CH(CH₃)₂), 24.0 (4xCH₃, CH(CH₃)₂), 28.7 (4xCH, CH(CH₃)₂), 116.4 (2xCH, Ce), 123.7 (2xCH, CHimidazolylidene), 124.7 (4xCH, Ca), 131.1 (2xCH, Cb), 135.1 (2xC, Caromatic-Nimidazolylidene), 136.7 (2xCH, Cd), 144.6 (2xCH, Cc), 145.2 (4xC, CaromaticCH(CH₃)₂), 154.6 (2xC, CaromaticNdpa), 182.0 (C, CuCimidazolylidene) (signals of the CF₃ substituent and the quaternary carbon bearing the CF₃ substituent were not observed). ¹⁹F-NMR (CDCl₃, 376 MHz): δ -71.7 (d, ¹J_{19F-31P} = 710 Hz, 6F), -61.2 (s, 6F) ppm. ³¹P-NMR (CDCl₃, 160 MHz): δ -144.0 (sept, ¹J_{31P-19F} = 710 Hz, 1P) ppm. IR (neat) ν 2965, 1631, 1493, 1472, 1405, 1321, 1127, 1080, 837 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₇H₄₃N₅C₁₂Cu [M-PF₆]⁺: 758.2719; found: 758.2698.

[Cu(IPr)(L3)][PF₆] (12)

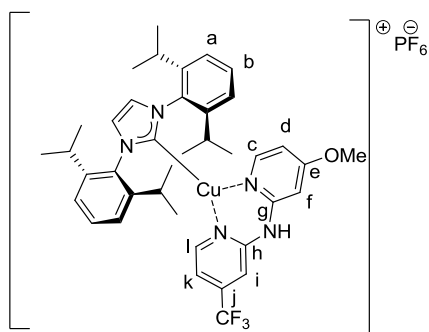
Using copper complex **1** (302 mg, 0.62 mmol) and ligand **L3** (200 mg, 0.65 mmol) and following the general procedure **D1** gave a mixture of expected complex **12** and starting materials (**1** and **L3**). After a recrystallization by slow gas diffusion of pentane in a dichloromethane solution of the crude mixture, the pure complex **12** was obtained as white solid (95 mg, 17% yield).

Using copper complex **16** (155 mg, 0.33 mmol), ligand **L3** (101 mg, 0.33 mmol), HBF₄·Et₂O (45 μL, 0.33 mmol) and following the general procedure **D2**, the complex **12** was obtained as an off-white powder (185 mg, 77% yield). ¹H-NMR (CDCl₃, 500 MHz): δ 1.02 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 1.18 (d, *J* = 6.9 Hz, 12H, CH(CH₃)₂), 2.56 (sept, *J* = 6.9 Hz, 4H, CH(CH₃)₂), 6.16 (d, *J* = 5.4 Hz, 2H, Hc), 6.46 (d, *J* = 5.4 Hz, 2H, Hd), 7.22 (s, 2H, CHimidazolylidene), 7.31 (d, *J* = 7.8 Hz, 4H, Ha), 7.42 (s, 2H, He), 7.57 (t, *J* = 7.8 Hz, 2H, Hb), 8.71 (s, 1H, NH). ¹³C-NMR (CDCl₃, 125 MHz): δ 23.8 (s, 4xCH₃, CH(CH₃)₂), 24.5 (s, 4xCH₃, CH(CH₃)₂), 28.8 (s, 4xCH, CH(CH₃)₂), 112.2 (q, ³*J*_{C-F} = 4.0 Hz, 2xCH, Ce) 112.4 (q, ³*J*_{C-F} = 4.0 Hz, 2xCH, Cd), 123.2 (q, ¹*J*_{C-F} = 274 Hz, 2x CF₃), 123.7 (s, 2xCH, CHimidazolylidene), 124.9 (s, 4xCH, Ca), 130.9 (s, 2xCH, Cb), 135.7 (s, 2xC, Caromatic-Nimidazolylidene), 141.3 (q, ²*J*_{C-F} = 35.1 Hz, 2xC, Caromatic-CF₃), 146.2 (s, 4xC, CaromaticCH(CH₃)₂), 148.9 (s, 2xCH, Cc), 153.1 (2xC, CaromaticNdpa), 181.8 (s, C, CuCimidazolylidene). ¹⁹F-NMR (CDCl₃, 376 MHz): δ - 72.1 (d, ¹*J*_{19F-31P} = 713 Hz, 6F), - 65.7 (s, 6F) ppm. ³¹P-NMR (CDCl₃, 160MHz): δ - 144.0 (sept, ¹*J*_{31P-19F} = 713 Hz, 1P). IR (neat): ν 3392, 2967, 1640, 1536, 1480, 1312, 1183, 1145, 836 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₉H₄₃N₅F₆Cu [M-PF₆]⁺: 758.2719; found: 758.2715.

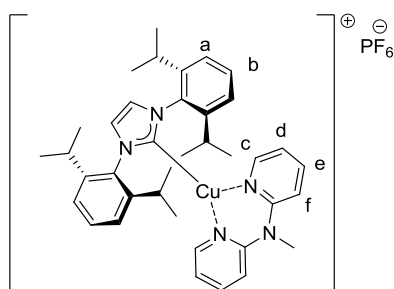
[Cu(IPr)(L4)][PF₆] (**13**)



Using copper complex **1** (150 mg, 0.30 mmol) and ligand **L4** (73.0 mg, 0.32 mmol) and following the general procedure **D1**, the complex **13** was obtained as white solid (236 mg, 95% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.09 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 1.23 (d, *J* = 6.8 Hz, 12H, CH(CH₃)₂), 2.65 (sept, *J* = 6.8 Hz, 4H, CH(CH₃)₂), 3.81 (s, 6H, OCH₃), 5.85 (s, 4H, Hc and Hd), 6.58 (s, 2H, He), 7.20 (s, 2H, CHimidazolylidene), 7.34 (d, *J* = 7.8 Hz, 4H, Ha), 7.57 (t, *J* = 7.8 Hz, 2H, Hb), 8.00 (s, 1H, NH) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 23.9 (4xCH₃, CH(CH₃)₂), 24.2 (4x CH₃, CH(CH₃)₂), 28.7 (4xCH, CH(CH₃)₂), 55.8 (2x CH₃, OCH₃), 96.2 (2xCH, Ce), 106.9 (2xCH, Cd), 123.3 (2xCH, CHimidazolylidene), 124.7 (4xCH, Ca), 130.5 (2xCH, Cb), 136.0 (2xC, Caromatic-Nimidazolylidene), 146.0 (4xC, CaromaticCH(CH₃)₂), 148.3 (2xCH, Cc), 155.0 (2xC, CaromaticN dpa), 167.2 (2xC, Caromatic-OCH₃), 183.8 (C, CuCimidazolylidene) ppm. IR (neat) ν 3408, 2965, 1629, 1592, 1470, 840 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₉H₄₉N₅O₂Cu [M-PF₆]⁺: 682.3182; found: 682.3214.

[Cu(IPr)(L5)][PF₆] (14)

Using copper complex **1** (161 mg, 0.33 mmol) and ligand **L5** (93.3 mg, 0.35 mmol) and following the general procedure **D1**, the complex **15** was obtained as white solid (262 mg, 92% yield). ¹H-NMR (CDCl₃, 400 MHz): δ 1.09 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 1.24 (d, *J* = 6.7 Hz, 12H, CH(CH₃)₂), 2.64 (sept, *J* = 6.7 Hz, 4H, CH(CH₃)₂), 3.82 (s, 3H, OCH₃), 5.85 (d, *J* = 6.6 Hz, 1H, Hc), 5.94 (dd, *J* = 6.4 and 2.2 Hz, 1H, Hd), 6.20 (d, *J* = 5.6 Hz, 1H, Hl), 6.42 (d, *J* = 5.6 Hz, 1H, Hk), 6.71 (d, *J* = 2.2 Hz, 1H, Hf), 7.24 (s, 2H, CHimidazolylidene), 7.33 (s, 1H, Hi), 7.36 (d, *J* = 7.8 Hz, 4H, Ha), 7.60 (t, *J* = 7.8 Hz, 2H, Hb), 8.37 (s, 1H, NH) ppm. ¹⁹F-NMR (CDCl₃, 376 MHz): δ -71.8 (d, *J* = 713 Hz, 6F, PF₆ anion), -65.7 (s, 3F) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 23.9 (s, 4xCH₃, CH(CH₃)₂), 24.3 (s, 4xCH₃, CH(CH₃)₂), 28.7 (s, 4xCH, CH(CH₃)₂), 56.0 (s, CH₃, OCH₃), 96.9 (s, CH, Cf), 107.8 (s, CH, Cd), 111.2 (q, ³*J*_{13C-19F} = 2.9 Hz, CH, Ck), 111.5 (q, ³*J*_{13C-19F} = 3.9 Hz, CH, Ci), 121.8 (q, ¹*J*_{13C-19F} = 274 Hz, CF₃), 123.5 (s, 2xCH, CHimidazolylidene), 124.8 (s, 4xCH, Ca), 130.7 (s, 2xCH, Cb), 135.9 (s, C, CaromaticNimidazolylidene), 140.7 (q, ²*J*_{13C-19F} = 34.9 Hz, C, Cj), 146.1 (s, 4xC, Caromatic-CH(CH₃)₂), 148.4 (s, 1xCH, Cc), 148.9 (s, 1xCH, Cl), 153.7 (s, C, Ch), 154.3 (s, C, Cg), 167.6 (s, C, Ce), 182.8 (s, C, Cucimidazolylidene) ppm. IR (neat) ν 3401, 2968, 1630, 1578, 1538, 1473, 1421, 1189, 1174, 1140, 857, 836 cm⁻¹. HRMS (ESI): *m/z* calcd for C₃₉H₄₆N₅O₃Cu [M-PF₆]⁺: 720.2950; found: 720.2939.

[Cu(IPr)(L6)][PF₆] (15)

Using copper complex **1** (161 mg, 0.333 mmol) and ligand **L6** (65.0 mg, 0.35 mmol) and following the general procedure **D1**, the complex **15** was obtained as white powder (204 mg, 79% yield). ¹H-

NMR (CDCl₃, 400 MHz): δ 1.08 (d, $J = 6.7$ Hz, 12H, CH(CH₃)₂), 1.22 (d, $J = 6.7$ Hz, 12H, CH(CH₃)₂), 2.63 (sept, $J = 6.7$ Hz, 4H, CH(CH₃)₂), 3.34 (s, 3H, CH₃N), 6.63 (d, $J = 4.6$ Hz, 4H, Hc et Hd), 7.15 (d, $J = 8.6$ Hz, 2H, Hf), 7.26 (s, 2H, CHimidazolylidene), 7.27 (d, $J = 7.8$ Hz, 4H, Ha), 7.52 (t, $J = 7.8$ Hz, 2H, Hb), 7.73 (tt, $J = 6.4, 2.6$ Hz, 2H, He) ppm. ¹H-NMR (d₆-DMSO, 400 MHz): δ 1.08 (d, $J = 6.7$ Hz, 12H, CH(CH₃)₂), 1.19 (d, $J = 6.7$ Hz, 12H, CH(CH₃)₂), 2.56 (sept, $J = 6.7$ Hz, 4H, CH(CH₃)₂), 3.32 (s, 3H, CH₃N), 6.82 (t, $J = 6.4$ Hz, 2H, Hc), 7.02 (s, 2H, Hd), 7.25 (d, $J = 8.5$ Hz, 2H, Hf), 7.36 (d, $J = 7.8$ Hz, 4H, Ha), 7.54 (t, $J = 7.8$ Hz, 2H, Hb), 7.80 (t, $J = 7.1$ Hz, 2H, He), 7.91 (s, 2H, CHimidazolylidene) ppm. ¹³C-NMR (CDCl₃, 100 MHz): δ 24.0 (4xCH₃, CH(CH₃)₂), 24.1 (4xCH₃, CH(CH₃)₂), 28.7 (4xCH, CH(CH₃)₂), 39.2 (CH₃, CH₃-N), 114.6 (2xCH, Cf), 118.9 (2xCH, Cd), 123.3 (2xCH, CHimidazolylidene), 124.4 (4xCH, Ca), 130.5 (2xCH, Cb), 135.7 (2xC, Caromatic-Nimidazolylidene), 140.1 (2xCH, Ce), 145.8 (4xC, CaromaticCH(CH₃)₂), 147.2 (2xCH, Cc), 155.5 (2xC, CaromaticNH dpa), 183.0 (s, C, CuCimidazolylidene) ppm. IR (neat): ν 2962, 1595, 1575, 1460, 1436, 1347, 837 cm⁻¹. HRMS (ESI): m/z calcd for C₃₈H₄₇CuN₅ [M-PF₆]⁺: 636.3127; found: 636.3109.

Part 5: Crystallographic data of [Cu(NHC)(N[^]N)][X] complexes **7-11** and **13-15**.

General Considerations. Crystallographic data sets were collected from single crystal samples. Collections were performed using a Bruker Kappa APEXII CCD diffractometer. The initial unit cell parameters were determined by a least-squares fit of the angular setting of strong reflections, collected by a 6.0° scan in 12 frames over three different parts of the reciprocal space (36 frames total). Cell refinement and data reduction were performed with SAINT (Bruker AXS). Absorption correction was done by multiscan methods using SADABS-2012/1 (Bruker AXS). The structure was solved by direct methods and refined using either SHELXL-97 or SHELXL-2013 (Sheldrick). All non-H atoms were refined by full-matrix least-squares with anisotropic displacement parameters while hydrogen atoms were placed in idealized positions. Crystal data and details of the data collection and refinement are summarized in Table S1, S2 and S3. CCDC numbers (1402282-1402289) contain the supplementary crystallographic data for this article. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

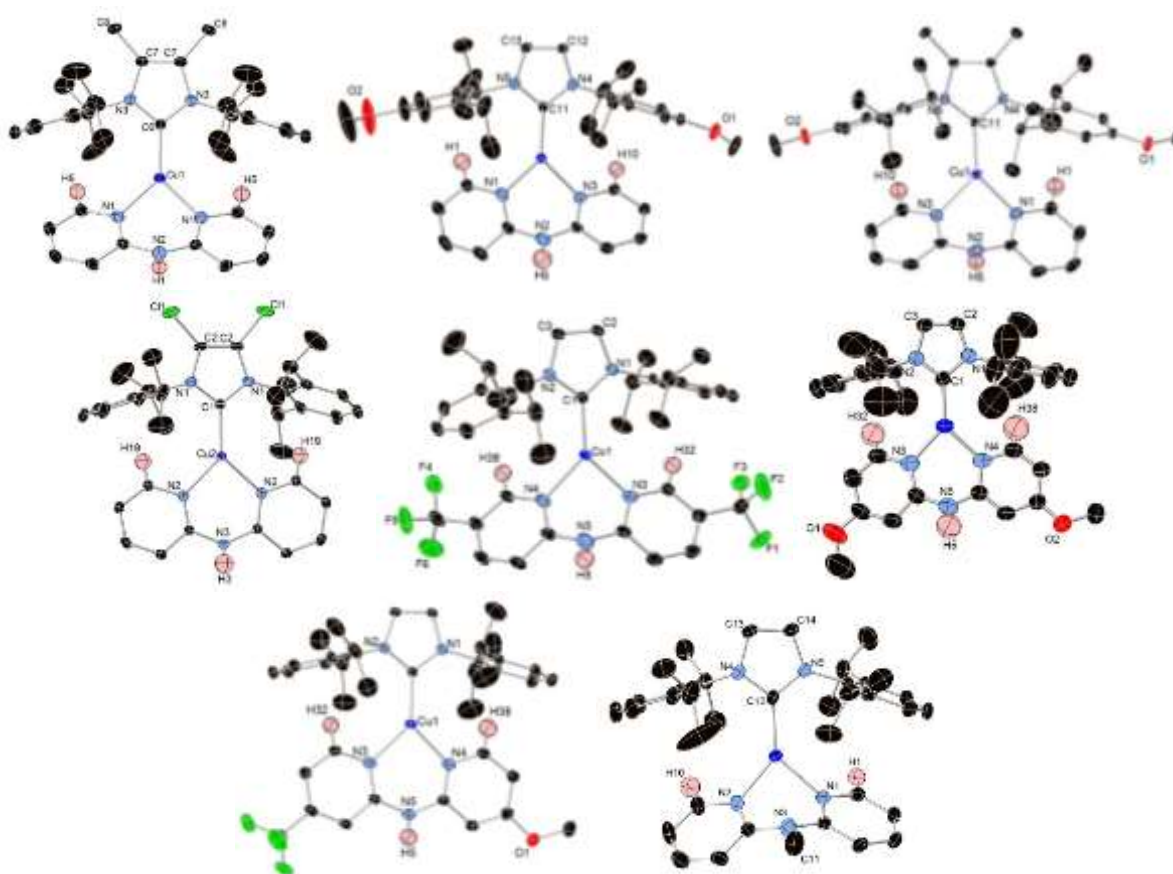


Figure S1. Thermal ellipsoid representations (50% probability) of [Cu(^{Me}IPr(L1))[PF₆] (**7**), [Cu(IPr^{OMe})(L1))[PF₆] (**8**), [Cu(^{Me}IPr^{OMe})(L1))[PF₆] (**9**), [Cu(^{Cl}IPr)(L1))[PF₆] (**10**), [Cu(IPr)(L2))[PF₆] (**11**), [Cu(IPr)(L4))[PF₆] (**13**), [Cu(IPr)(L5))[PF₆] (**14**) and [Cu(IPr)(L6))[PF₆] (**15**) complexes. Some hydrogen atoms and counteranion were omitted for clarity.

Table S1. Crystallographic data of [Cu(NHC)(N^N)][X] complexes **7-9**.

	[Cu(^{Me} IPr)(L1)] [PF ₆] (7)	[Cu(IPr ^{MeO})(L1)] [PF ₆] (8)	[Cu(^{Me} IPr ^{MeO})(L1)] [PF ₆] (9)
Formula	C ₃₉ H ₄₉ CuF ₆ N ₅ P, CH ₂ Cl ₂	C ₃₉ H ₄₉ CuF ₆ N ₅ O ₂ P	C ₄₁ H ₅₃ CuF ₆ N ₅ O ₂ P
M/g.mol ⁻¹	881.26	828.34	856.39
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Flack parameter			
Space group	<i>Pnma</i>	<i>C 2/c</i>	<i>C 2/c</i>
<i>a</i> / Å	14.7051(6)	27.2839(9)	21.8506(6)
<i>b</i> / Å	18.4222(7)	13.0191(4)	13.9457(4)
<i>c</i> / Å	15.3575(6)	25.8111(8)	27.2161(8)
<i>α</i> / °	90	90.00	90.00
<i>β</i> / °	90	117.2230(12)	96.4260(10)
<i>γ</i> / °	90	90.00	90.00
<i>V</i> / Å ³	4160.4(3)	8152.8(5)	8241.2(4)
<i>Z</i>	4	8	8
<i>μ</i> / mm ⁻¹	0.754	0.642	0.637
<i>ρ</i> _{calcd} / g.cm ⁻³	1.407	1.350	1.380
<i>λ</i> (Mo K _α)/ mm ⁻¹	0.71073	0.71073	0.71073
<i>T</i> / K	150(2)	150(2)	150(2)
No of reflections	42453	38327	45099
No of unique reflections	5324	10167	7778
<i>R</i> _{int}	0.0335	0.0297	0.0331
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0383, 0.1025	0.0541, 0.1487	0.0335, 0.0810
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0453, 0.1076	0.0635, 0.1576	0.0395, 0.0839
GOF	1.037	1.033	1.045

Table S2. Crystallographic data of [Cu(NHC)(N[^]N)][X] complexes **10**, **11** and **13**.

	[Cu(^{Cl} IPr)(L1)] [PF ₆] (10)	[Cu(IPr)(L2)] [PF ₆] (11)	[Cu(IPr)(L4)] [PF ₆] (13)
Formula	C ₃₇ H ₄₃ Cl ₂ CuF ₆ N ₅ P, 2CH ₂ Cl ₂	C ₃₉ H ₄₃ CuF ₁₂ N ₅ P	C ₃₉ H ₄₉ CuF ₆ N ₅ O ₂ P
M/g.mol ⁻¹	1007.02	904.29	828.34
Crystal system	Monoclinic	Monoclinic	Monoclinic
Flack parameter			
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> / Å	17.1708(7)	15.6210(7)	39.1885(10)
<i>b</i> / Å	19.8436(8)	12.3465(5)	11.3554(3)
<i>c</i> / Å	15.0379(7)	21.1831(7)	20.4130(5)
<i>α</i> / °	90	90	90
<i>β</i> / °	117.513(2)	93.409(2)	104.6500(10)
<i>γ</i> / °	90	90	90
<i>V</i> / Å ³	4544.4(3)	4078.2(3)	8788.5(4)
<i>Z</i>	4	4	8
<i>μ</i> / mm ⁻¹	0.928	0.665	0.595
<i>ρ</i> _{calcd} / g.cm ⁻³	1.472	1.473	1.252
<i>λ</i> (Mo K _α)/ mm ⁻¹	0.71073	0.71073	0.71073
<i>T</i> / K	150(2)	150(2)	291(2)
No of reflections	45581	32146	45972
No of unique reflections	6290	9326	8834
<i>R</i> _{int}	0.0327	0.0256	0.0439
<i>R</i> ₁ , w <i>R</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0425, 0.0989	0.0406, 0.1067	0.0609, 0.1767
<i>R</i> ₁ , w <i>R</i> ₂ (all data)	0.0521, 0.1051	0.0514, 0.1131	0.1068, 0.1938
GOF	0.969	1.038	1.050

Table S3. Crystallographic data of [Cu(NHC)(N[^]N)][X] complexes **14** and **15**.

	[Cu(IPr)(L5)][PF ₆] (14)	[Cu(IPr)(L6)][PF ₆] (15)
Formula	C ₃₉ H ₄₆ CuF ₉ N ₅ OP	C ₃₈ H ₄₇ CuF ₆ N ₅ P, CHCl ₃
M/g.mol ⁻¹	866.32	901.68
Crystal system	Monoclinic	Monoclinic
Flack parameter		
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> / Å	38.5295(8)	10.9223(6)
<i>b</i> / Å	11.3630(2)	30.7961(19)
<i>c</i> / Å	20.2769(4)	12.5703(9)
<i>α</i> / °	90	90.00
<i>β</i> / °	105.2020(10)	91.537(2)
<i>γ</i> / °	90	90.00
<i>V</i> / Å ³	8566.8(3)	4226(5)
<i>Z</i>	8	4
<i>μ</i> / mm ⁻¹	0.622	0.805
<i>ρ</i> _{calc} / g.cm ⁻³	1.343	1.417
<i>λ</i> (Mo K _α)/ mm ⁻¹	0.71073	0.71073
<i>T</i> / K	150(2)	150(2)
No of reflections	95824	16799
No of unique reflections	13125	7068
<i>R</i> _{int}	0.0365	0.0241
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0444, 0.1199	0.0512, 0.1178
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0555, 0.1256	0.0646, 0.1247
GOF	1.046	1.085

Measures of the angle formed by the imidazole ring and the plan including the three nitrogen atoms of the dpa ligand in copper complexes **6-11** and **13-15**.

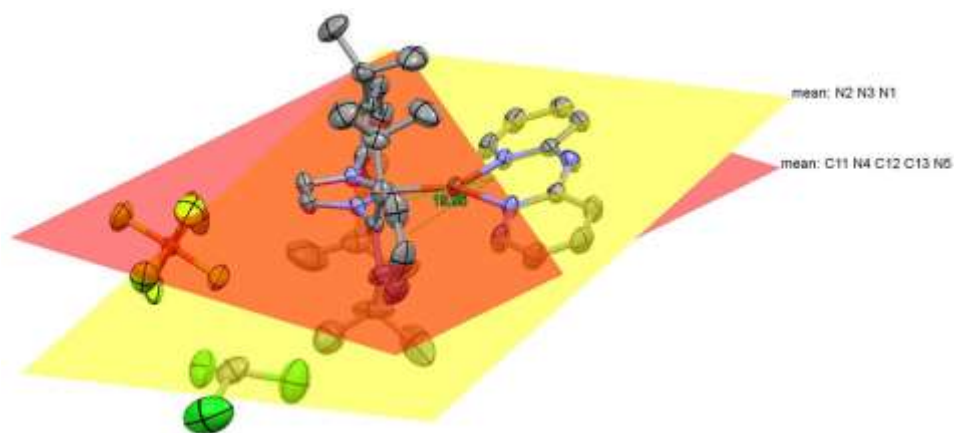


Figure S2. Complex $[\text{Cu}(\text{IPr})(\text{L1})][\text{PF}_6]$ (**6**).

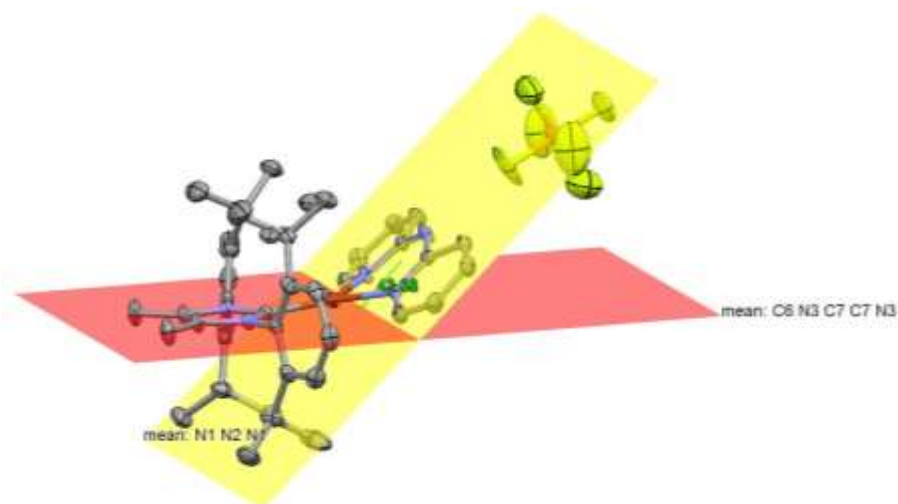


Figure S3. Complex $[\text{Cu}(\text{MeIPr})(\text{L1})][\text{PF}_6]$ (**7**).

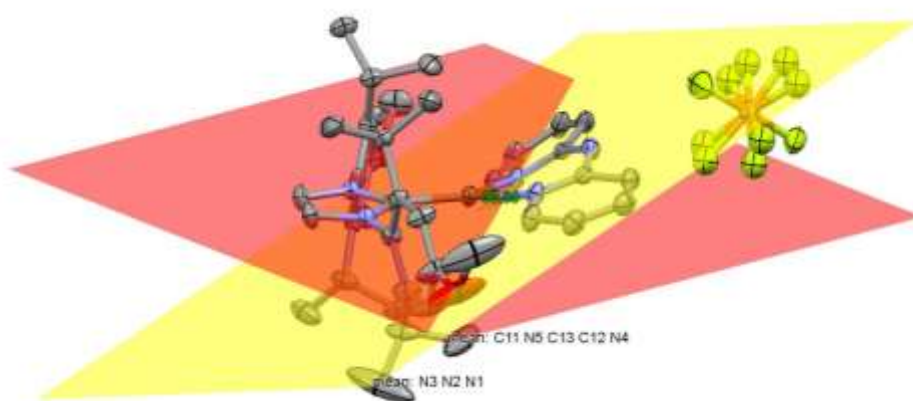


Figure S4. Complex $[\text{Cu}(\text{IPr}^{\text{MeO}})(\text{L1})][\text{PF}_6]$ (**8**).

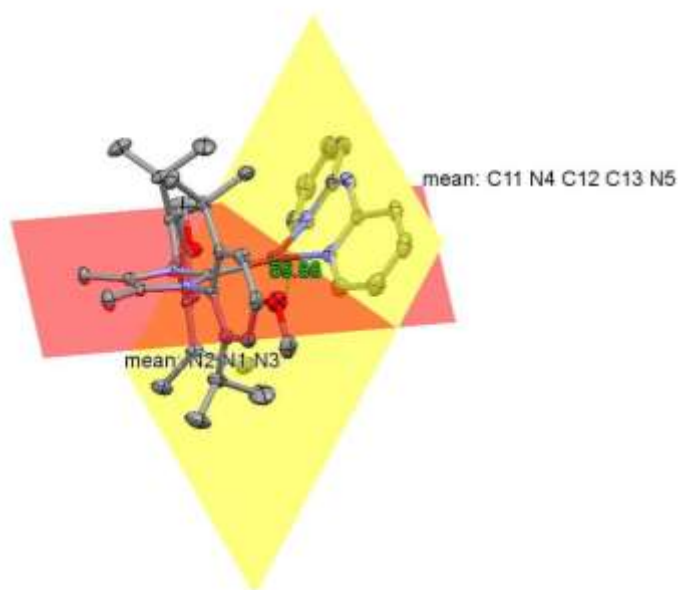


Figure S5. Complex $[\text{Cu}^{\text{MeIPr}^{\text{MeO}}}(\text{L1})][\text{PF}_6]$ (**9**).

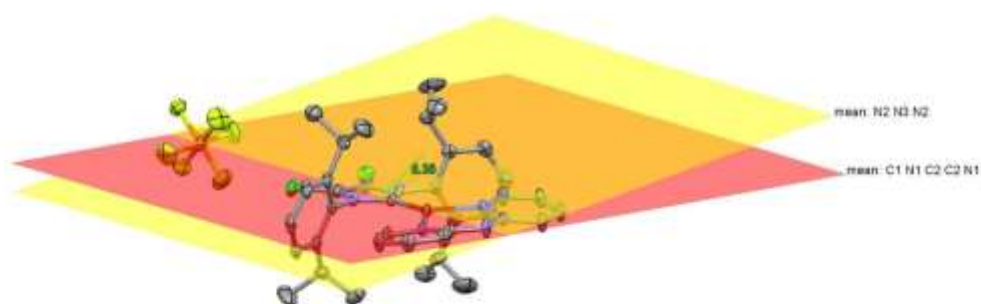


Figure S6. Complex $[\text{Cu}^{\text{ClIPr}}(\text{L1})][\text{PF}_6]$ (**10**).

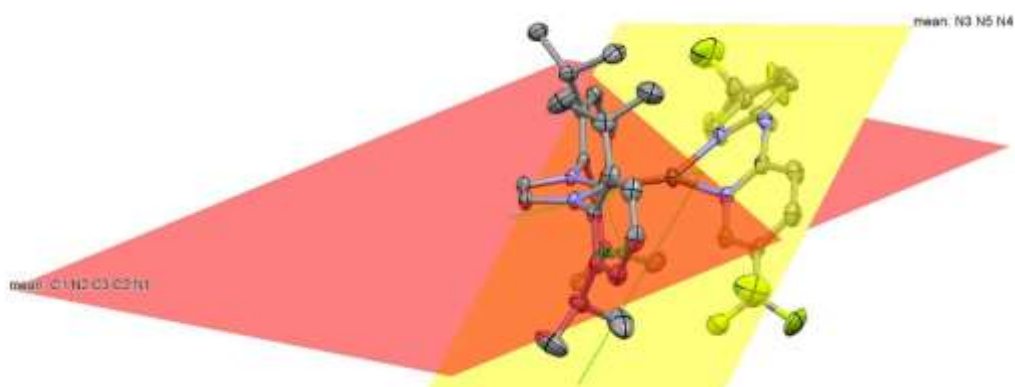


Figure S7. Complex $[\text{Cu}(\text{IPr})(\text{L2})][\text{PF}_6]$ (**11**).

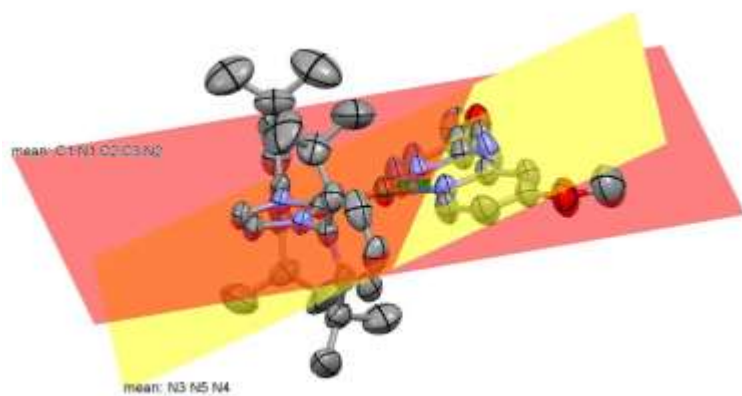


Figure S8. Complex $[\text{Cu}(\text{IPr})(\text{L4})][\text{PF}_6]$ (**13**).

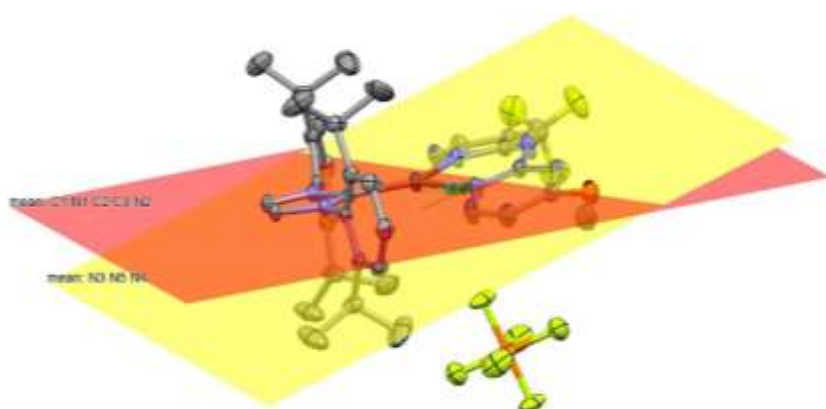


Figure S9. Complex $[\text{Cu}(\text{IPr})(\text{L5})][\text{PF}_6]$ (**14**).

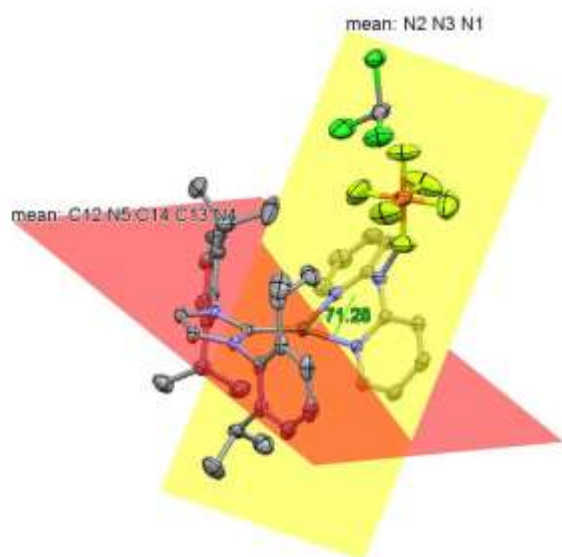


Figure S10. Complex $[\text{Cu}(\text{IPr})(\text{L6})][\text{PF}_6]$ (**15**).

Part 6: Photophysical data of [Cu(NHC)(N[^]N)][X] complexes **7-15**

General Considerations. UV-visible absorption spectra were measured at room temperature in chloroform on a Jenway 6715 UV/vis spectrometer, wavelengths are given in nm and extinction coefficients ϵ are presented in $\text{L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1}$. Steady-state emission spectra and emission lifetime were recorded with solid-state on an Horiba Jobin Yvon Fluoromax-4P spectrofluorometer. For measuring absolute solid-state emission quantum yields, an Horiba Jobin Yvon integrating sphere F-3018 was equipped to the Fluoromax-4P spectrometer.

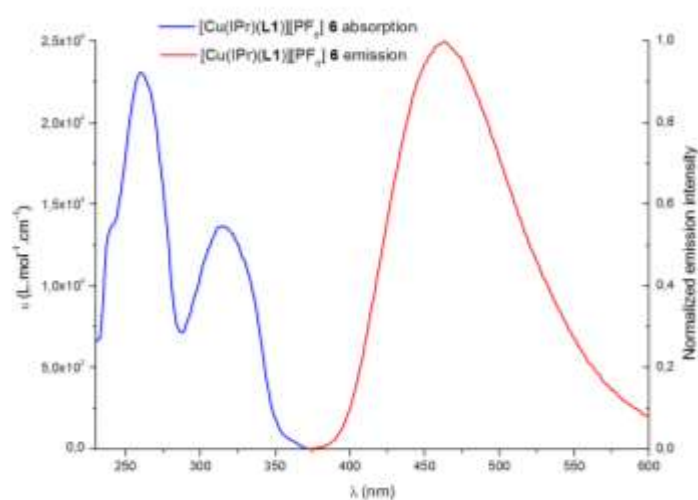


Figure S11. Absorption (in CHCl_3) and normalized emission (in solid state) spectra of complex **6**.

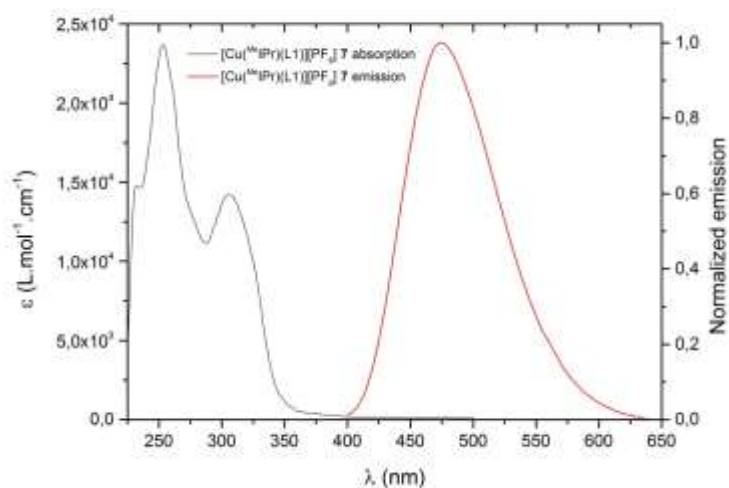


Figure S12. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **7**.

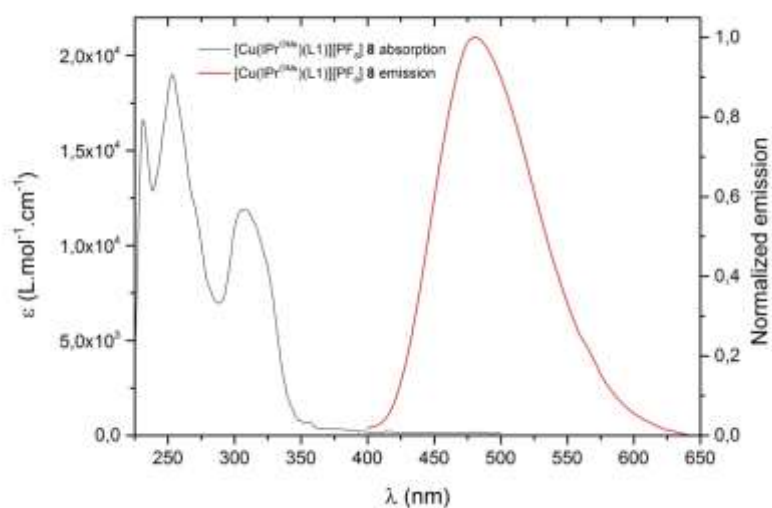


Figure S13. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **8**.

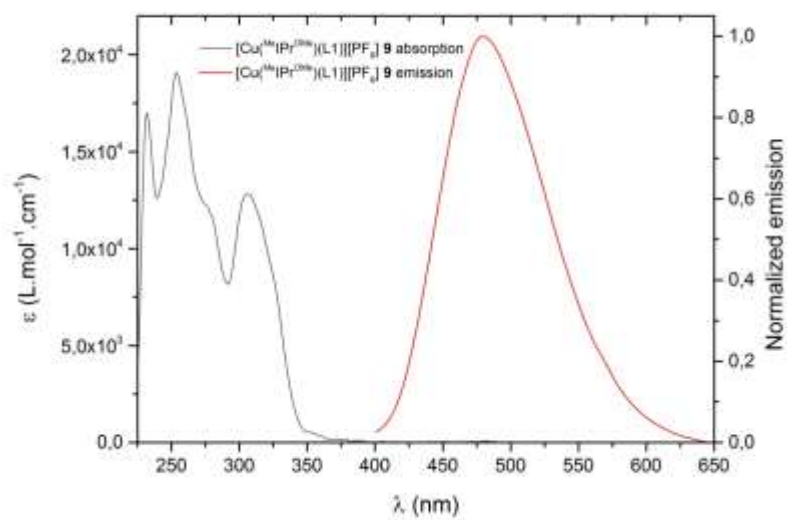


Figure S14. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **9**.

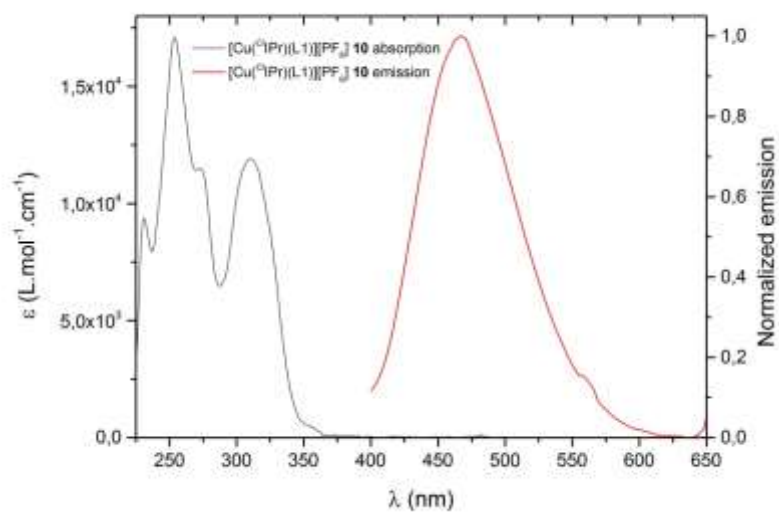


Figure S15. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **10**.

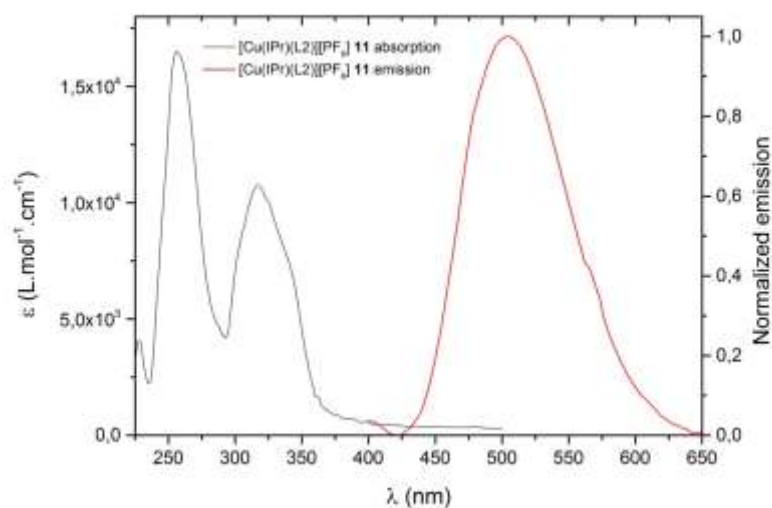


Figure S16. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **11**.

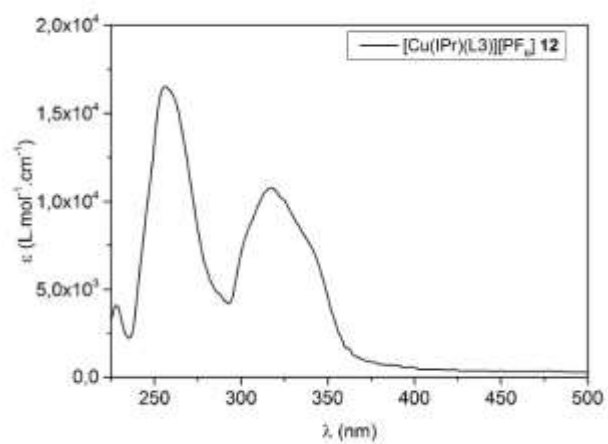


Figure S17. Absorption (in CH₂Cl₂) spectrum of complex **12**.

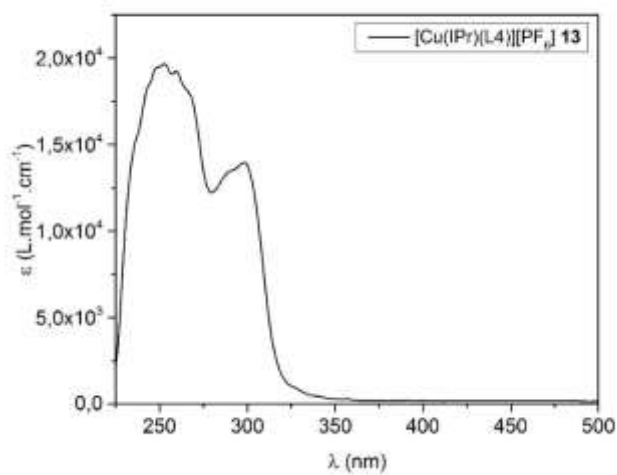


Figure S18. Absorption (in CH₂Cl₂) spectrum of complex **13**.

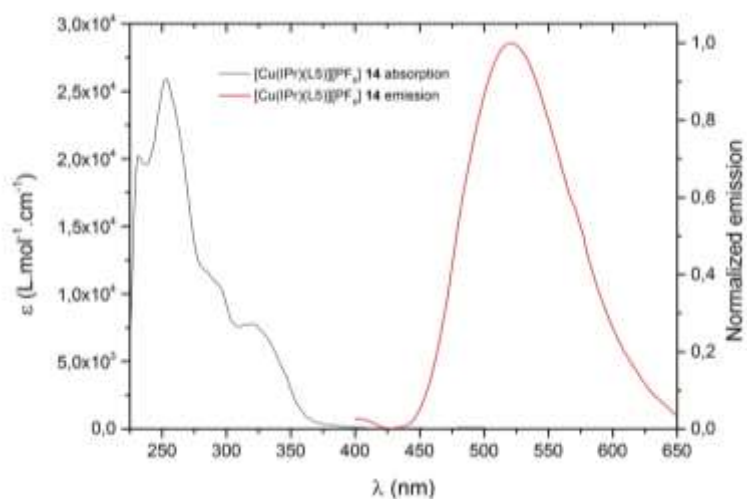


Figure S19. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **14**.

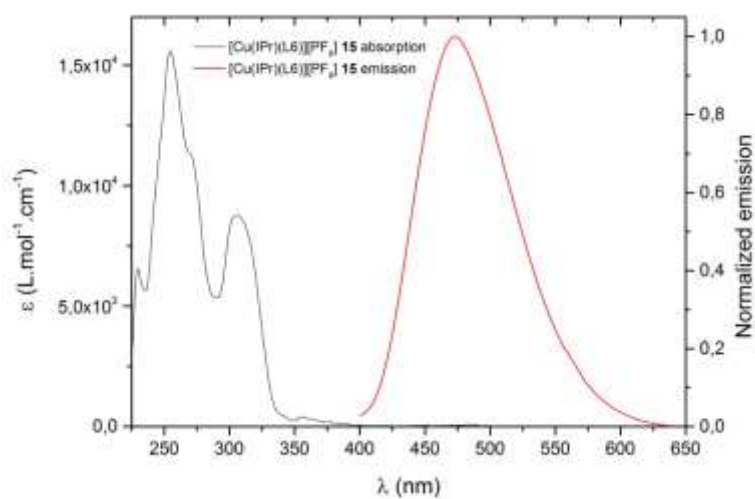


Figure S20. Absorption (in CH_2Cl_2) and normalized emission (in solid state) spectra of complex **15**.

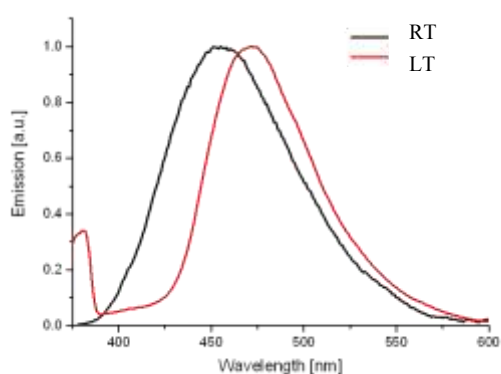


Figure S21. Emission spectra (in solid state) of complex **6** at 298 K (RT) and 77 K (LT).

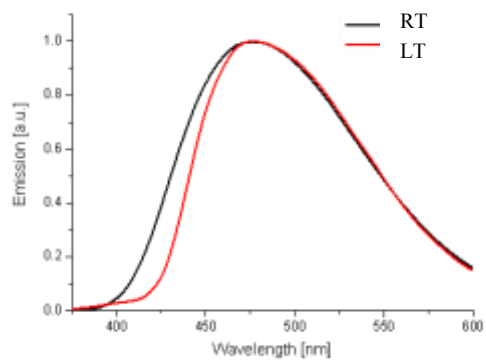


Figure S22. Emission spectra (in solid state) of complex **9** at 298 K (RT) and 77 K (LT).

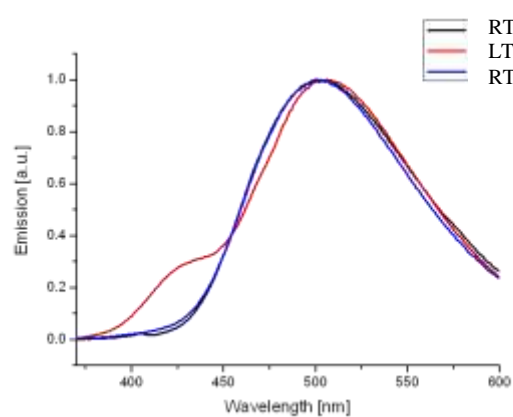


Figure S23. Emission spectra (in solid state) of **14** at 298 K (RT) and 77 K (LT).

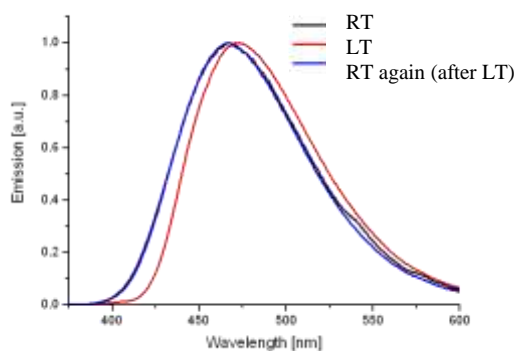


Figure S24. Emission spectra (in solid state) of complex **15** at 298 K (RT) and 77 K (LT).

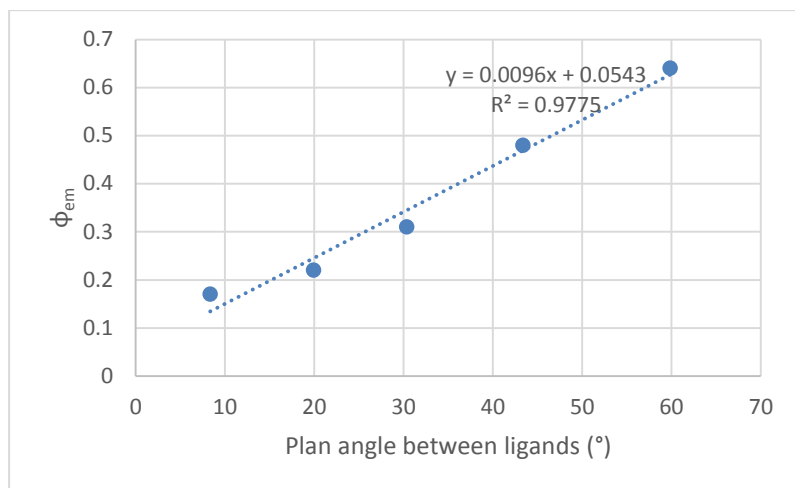


Figure S25. Correlation between ϕ_{em} and the plan angle between ligands for complexes **6-10**.

Part 7: DFT and TD-DFT studies on [Cu(NHC)(N[^]N)]⁺[X] complexes

Conformational Features and Binding Energies. The following complexes were studied [Cu(IPr)(L1)]⁺, [Cu^(Me)(IPr)(L1)], [Cu(IPr^(MeO))(L1)]⁺, [Cu^(Me)(IPr^(MeO))(L1)]⁺, [Cu^(Cl)(IPr)(L1)]⁺, [Cu(IPr)(L2)]⁺, [Cu(IPr)(L3)]⁺, [Cu(IPr)(L4)]⁺, [Cu(IPr)(L5)]⁺ and [Cu(IPr)(L6)]⁺ corresponding to complexes **6**, **7**, **8**, **9**, **10**, **11**, **12**, **13**, **14**, and **15**, respectively. It must be stressed that counterions were not included in calculations. [Cu(IPr)(L1)]⁺ was used as the reference to assess and rationalize the first experimental results.

Binding energies were calculated as follows:

$$\Delta E_{binding} = E_{complex} - E_{dpa} - E_{Cu(NHC)}$$

where $E_{complex}$, E_{dpa} and $E_{Cu(NHC)}$ energies were calculated from optimized geometries of complexes, corresponding standalone dpa (i.e., L1 to L6) and standalone Cu-NHC molecule. Such calculations were performed in vacuum at the ω B97X-D/6-31+G(d,p)/SDD level of theory. It must be underlined that such approach aims only at providing some trends on experimental yield based on electronic and conformational features. While most of the complexes exhibit binding energies lower than -63 kcal.mol⁻¹, the highest binding energies were obtained for complexes with CF₃-disubstituted ligands, in very good agreement with the lowest synthesis yield in this series (i.e., $\Delta E_{binding}$ ca. -58 kcal.mol⁻¹). The electron-acceptor character of the CF₃ groups decreases the electron population on N_{ligand} atoms weakening N_{dpa}...Cu bonds. As summarized in Table S5, the presence of electron-acceptor moieties either on NHC or dpa (e.g., CF₃ or Cl) might lead to a higher charge on the Cu-atom and, in turn, to less stabilized complexes (e.g., q(Cu) = 0.50, 0.48 and 0.44 for [Cu^(Cl)(IPr)(L1)]⁺, [Cu(IPr)(L3)]⁺ and [Cu(IPr)(L1)]⁺, respectively). It must be stressed that Cu-atom charge transfer is not enough to rationalize the stability of complexes. Indeed, [Cu(IPr)(L2)]⁺ exhibits a lower Cu-charge than [Cu(IPr)(L1)]⁺ while binding energy is significantly higher (see Table S4). The lower stability of [Cu(IPr)(L2)]⁺ may be explained by the significantly higher dpa ligand twist with respect to other complexes (see below).

Since N_{imidazole}-C_{carbene}...Cu-N_{dpa} dihedral angle has been shown to play a crucial role in the photoluminescence features,^{17d} S₀ ground state structures were optimized breaking the C_s symmetry to C₁ point group contrary to our previous study. Theoretical calculations exhibit a very good agreement with respect to crystallographic data. RMSD on relevant distances and angles are 0.01 Å, 0.04 Å and 2.5° respectively for Cu-C_{carbene}, Cu...N_{dpa} distances and N_{dpa}...Cu...N_{dpa} angle (Table S5). It must be pointed out that significant differences were obtained concerning values of N_{imidazole}-C_{carbene}...Cu-N_{dpa} dihedral angles (RMSD being 17.9°). Besides this fact, the crystallographic global unsymmetrical shape of complexes and the trend between several complexes were successfully established. Differences between XRD and calculations may be attributed to the absence of counterions in calculations. It is worth noting that [Cu(IPr)(L2)]⁺ is significantly twisted with respect to the plane

formed by NHC ring (*i.e.*, calculated $N_{\text{imidazole}}\text{-C}_{\text{carbene}}\text{-Cu-N}_{\text{dpa}}$ dihedral angles) are -28.7 and -15.7° , respectively. Due to the presence of the steric bulky *iso*-propyl moieties on NHC closed to dpa CF_3 moieties, $[\text{Cu}(\text{IPr})(\mathbf{L2})]^+$ is much less stabilized, explaining the low yield obtained during synthesis.

Electronic structures. As observed in our previous study, most of the complex frontier orbital distribution showed metal ligand charge transfer (MLCT) feature. For instance, in $[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$ complex, the highest occupied molecular orbital (HOMO) is mainly located on the Cu-atom and $\mathbf{L1}$, while LUMO is mainly located on the $\mathbf{L1}$ ligand (Figure S26). NHC molecule is not involved in $[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$ LUMO contrary to the corresponding theoretical boron-based model system. In our complexes, the presence of *N*-atom bridge instead of $\text{B}(\text{Me})_2$ increases the π -delocalization in dpa. This leads to an inversion of unoccupied molecular orbitals located on NHC and dpa ligand with respect to boron-based systems, highlighting the differences between both families of complexes.

NHC-tuned complexes exhibit various HOMO localizations whereas LUMOs remain on dpa molecule. In $[\text{Cu}(\text{MeIPr})(\mathbf{L1})]^+$ and $[\text{Cu}(\text{ClIPr})(\mathbf{L1})]^+$ complexes, the presence of electron donor moieties leads to a relevant contribution of the NHC imidazole ring to the HOMO. This effect is significantly lower in $[\text{Cu}(\text{ClIPr})(\mathbf{L1})]^+$, owing to the inherent strong inductive electron-acceptor effect of chlorine atom. Interestingly, the strong contribution of NHC in $[\text{Cu}(\text{MeIPr})(\mathbf{L1})]^+$ is correlated to the contribution of the d_{z^2} orbital of Cu-atom contrary to the contribution of d_{xy} orbital in all the other complexes. $[\text{Cu}(\text{IPr}^{\text{OMe}})(\mathbf{L1})]^+$ and $[\text{Cu}(\text{MeIPr}^{\text{OMe}})(\mathbf{L1})]^+$ complexes present a very similar HOMO topology, highlighting the prevalence of methoxy electronic effects to methyl ones. The presence of methoxy moieties drastically decreases the dpa contribution in the HOMO, owing to high π -delocalization over NHC phenyl rings. Therefore, these complexes exhibit a larger MLCT with respect to $[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$ (Figure S26). However, NHC contribution to HOMO is strictly localized on phenyl rings, since the π -conjugation induced by the methoxy groups is blocked by the *N*-heterocyclic ring. HOMO-LUMO gaps ($\Delta E^{\text{H/L}}$) are not significantly affected by NHC-tuning ($\Delta E^{\text{H/L}}$ ca. 8.4 eV). Occupied and unoccupied molecular orbitals are (un)stabilized by electron-acceptor(donor) groups within the same order of magnitude (Table S4). This is in good agreement with the experimental maxima emission wavelengths measured for **6-10**. Concerning dpa-tuned complexes, they exhibit an almost symmetrical LUMO localization on dpa except for $[\text{Cu}(\text{IPr})(\mathbf{L5})]^+$. This “push-pull” system along dpa moiety leads to unsymmetrical LUMO localization on pyridine ring bearing CF_3 group due to its electron-acceptor feature.

In all complexes, the dpa contribution to HOMO is significantly lowered by substitution pattern with respect to the $[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$ unsubstituted complex. Thus, they exhibit a stronger separation between HOMO and LUMO, which might increase the MLCT character. While HOMO and LUMO distributions are rather similar between these complexes, these energies are significantly affected by the above-mentioned electronic effects. Before going further, it must be mentioned that range-

separated functional are known to well-describe semi-quantitatively MO energies but overestimate H-L gaps.

In detail, electron-donor ligands (*i.e.*, **L4** and **L6**) destabilize the energies of both HOMOs and LUMOs. In case of π -conjugated electron donor such as $[\text{Cu}(\text{IPr})(\mathbf{L4})]^+$, the LUMO destabilization is more important than that noted for the HOMO, leading to a higher HOMO-LUMO gap (ca. 8.7, 8.1 and 8.4 eV for $[\text{Cu}(\text{IPr})(\mathbf{L4})]^+$, and $[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$, respectively). In $[\text{Cu}(\text{IPr})(\mathbf{L2})]^+$ and $[\text{Cu}(\text{IPr})(\mathbf{L3})]^+$, both $\Delta E^{\text{H/L}}$ gap are lowered by electron-acceptor CF_3 groups (*i.e.*, $\Delta E^{\text{H/L}} = 7.7$ and 8.1 eV, respectively). The presence of CF_3 moieties strongly stabilizes the LUMO energies with the same order of magnitude (ca. -0.8 eV) for both complexes. However, the HOMO stabilization is greater for $[\text{Cu}(\text{IPr})(\mathbf{L3})]^+$ with respect to that of $[\text{Cu}(\text{IPr})(\mathbf{L2})]^+$ (*e.g.*, -0.4 and -0.2 eV, respectively). Electronic effects of the N-atom bridge, CF_3 groups and *N*-heterocyclic atoms of dpa molecule are synergic in $[\text{Cu}(\text{IPr})(\mathbf{L2})]^+$ contrary to $[\text{Cu}(\text{IPr})(\mathbf{L3})]^+$. The π -conjugated *N*-heterocyclic contribution is stronger than the σ -inductive CF_3 effect. The former might screens CF_3 effects resulting to a lower HOMO stabilization. Furthermore, considering the whole **L2** ligand, electronic effects on one pyridine ring are opposite to those on the other ring. This leads to an imbalance in π -electron conjugation between both rings, explaining the unexpected twisted structure. In contrast, these effects are compensate in $[\text{Cu}(\text{IPr})(\mathbf{L3})]^+$ by the synergy between CF_3 moiety and the opposite pyridine ring through nitrogen bridged atom. Finally, stabilization in $[\text{Cu}(\text{IPr})(\mathbf{L5})]^+$ are weaker than in CF_3 -substituted complexes, as the presence of the electron-donor methoxy group partially compensates the effect of CF_3 (Figure S26).

Table S4. Binding Energies and HOMO-LUMO gap and HOMO, LUMO levels.

Complex	$\Delta E_{\text{binding}}$ (kcal.mol ⁻¹)	$\Delta E^{\text{H/L}}$ (eV)	E^{HOMO} (eV)	E^{LUMO} (eV)
$[\text{Cu}(\text{IPr})(\mathbf{L1})]^+$	-69.0	8.4	-10.6	-2.2
$[\text{Cu}(\text{MeIPr})(\mathbf{L1})]^+$	-67.8	8.3	-10.5	-2.2
$[\text{Cu}(\text{IPr}^{\text{OMe}})(\mathbf{L1})]^+$	-69.5	8.4	-10.5	-2.1
$[\text{Cu}(\text{MeIPr}^{\text{OMe}})(\mathbf{L1})]^+$	-68.3	8.3	-10.4	-2.1
$[\text{Cu}(\text{ClIPr})(\mathbf{L1})]^+$	-70.4	8.4	-10.7	-2.3
$[\text{Cu}(\text{IPr})(\mathbf{L2})]^+$	-58.5	7.7	-10.8	-3.1
$[\text{Cu}(\text{IPr})(\mathbf{L3})]^+$	-58.5	8.1	-11.1	-3.0
$[\text{Cu}(\text{IPr})(\mathbf{L4})]^+$	-71.5	8.7	-10.4	-1.7
$[\text{Cu}(\text{IPr})(\mathbf{L5})]^+$	-63.7	8.1	-10.7	-2.6
$[\text{Cu}(\text{IPr})(\mathbf{L6})]^+$	-71.0	8.3	-10.5	-2.2

Table S5. Selected theoretical bond lengths, angles and CHELPG Cu(I) charges of optimized copper complexes at the S_0 state as well as.

Complex	Cu-C _{carbene} (Å)	Cu-N _{dpa} (Å)	N _{dpa} -Cu-N _{dpa} (°)	C _{carbene} -Cu-N _{central dpa} (°)	Plane Angle (°)	Torsion Angle (°)	q(Cu) (e)
Cu(IPr)(L1)	1.917	2.089 2.091	88.935	158.09	21.91	-7.127 -0.814	0.440
Cu(MeIPr)(L1)	1.914	2.094 2.094	88.636	157.47	22.53	-3.567 3.547	0.412
Cu(IPr ^{OMe})(L1)	1.916	2.091 2.094	88.547	156.66	23.34	-7.393 1.085	0.466
Cu(MeIPr ^{OMe})(L1)	1.915	2.096 2.096	88.145	155.32	24.68	-5.171 5.169	0.475
Cu(ClIPr)(L1)	1.913	2.086 2.084	89.043	155.72	24.28	-13.628 -4.871	0.496
Cu(IPr)(L2)	1.912	1.982 2.016	88.385	154.95	25.06	-28.716 -15.758	0.417
Cu(IPr)(L3)	1.913	2.095 2.095	88.047	154.92	25.08	-5.061 5.609	0.480
Cu(IPr)(L4)	1.913	2.084 2.082	89.026	156.73	23.27	-6.739 0.090	0.459
Cu(IPr)(L5)	1.913	2.069 2.110	88.514	156.07	23.93	-6.533 1.706	0.443
Cu(IPr)(L6)	1.904	2.073 2.076	87.667	148.99	31.01	-9.375 -2.308	0.400

Table S6. Selected theoretical bond lengths and angles of optimized copper complexes at (a) the S_1 state and (b) T_1 state including S_1 - T_1 geometry root-mean squared-deviations.

(a)

Complex	Cu-C _{carbene} (Å)	Cu-N _{dpa} (Å)	N _{dpa} -Cu-N _{dpa} (°)	C _{carbene} -Cu-N _{central dpa} (°)	Plane Angle (°)	Torsion Angle (°)
Cu(IPr)(L1)	1.974	1.858 2.000	92.080	147.579	32.421	21.601 23.547
Cu(MeIPr)(L1)	1.974	1.862 1.995	92.105	146.189	33.811	18.344 17.623
Cu(IPr ^{OMe})(L1)	1.970	2.011 1.860	91.590	145.408	34.592	-15.537 -16.415
Cu(MeIPr ^{OMe})(L1)	1.974	2.023 1.864	91.561	142.321	37.679	6.992 -1.895
Cu(ClIPr)(L1)	1.973	1.857 1.994	91.720	145.273	34.727	18.405 18.997
Cu(IPr)(L2)	1.968	1.976 1.895	93.041	143.666	36.334	-18.806 -28.509
Cu(IPr)(L3)	1.968	1.868 1.998	92.157	144.895	35.105	25.092 18.403
Cu(IPr)(L4)	1.902	1.976 1.932	91.402	139.865	40.135	-19.460 -18.974
Cu(IPr)(L5)	1.972	1.864 2.005	90.940	139.433	40.567	-3.338 -15.132
Cu(IPr)(L6)	1.957	1.995 1.868	89.672	140.457	39.543	-9.981 -1.826

(b)

Complex	Cu-C _{carbene} (Å)	Cu-N _{dpa} (Å)	N _{dpa} -Cu-N _{dpa} (°)	C _{carbene} -Cu-N _{central dpa} (°)	Plane Angle (°)	Torsion Angle (°)	RMSD (T ₁ /S ₁)
Cu(IPr)(L1)	1.977	1.880 1.968	92.878	151.168	28.832	25.554 28.679	0.131
Cu(^{Me} IPr)(L1)	1.956	1.973 1.900	91.290	145.469	34.531	-14.212 -4.073	0.708
Cu(IPr ^{OMe})(L1)	1.976	1.973 1.884	92.494	149.210	30.790	-22.098 -23.079	0.202
Cu(^{Me} IPr ^{OMe})(L1)	1.978	1.972 1.894	92.391	147.804	32.196	-12.737 -17.738	0.541
Cu(^{Cl} IPr)(L1)	1.991	1.899 1.954	92.856	146.326	33.674	-8.515 -23.907	0.982
Cu(IPr)(L2)	1.967	1.971 1.906	92.687	146.110	33.890	-22.302 -28.999	0.091
Cu(IPr)(L3)	1.972	1.891 1.963	92.406	148.214	31.786	24.056 21.019	0.062
Cu(IPr)(L4)	1.923	1.973 1.909	91.377	142.701	37.299	-30.238 -14.446	0.172
Cu(IPr)(L5)	1.974	1.906 1.934	92.843	150.657	29.343	-26.860 -23.435	0.529
Cu(IPr)(L6)	1.977	1.880 1.968	92.878	151.168	28.832	25.554 28.679	0.080

Table S7. Calculated S₁→S₀ and T₁→S₀ emission properties, Singlet-Triplet splitting and experimental emission properties.

Complex	S ₁ →S ₀				T ₁ →S ₀				ΔE ST	Exp E _{em}
	E _{em}	RMSD	λ _{S1}	λ _{S0}	E _{em}	RMSD	λ _{T1}	λ _{S0}		
Cu(IPr)(L1)	3.00	0.755	0.65	0.61	2.59	0.868	0.24	0.66	0.35	2.54
Cu(^{Me} IPr)(L1)	2.98	0.484	0.68	0.60	2.75	0.324	0.15	0.59	0.24	2.61
Cu(IPr ^{OMe})(L1)	2.98	0.363	0.68	0.60	2.57	0.522	0.25	0.65	0.36	2.58
Cu(^{Me} IPr ^{OMe})(L1)	2.95	0.289	0.70	0.59	2.59	0.409	0.26	0.61	0.35	2.59
Cu(^{Cl} IPr)(L1)	3.04	0.786	0.61	0.61	2.79	0.318	0.12	0.58	0.29	2.65
Cu(IPr)(L2)	2.75	0.282	0.82	0.18	2.35	0.257	0.75	0.22	0.36	2.46
Cu(IPr)(L3)	2.68	0.673	0.72	0.62	2.27	0.702	0.39	0.65	0.37	2.25
Cu(IPr)(L4)	3.25	0.552	0.49	0.54	3.05	0.622	0.00	0.62	0.12	2.95
Cu(IPr)(L5)	2.61	0.456	0.80	0.69	2.21	0.717	0.48	0.74	0.36	2.38
Cu(IPr)(L6)	2.97	0.215	0.56	0.56	2.74	0.220	0.54	0.55	0.24	2.62

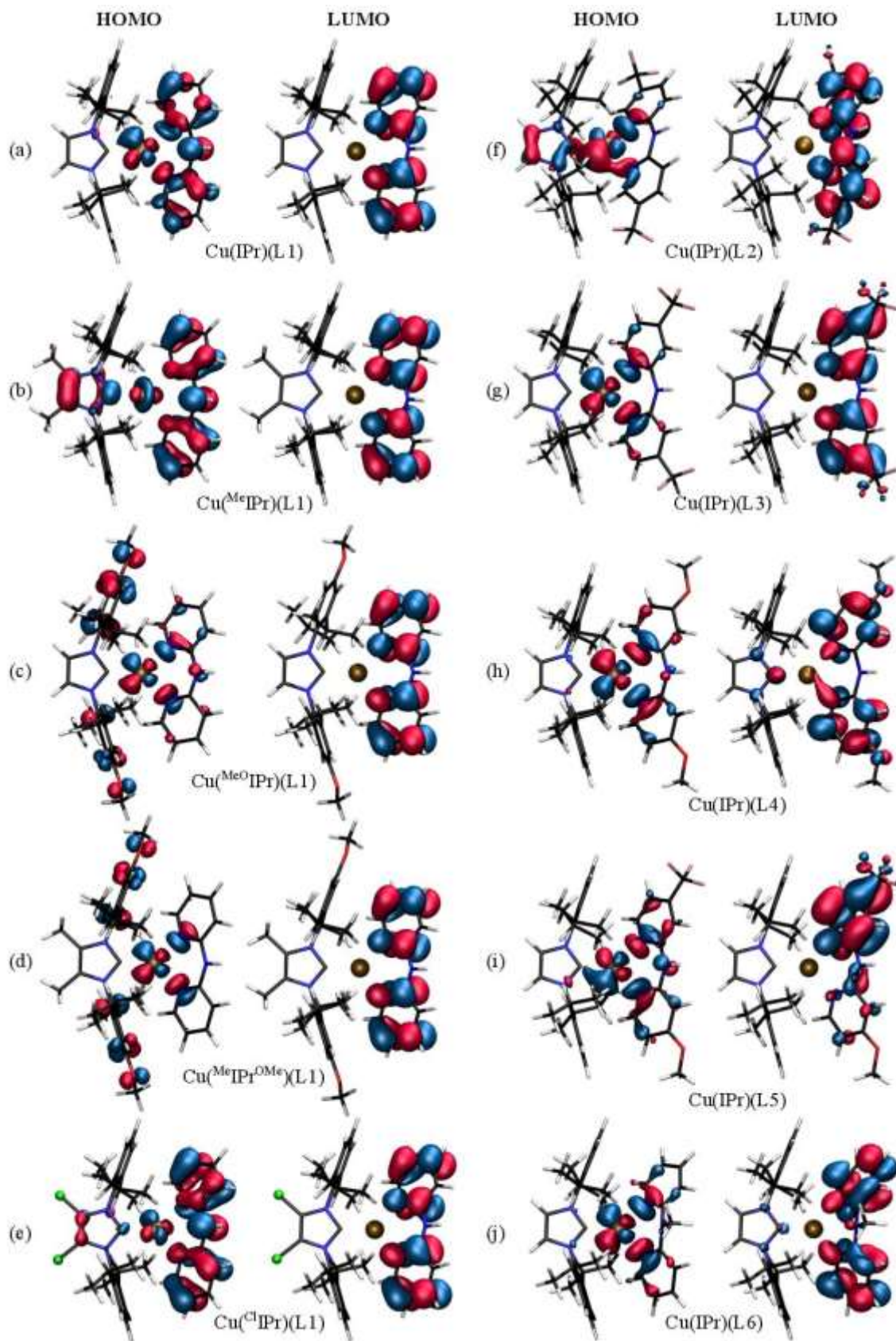


Figure S26. HOMO and LUMO distributions of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}^{\text{Me}}(\text{IPr})(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}^{\text{Me}}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}^{\text{Cl}}(\text{IPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j).

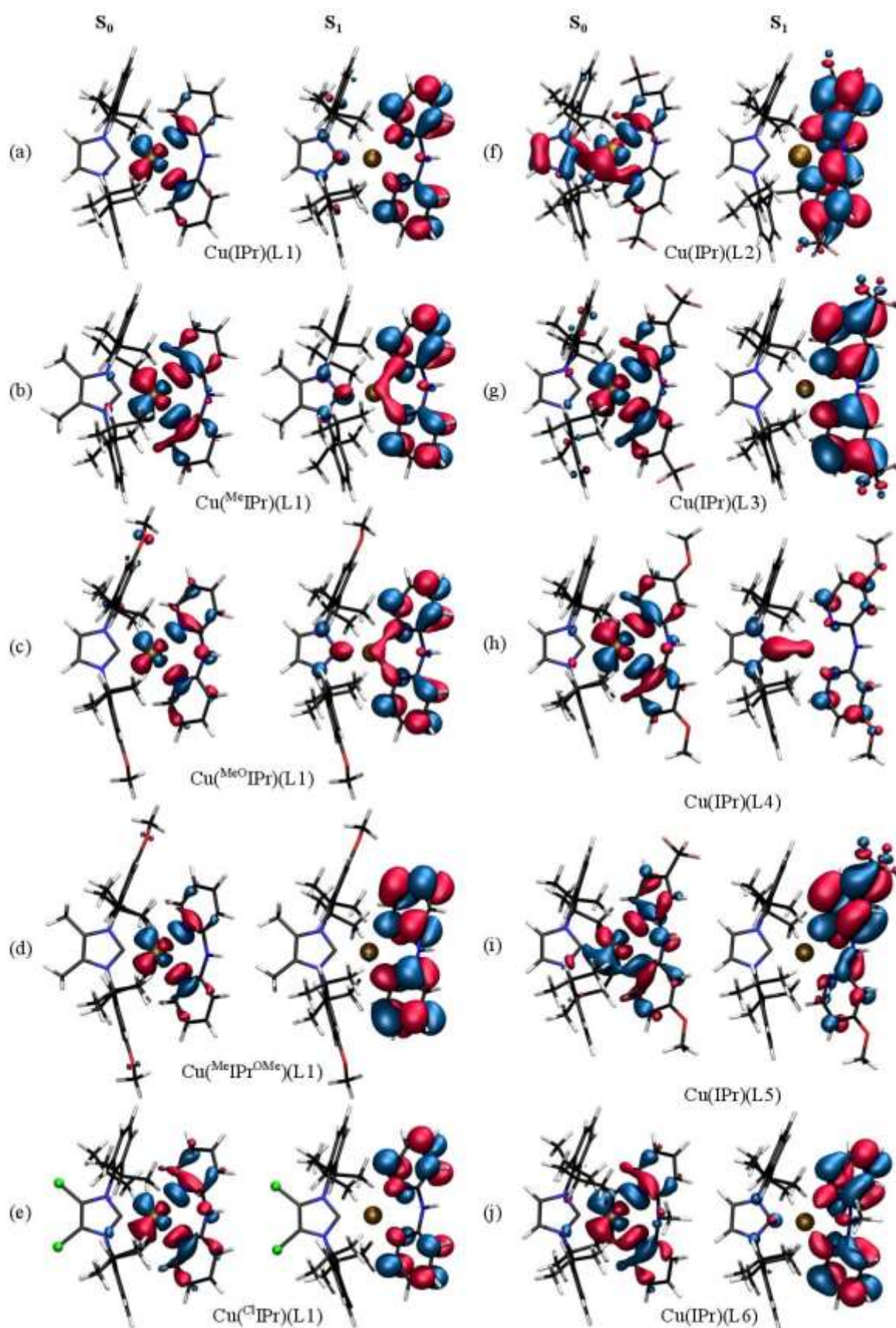


Figure S27. NTO distribution of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}(\text{MeIPr})(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}(\text{MeIPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}(\text{ClIPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j), S_0 - S_1 transitions.

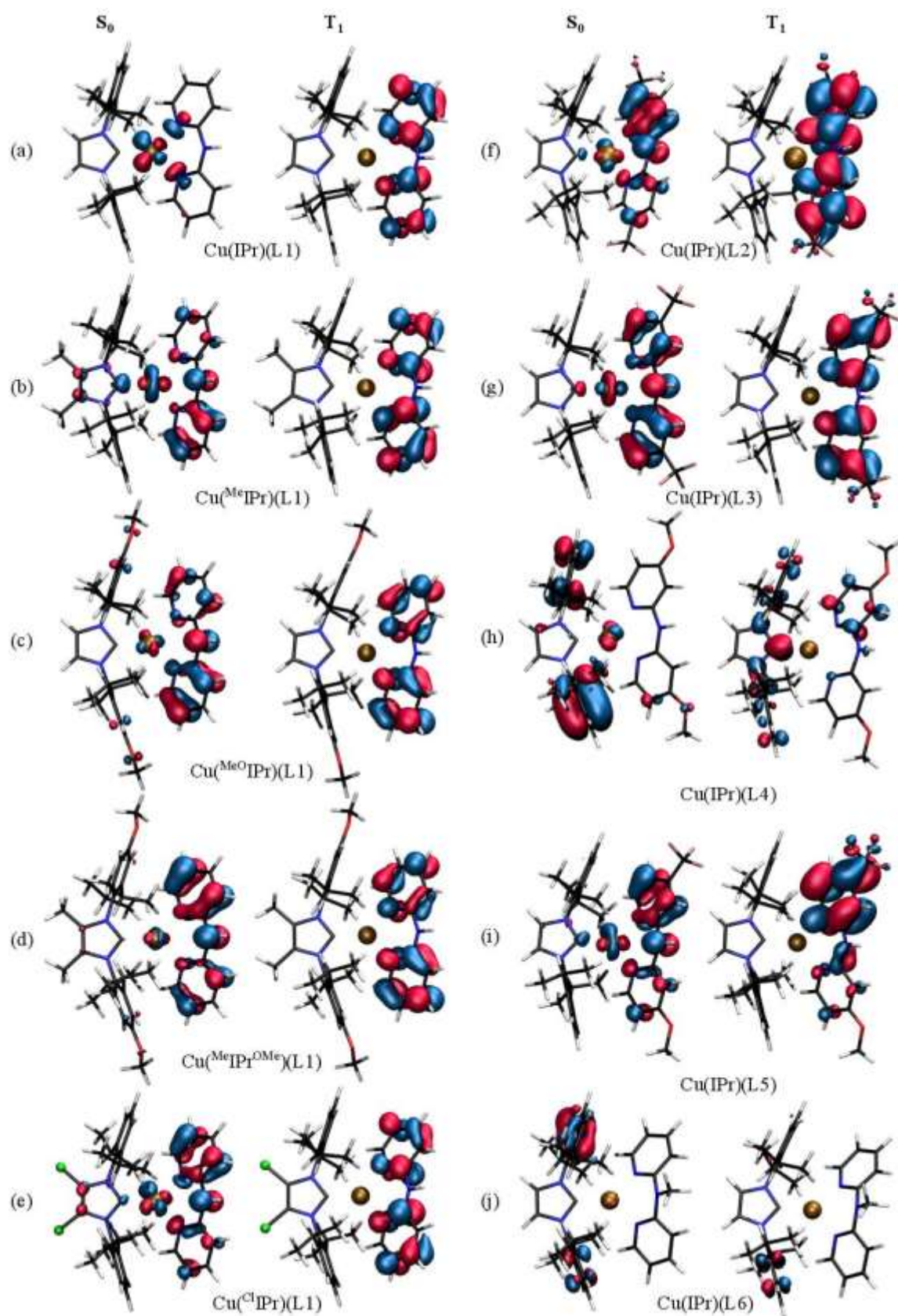


Figure S28. NTO distribution of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}^{\text{Me}}(\text{IPr})(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}^{\text{Me}}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}^{\text{Cl}}(\text{IPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j), S_0 - T_1 transitions.

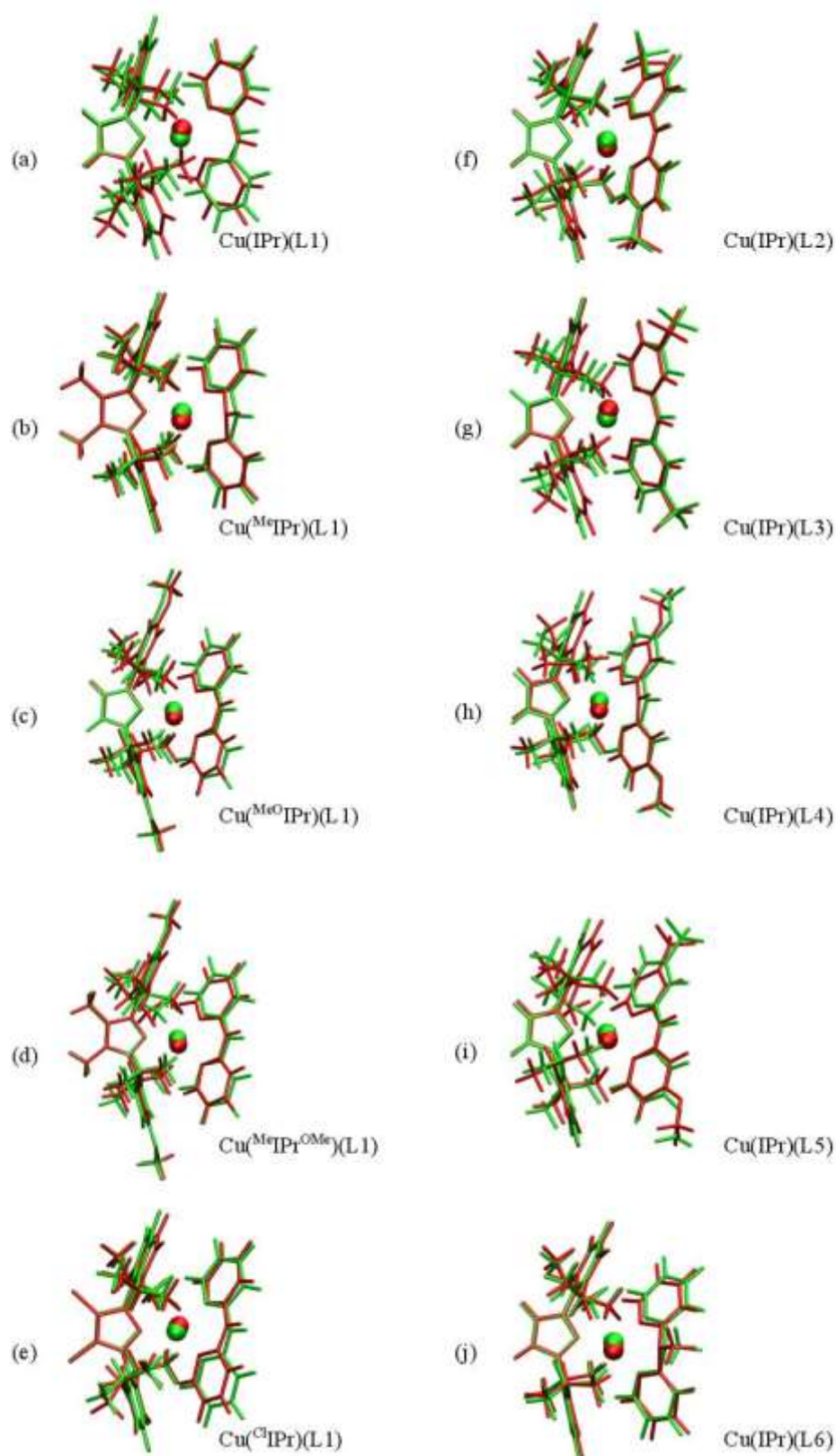


Figure S29. S_0/T_1 state superimpositions of studied complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}(\text{MeIPr})(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}(\text{MeIPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}(\text{CIPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j). S_0 and T_1 states are respectively depicted in green and red.

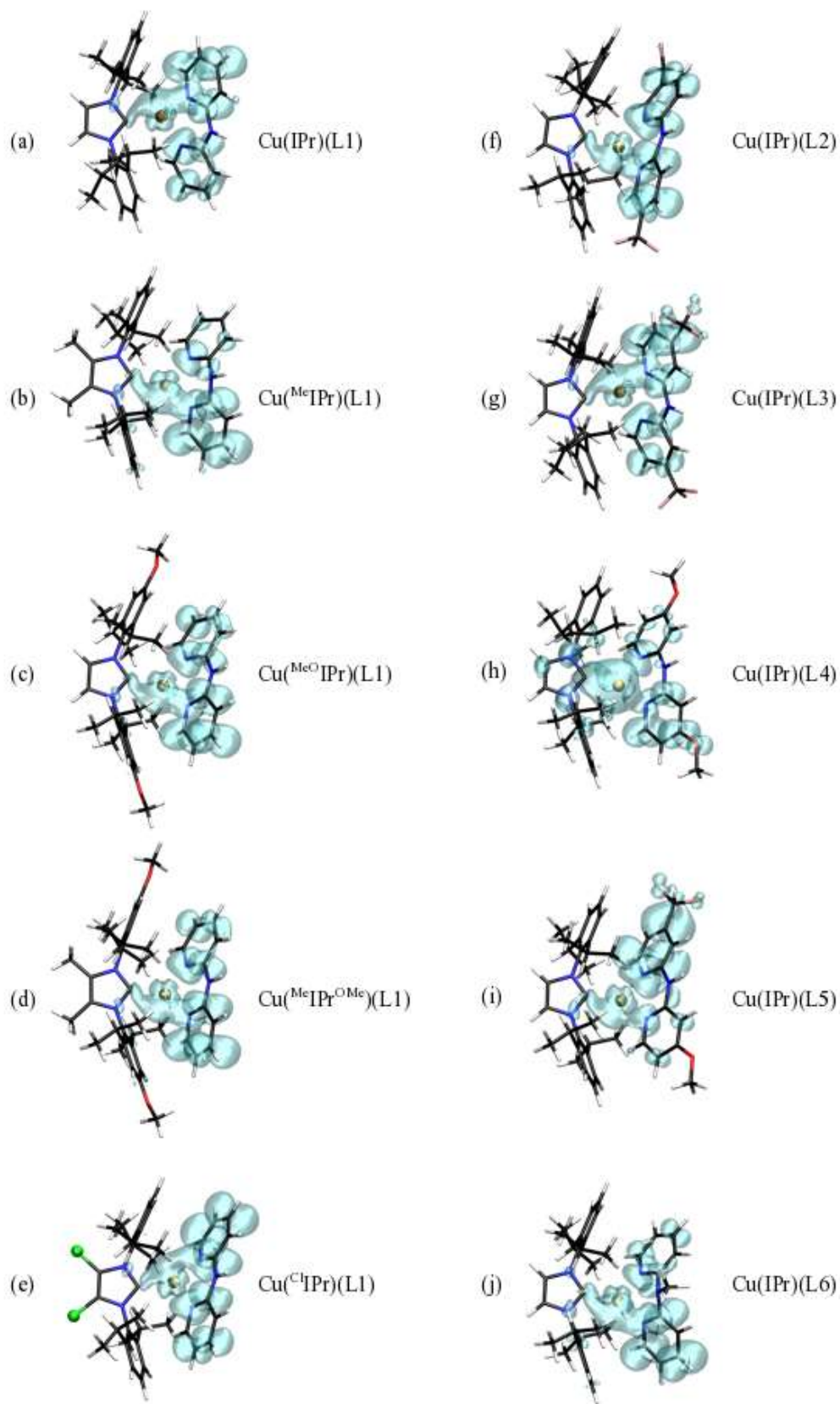
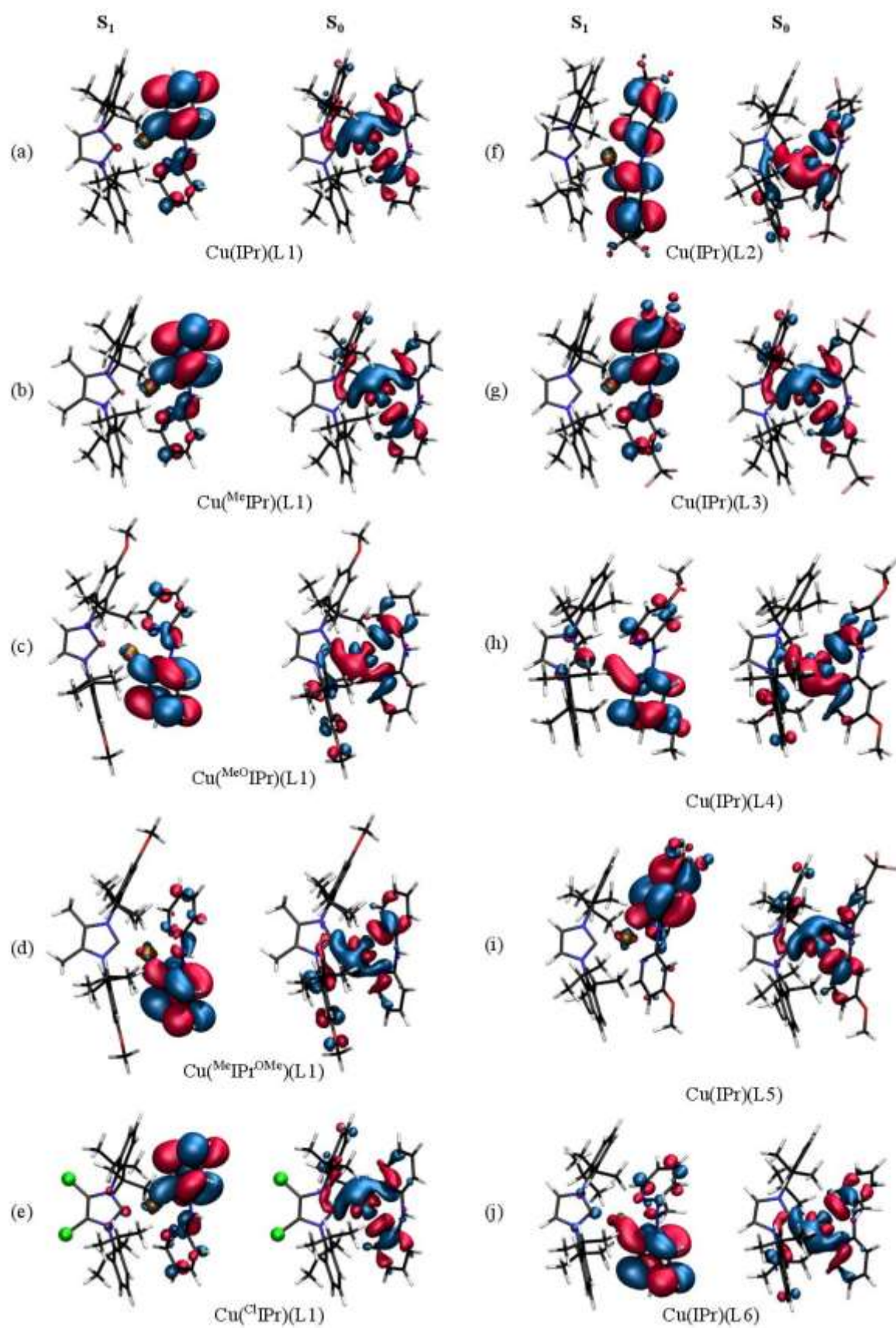
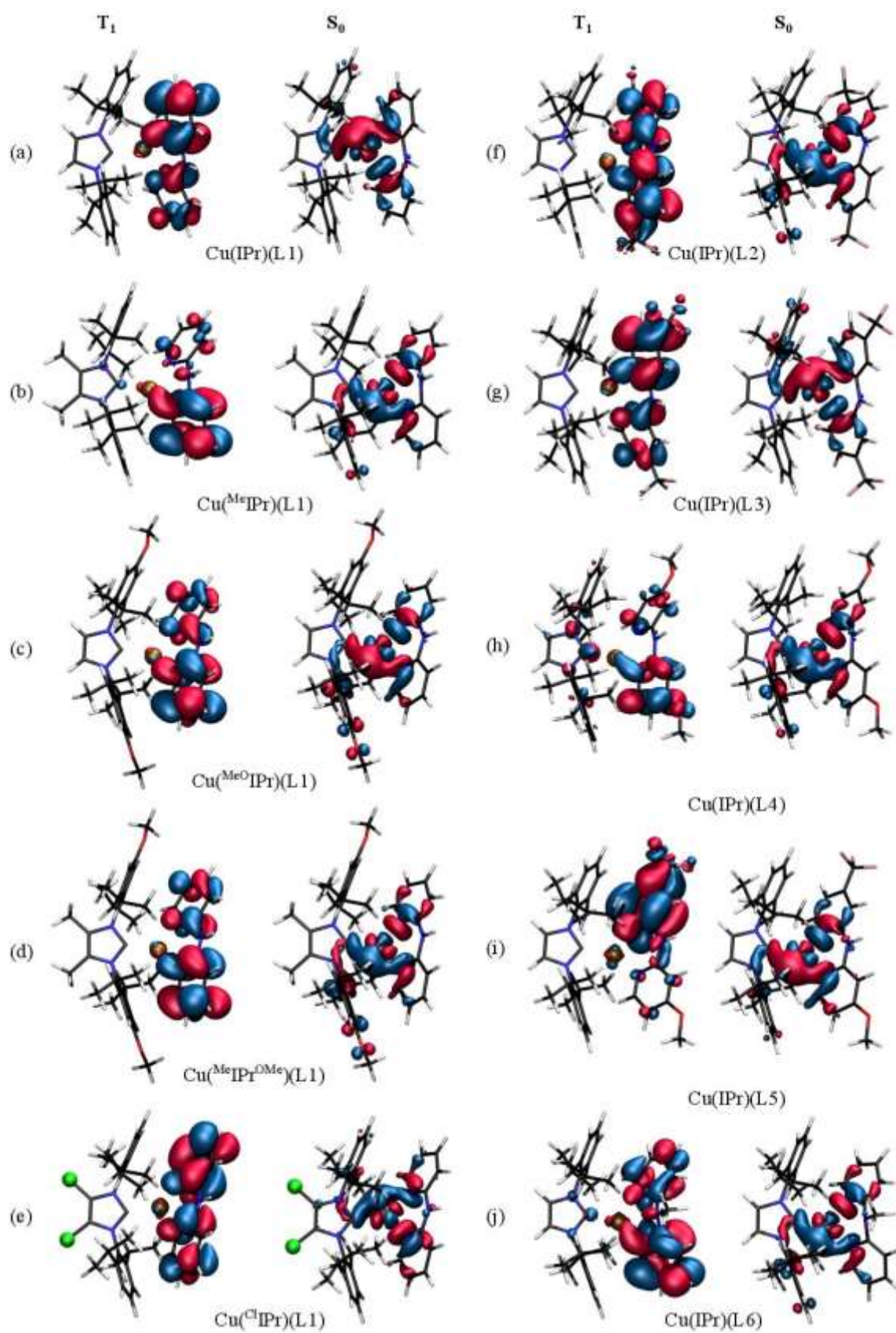


Figure S30. T_1 Spin distribution of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}^{\text{Me}}\text{IPr}(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}^{\text{Me}}\text{IPr}^{\text{OMe}}(\text{L1})]^+$ (d), $[\text{Cu}^{\text{Cl}}\text{IPr}(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j).



Figures S31. NTO distribution of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}^{\text{Me}}(\text{IPr})(\text{L1})]^+$ (b), $[\text{Cu}^{\text{OMe}}(\text{IPr})(\text{L1})]^+$ (c), $[\text{Cu}^{\text{Me}}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}^{\text{Cl}}(\text{IPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j), $S_1 \rightarrow S_0$ emission.



Figures S32. NTO distribution of copper complexes $[\text{Cu}(\text{IPr})(\text{L1})]^+$ (a), $[\text{Cu}(\text{MeIPr})(\text{L1})]^+$ (b), $[\text{Cu}(\text{IPr}^{\text{OMe}})(\text{L1})]^+$ (c), $[\text{Cu}(\text{MeIPr}^{\text{OMe}})(\text{L1})]^+$ (d), $[\text{Cu}(\text{CIPr})(\text{L1})]^+$ (e), $[\text{Cu}(\text{IPr})(\text{L2})]^+$ (f), $[\text{Cu}(\text{IPr})(\text{L3})]^+$ (g), $[\text{Cu}(\text{IPr})(\text{L4})]^+$ (h), $[\text{Cu}(\text{IPr})(\text{L5})]^+$ (i) and $[\text{Cu}(\text{IPr})(\text{L6})]^+$ (j), $T_1 \rightarrow S_0$ emission.

Complete absorption-emission diagrams of copper complexes **6-15**.

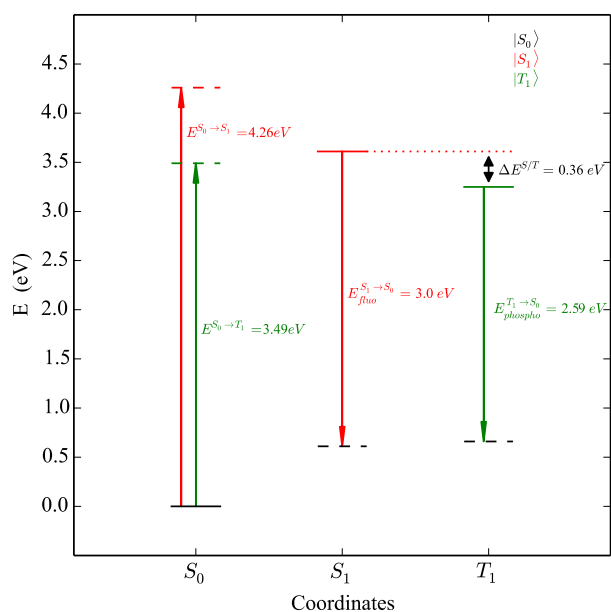


Figure S33. Complex 6.

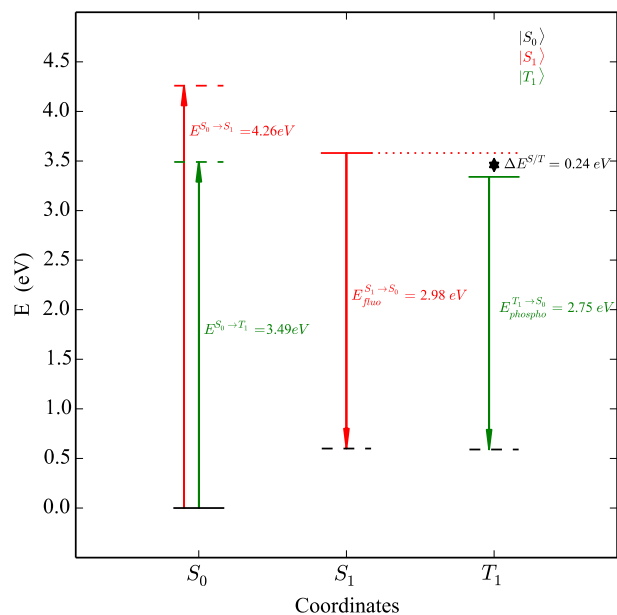


Figure S34. Complex 7.

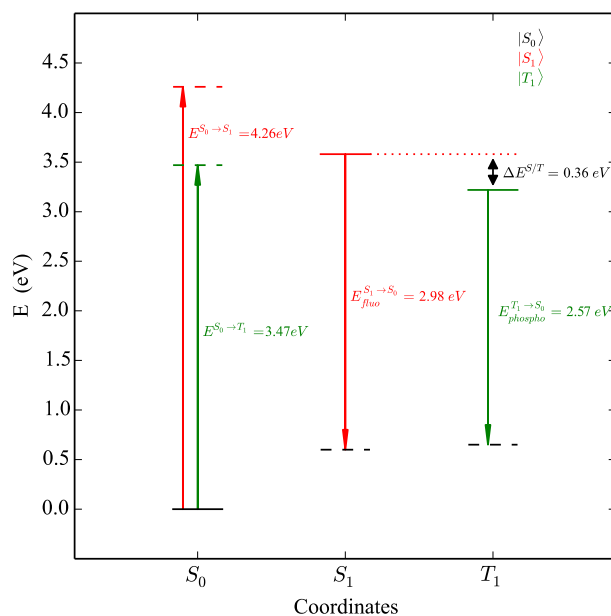


Figure S35. Complex 8.

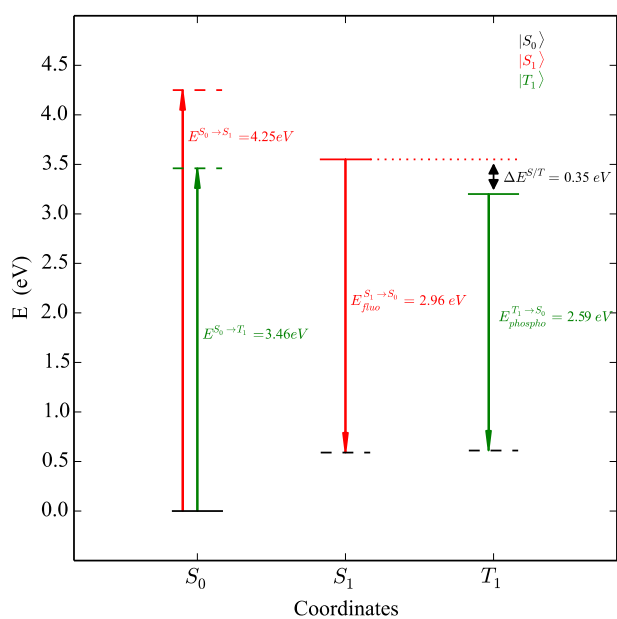


Figure S36. Complex 9.

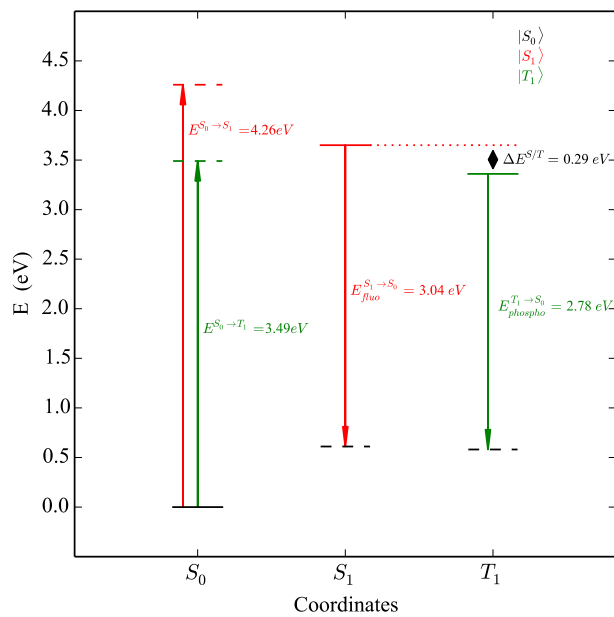


Figure S37. Complex 10.

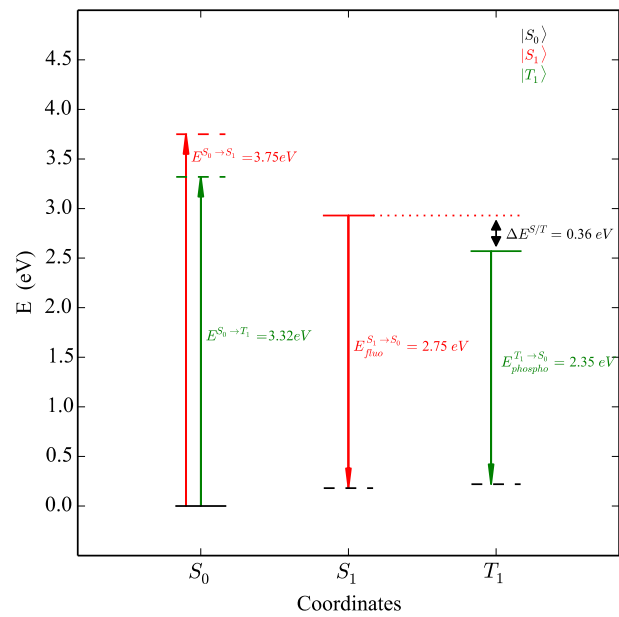


Figure S38. Complex 11.

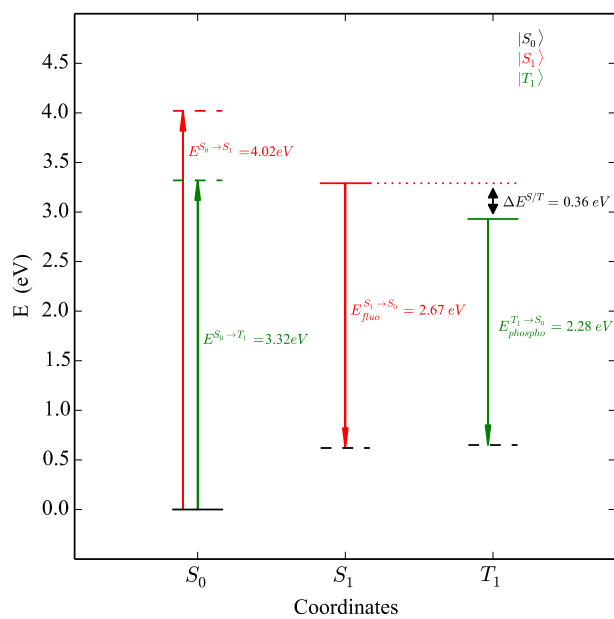


Figure S39. Complex 12.

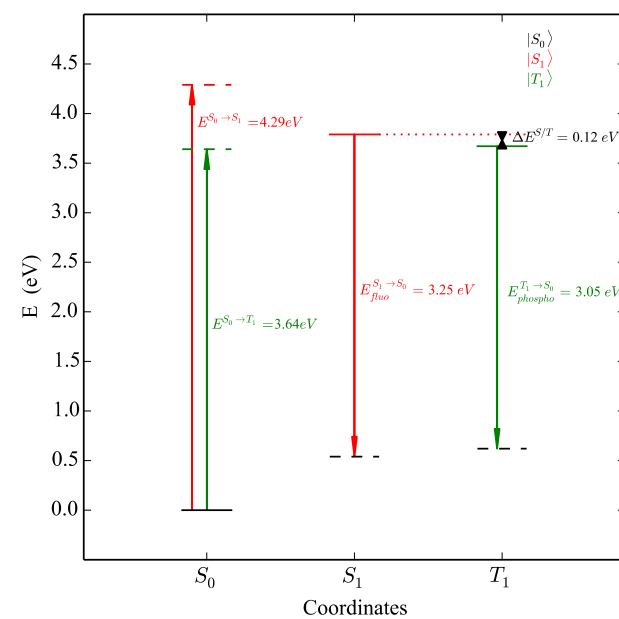


Figure S40. Complex 13.

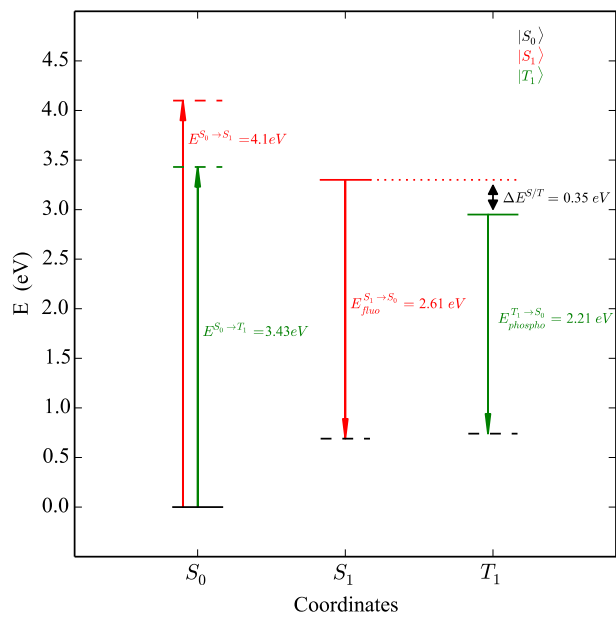


Figure S41. Complex 14.

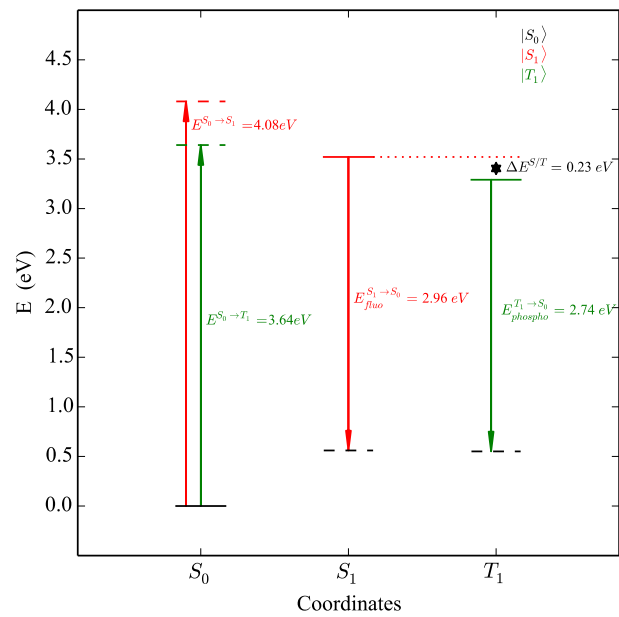


Figure S42. Complex 15.

Part 8. Device characterization

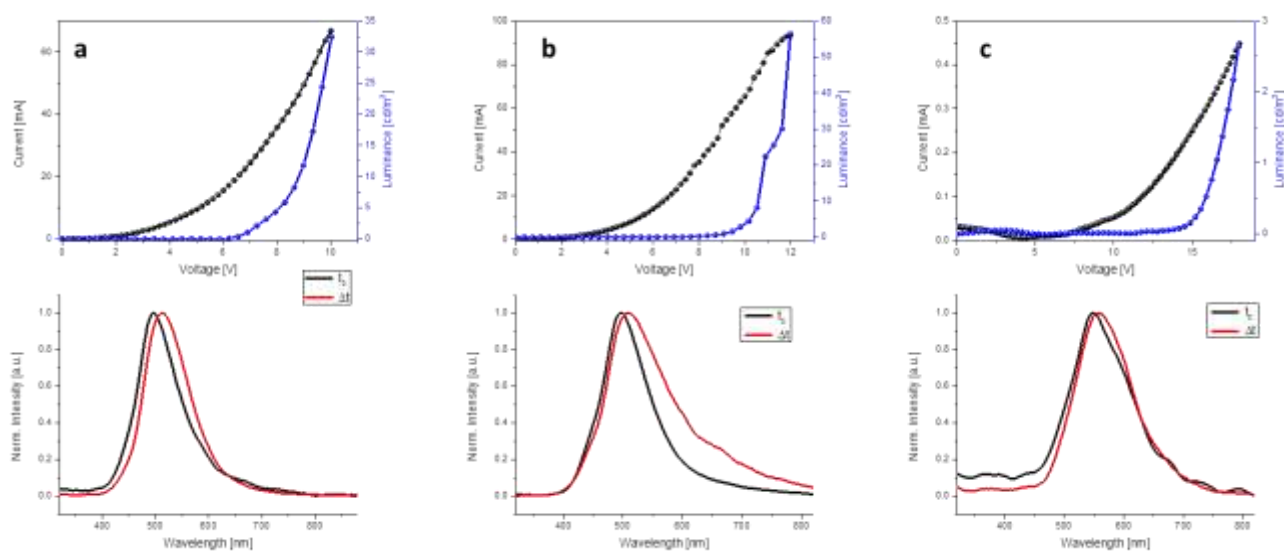


Figure S43. LIV of devices prepared with complex (a) **6**, (b) **9** and (c) **14** (top) and corresponding EL shift (bottom) from initial (black) to final (red) time of the LIV assay.

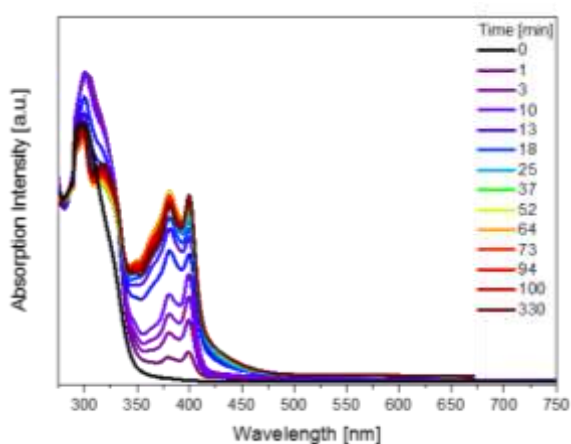


Figure S44. Absorption spectra over time of **17** (1×10^{-6} M) in THF under ambient conditions.

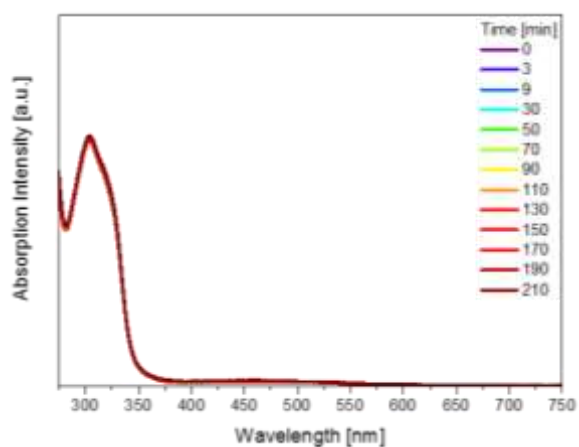


Figure S45. Absorption spectra over time of **17** in thin films prepared with the THF solution under ambient conditions.

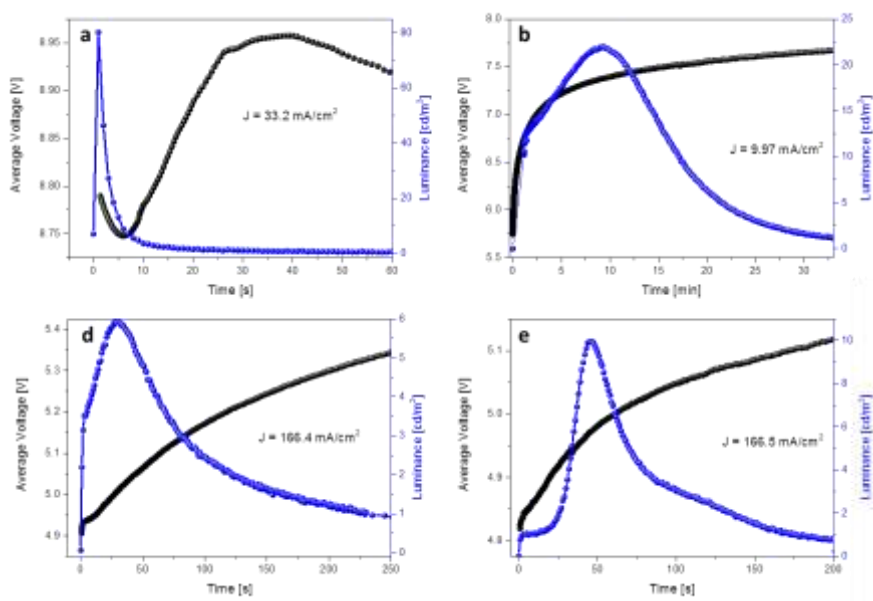


Figure S46. Lifetime measurements of blue LECs (17) at 5 mA (a) and 1.5 mA (b) galvanostatic pulsed driving scheme and 25 mA mode applied to 6 (d) and 9 (e), respectively.

Part 9: ^1H and ^{13}C NMR spectra of compounds

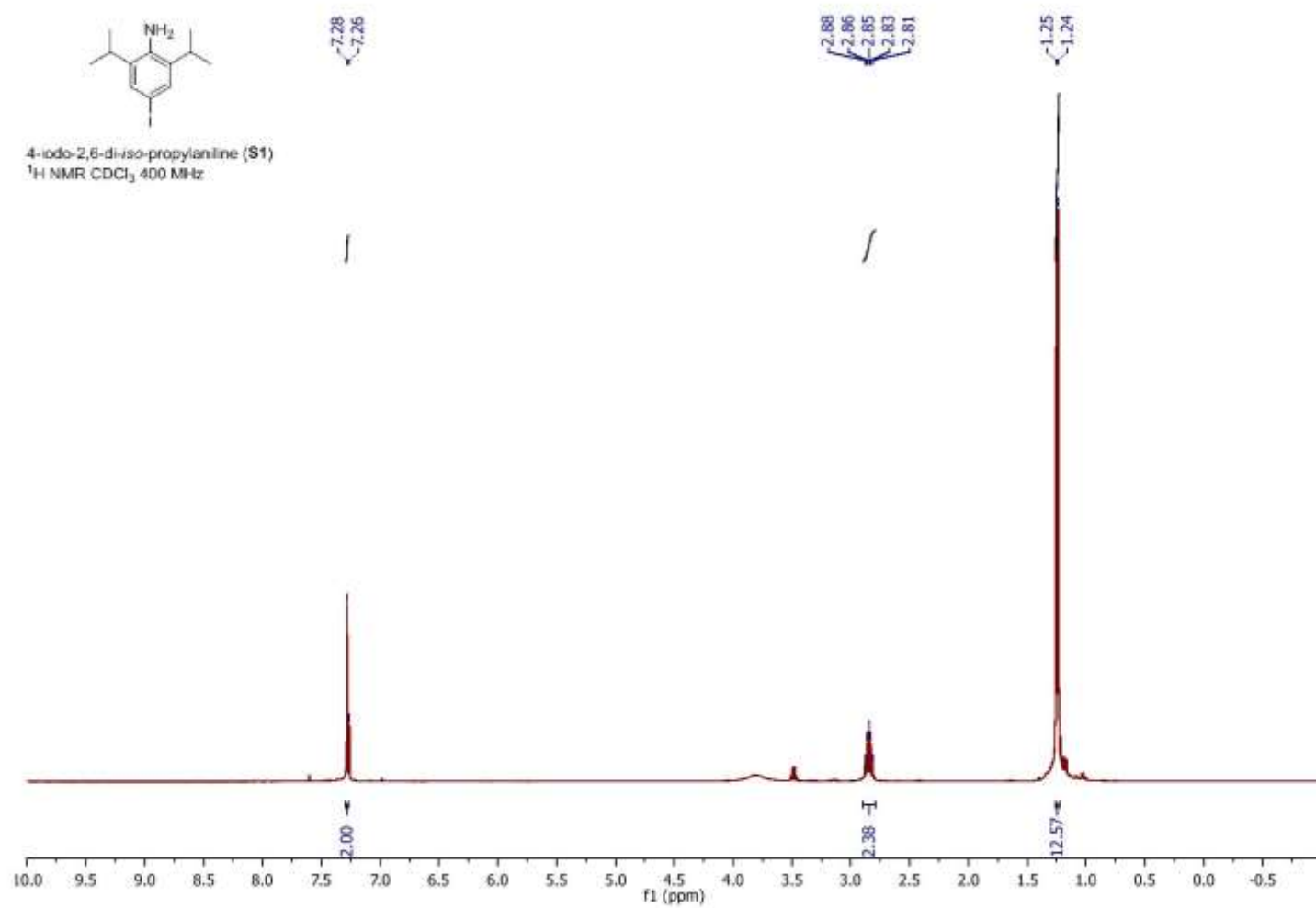


Figure S47. ^1H NMR spectra of compound S1.

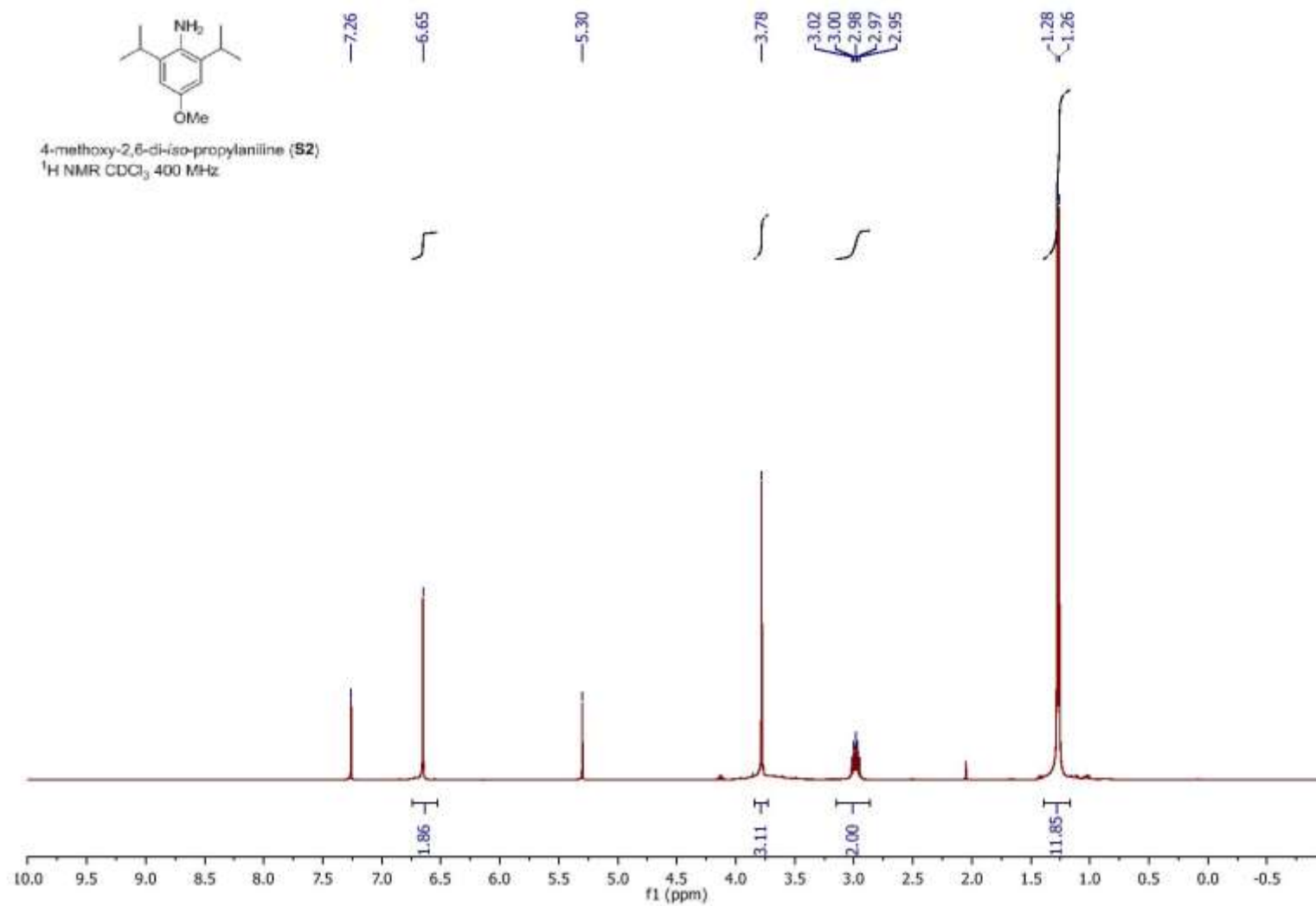


Figure S48. ¹H NMR spectra of compound **S2**.

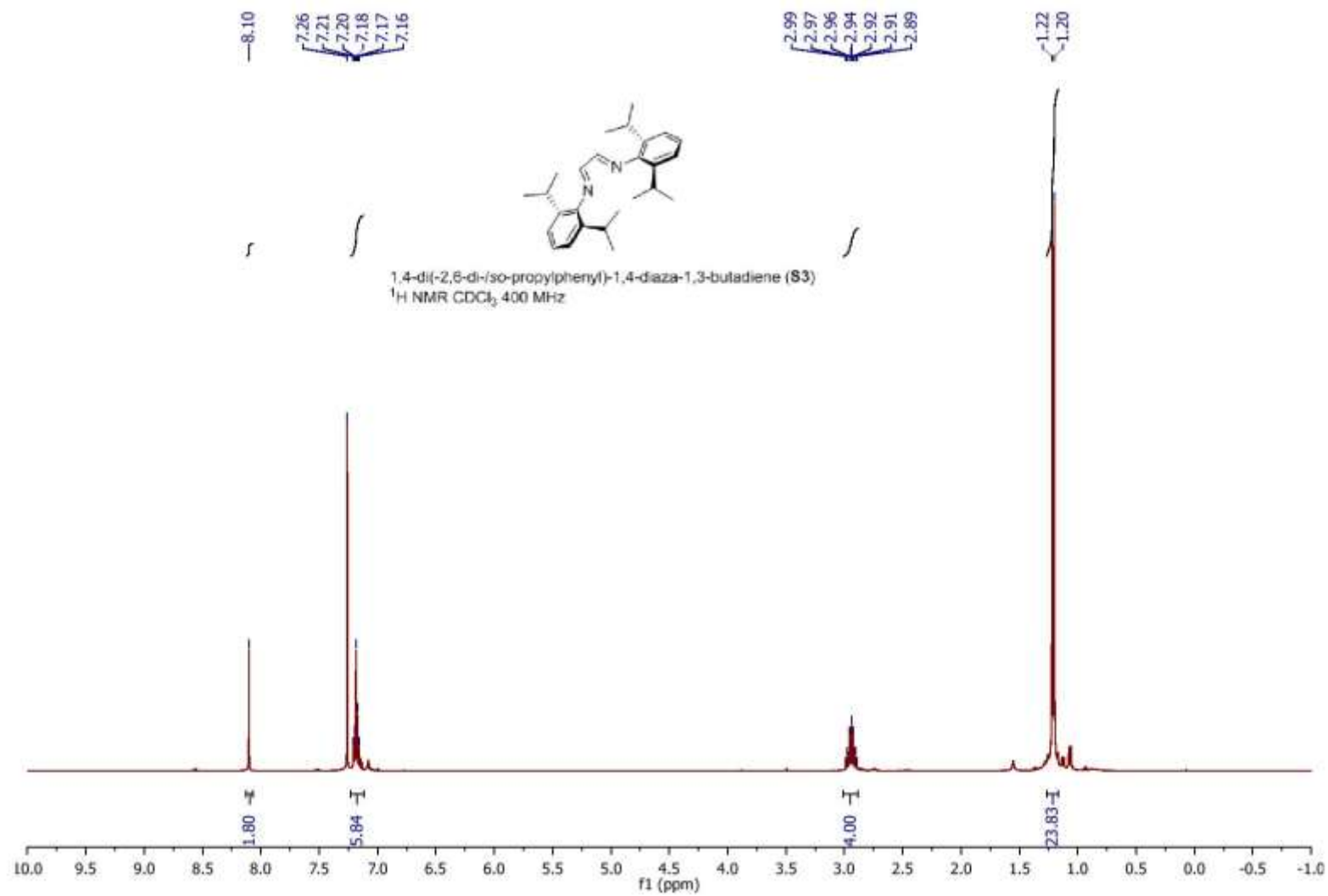


Figure S49. ¹H NMR spectra of compound S3.

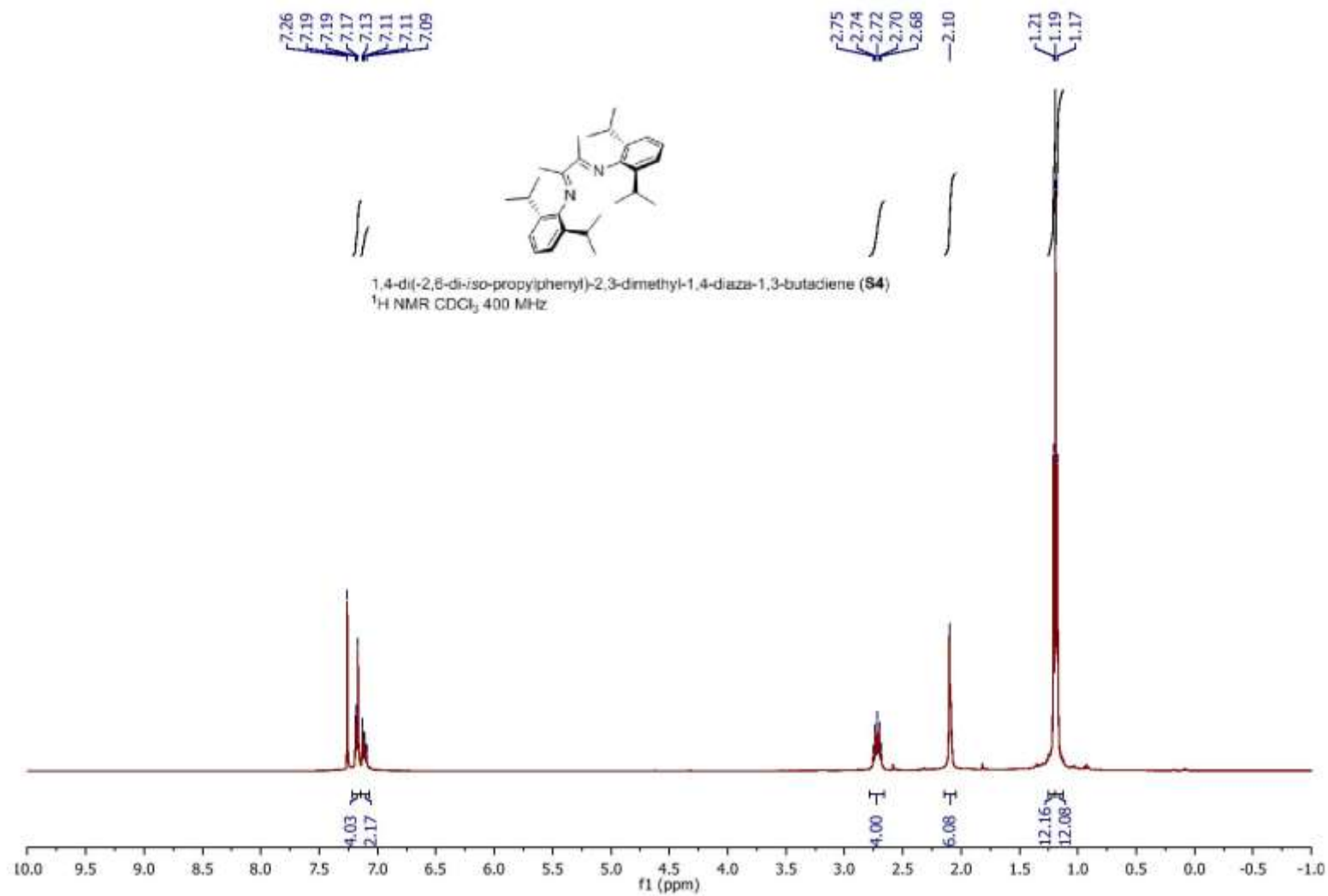


Figure S50. ¹H NMR spectra of compound **S4**.

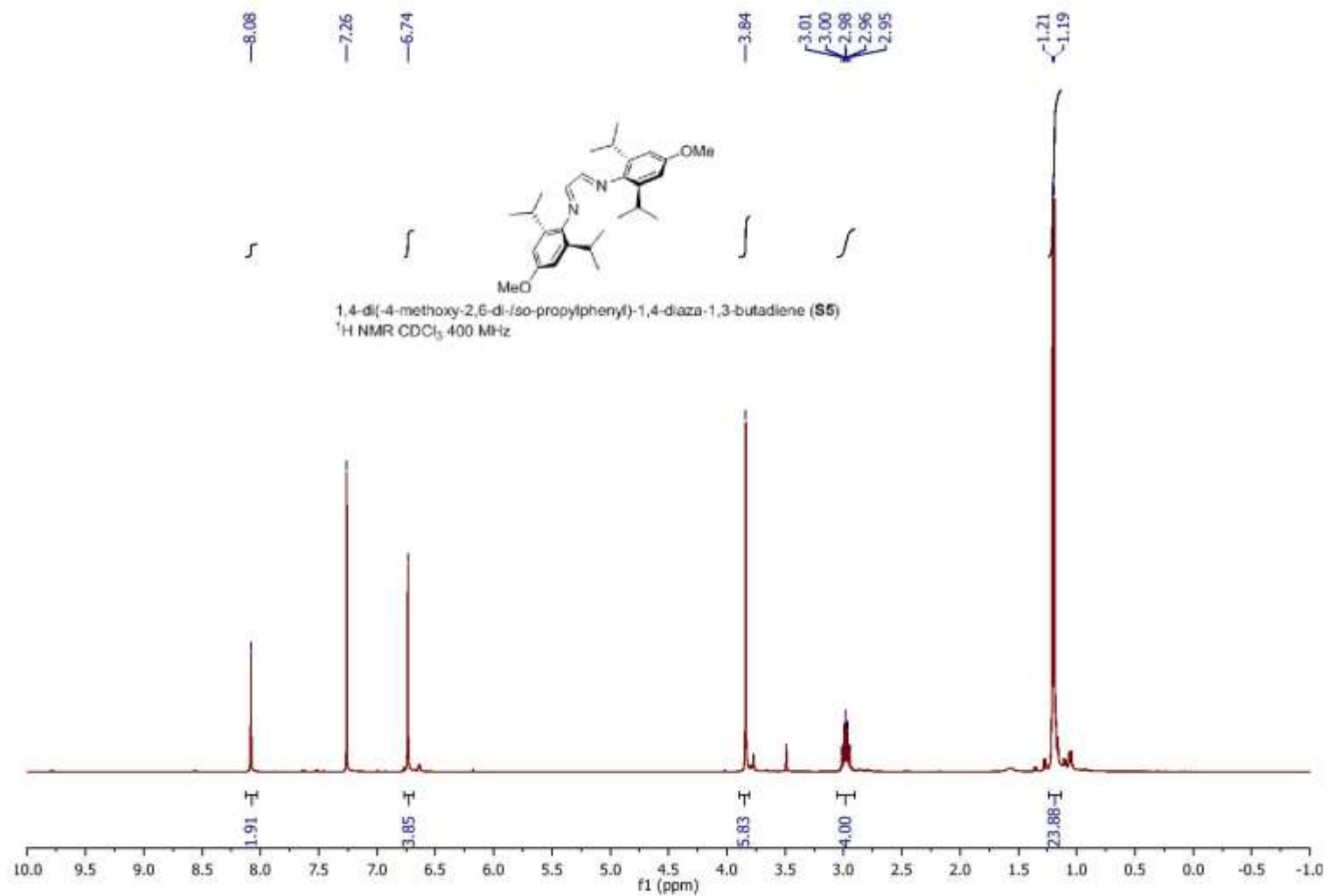


Figure S51. ¹H NMR spectra of compound **S5**.

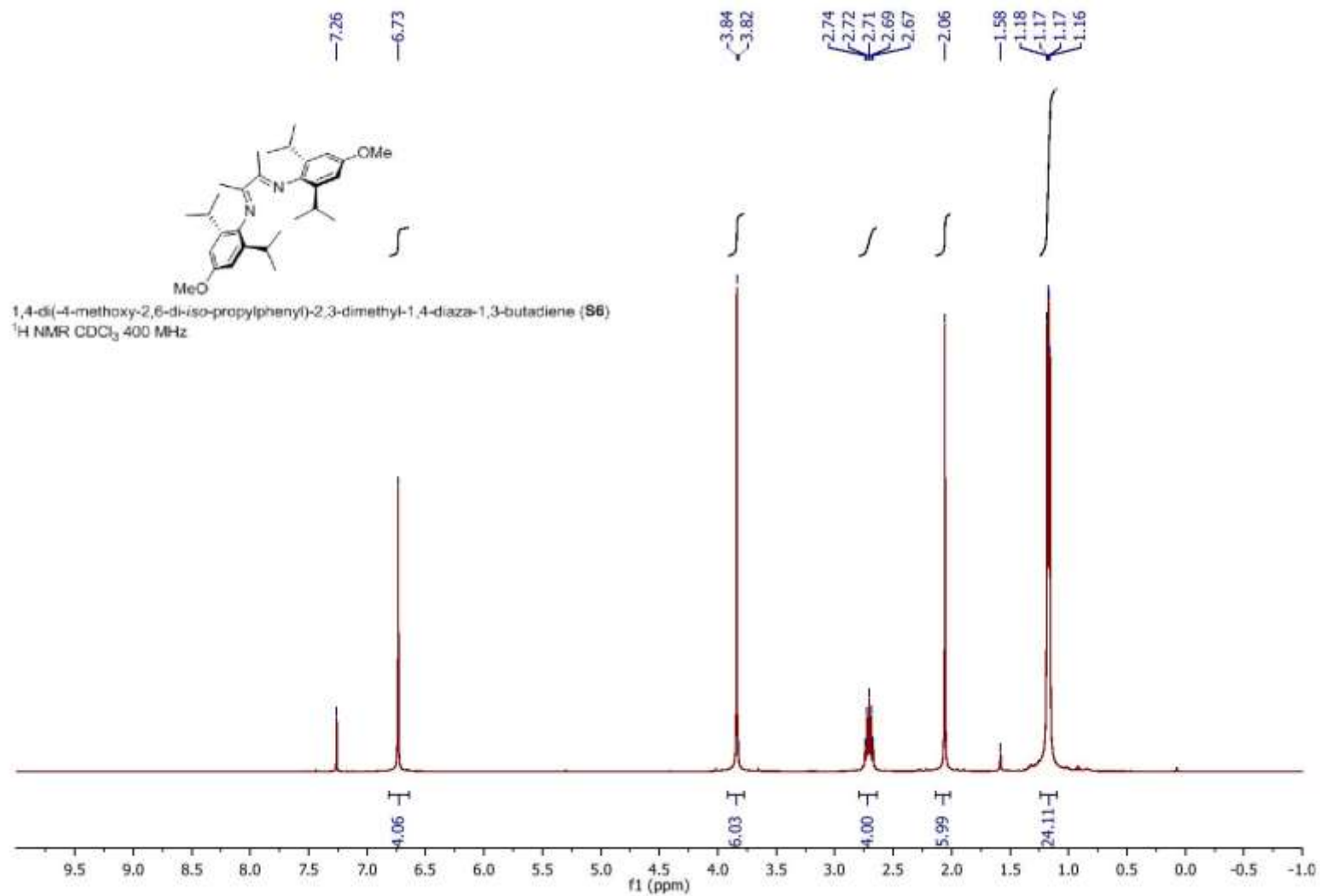


Figure S52. ¹H NMR spectra of compound **S6**.

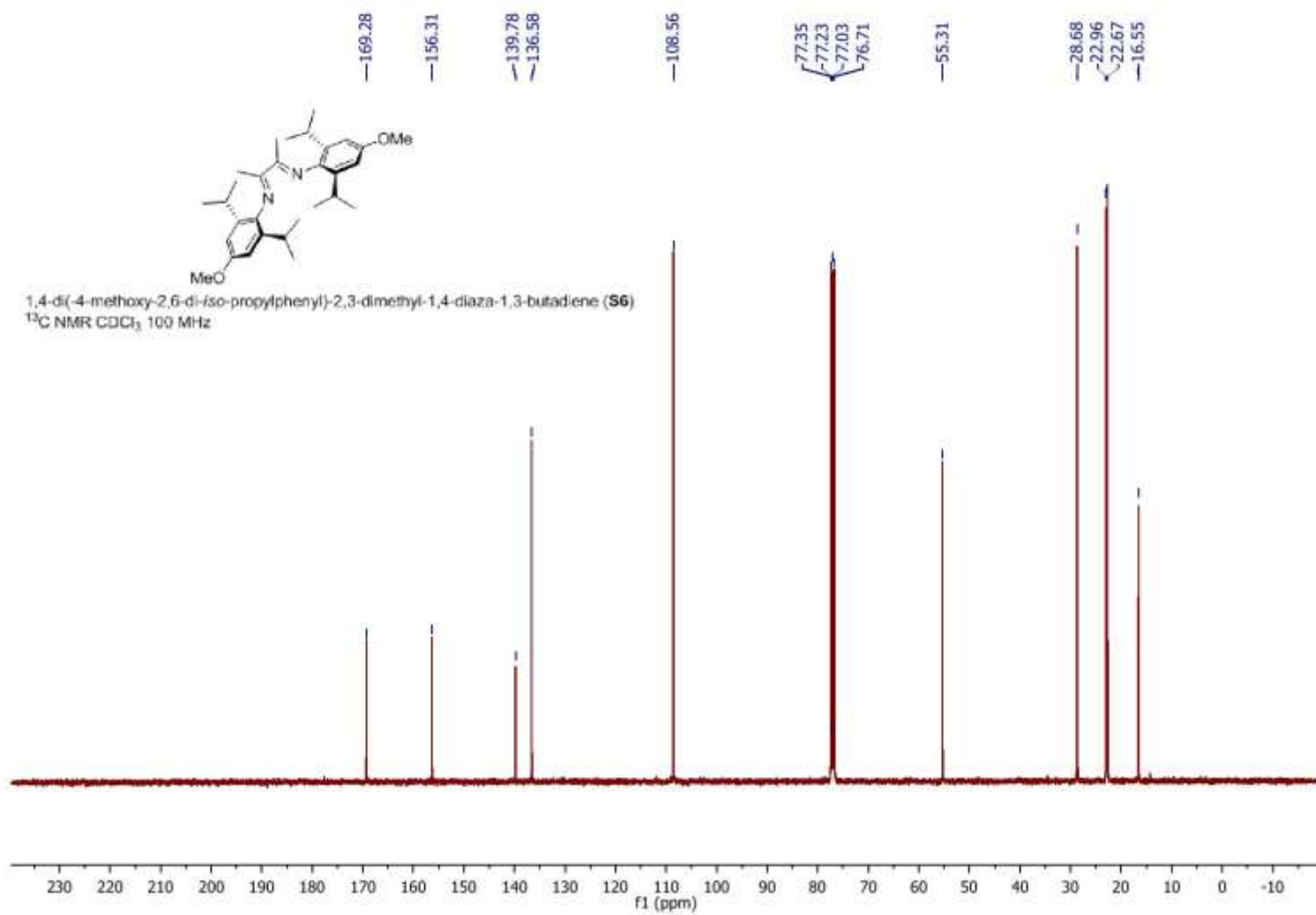


Figure S53. ¹³C NMR spectra of compound **S6**.

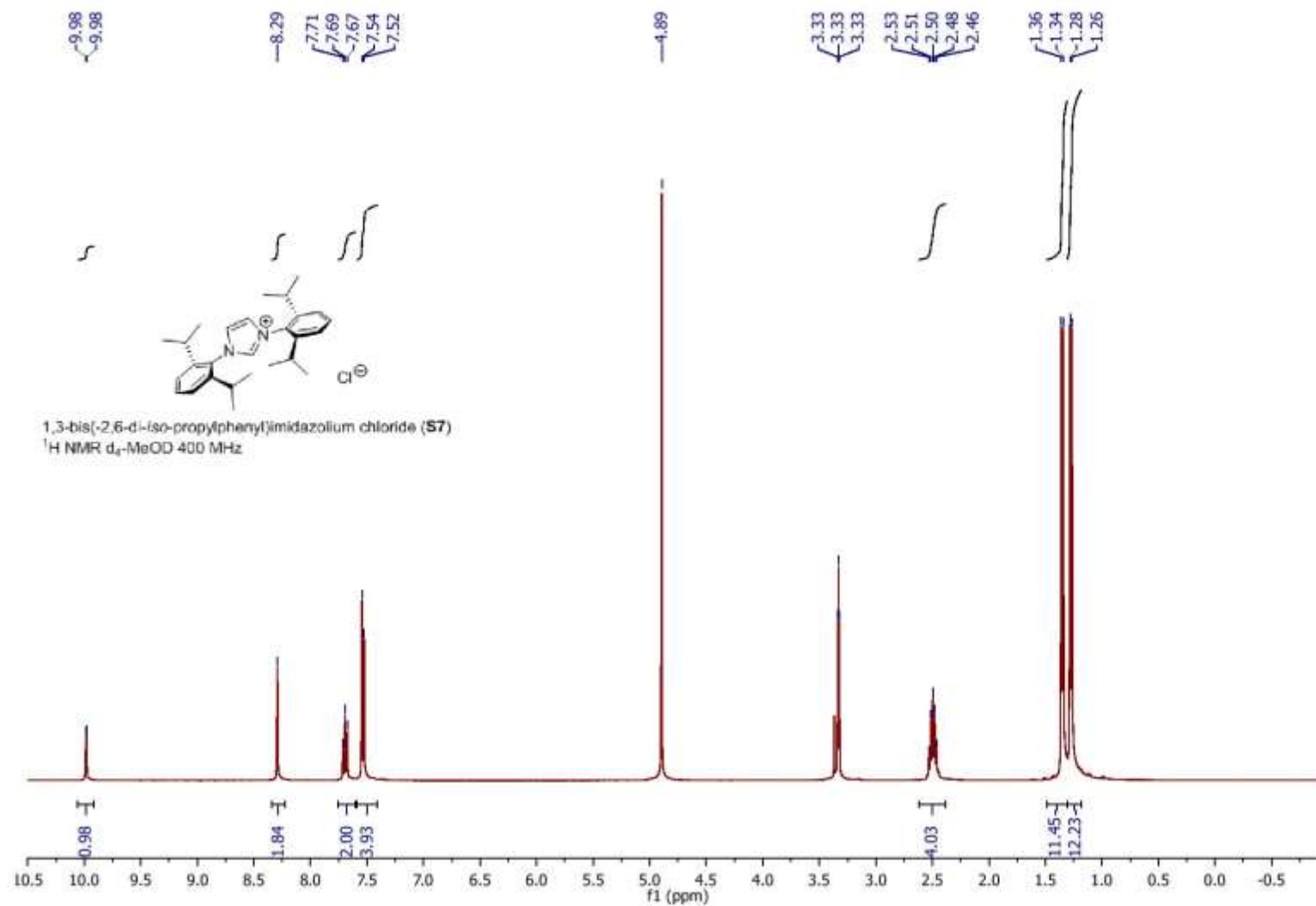


Figure S54. ¹H NMR spectra of compound **S7**.

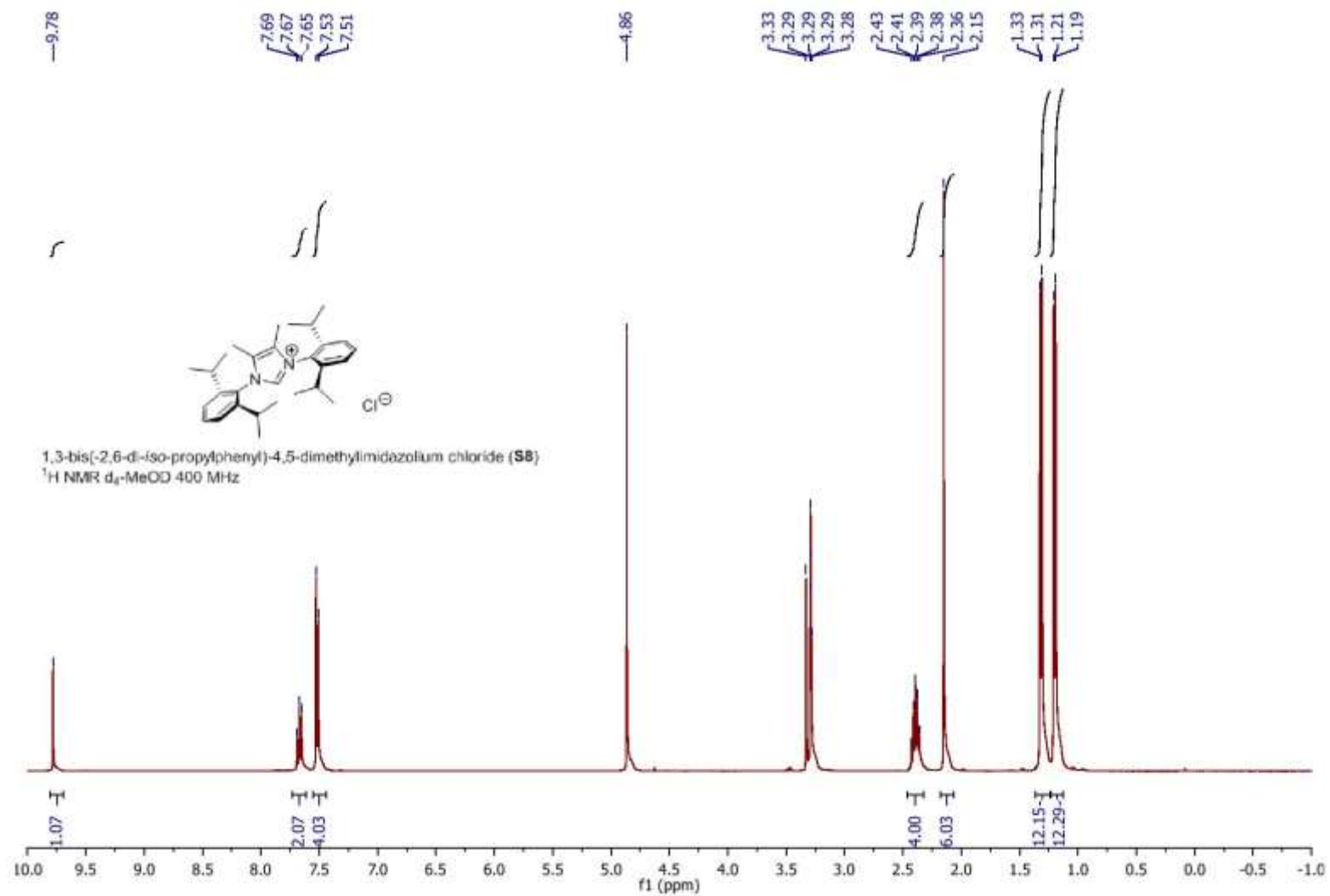


Figure S55. ¹H NMR spectra of compound **S8**.

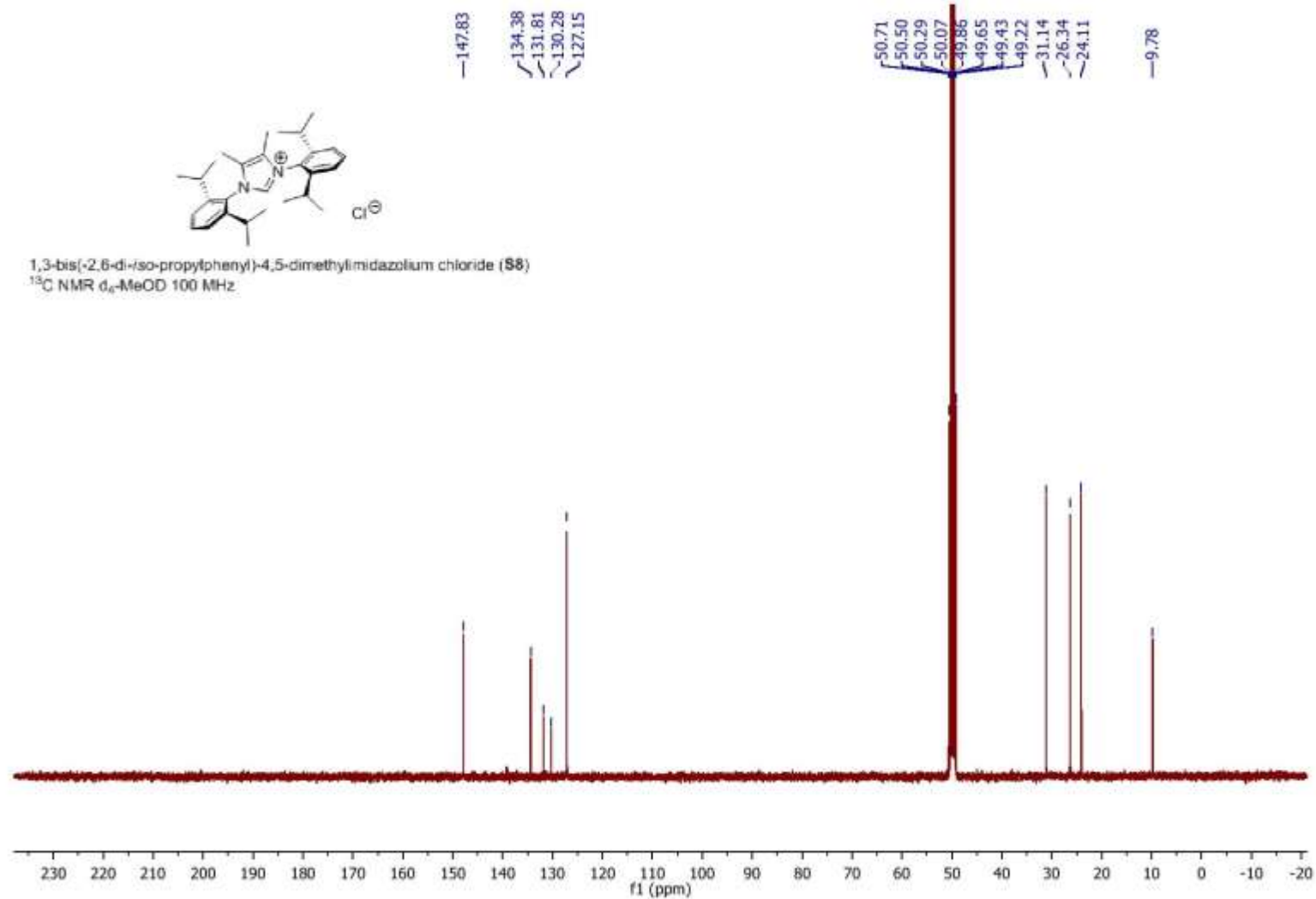


Figure S56. ¹³C NMR spectra of compound **S8**.

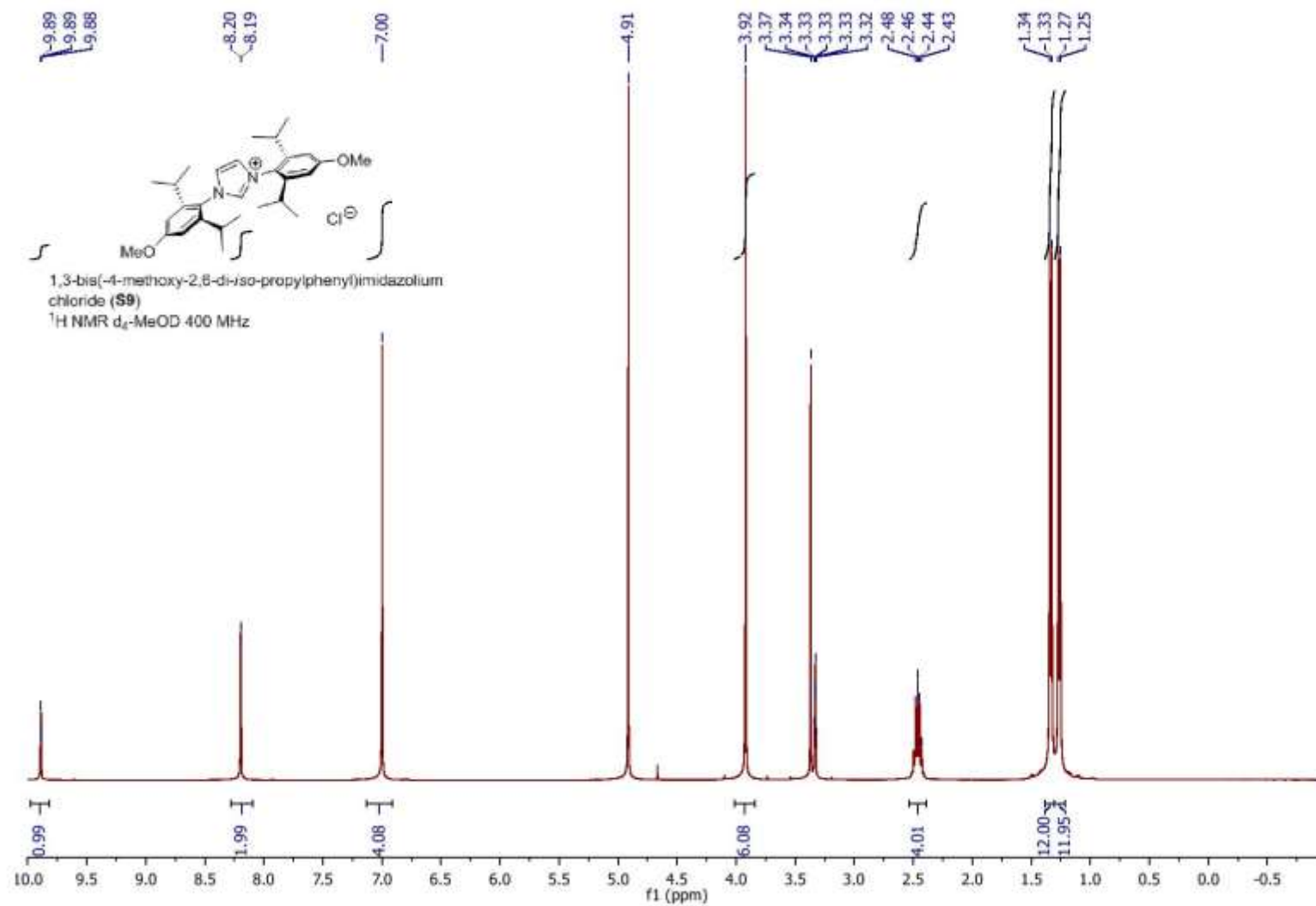


Figure S57. ¹H NMR spectra of compound **S9**.

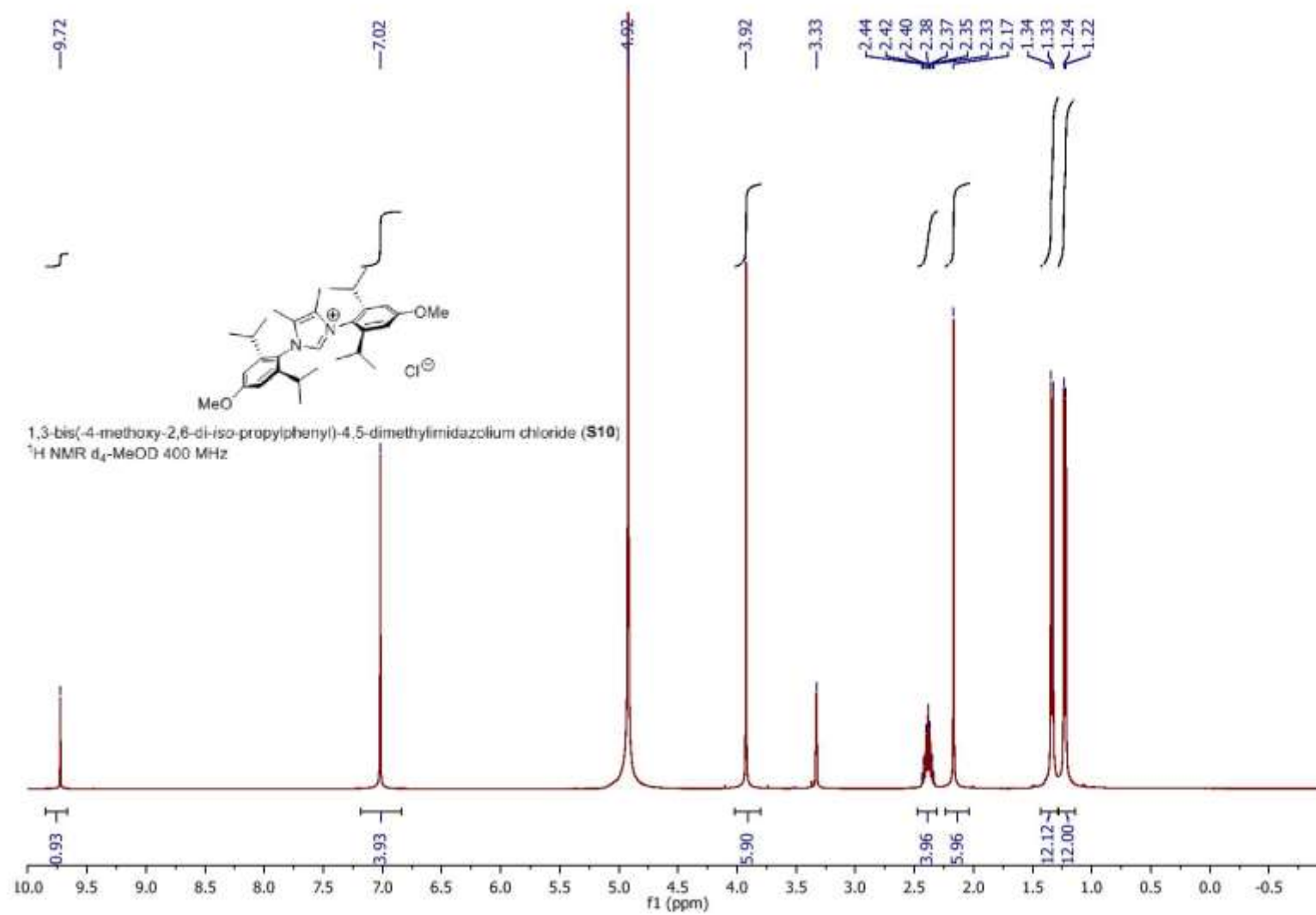


Figure S58. ¹H NMR spectra of compound **S10**.

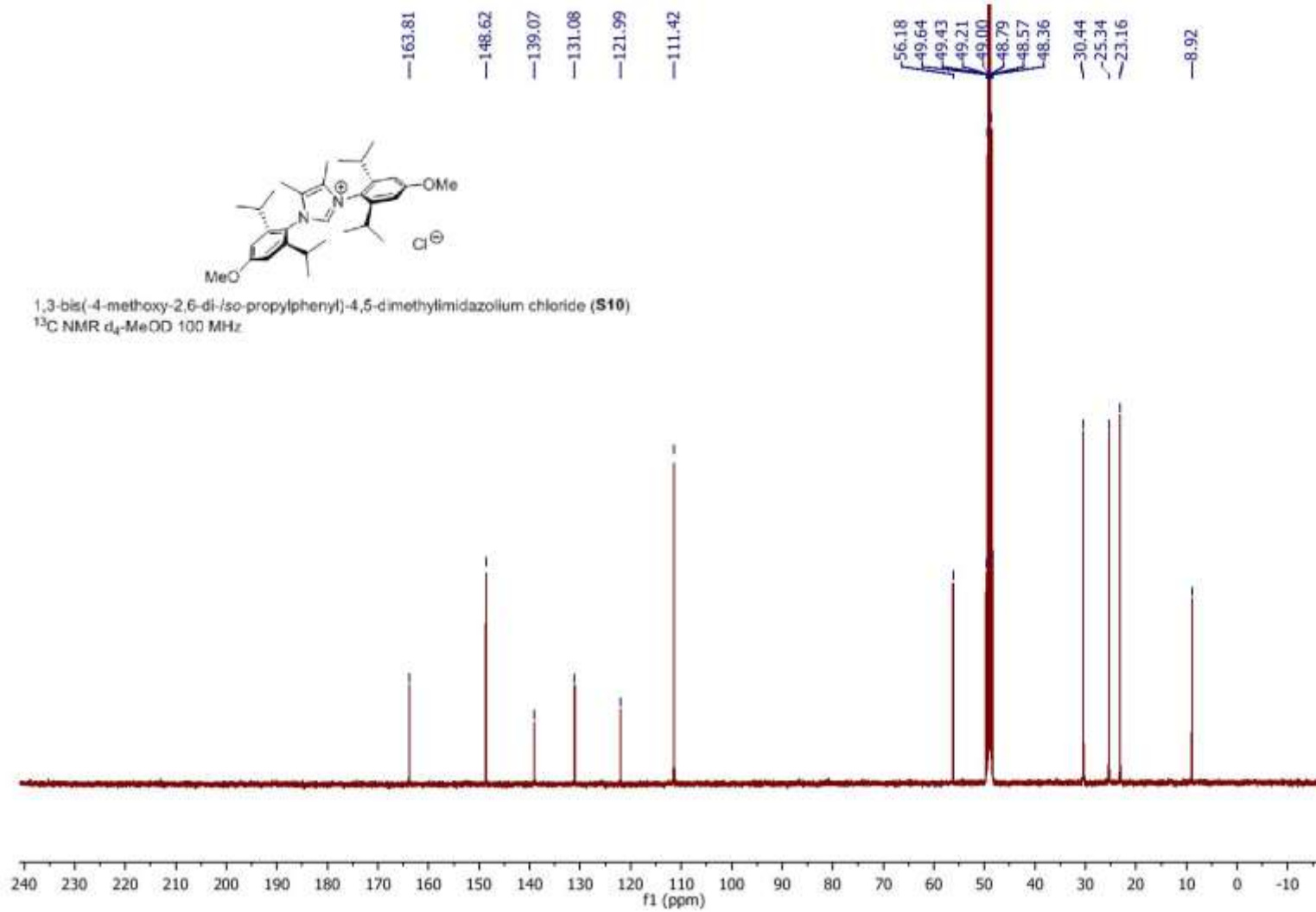


Figure S59. ^{13}C NMR spectra of compound **S10**.

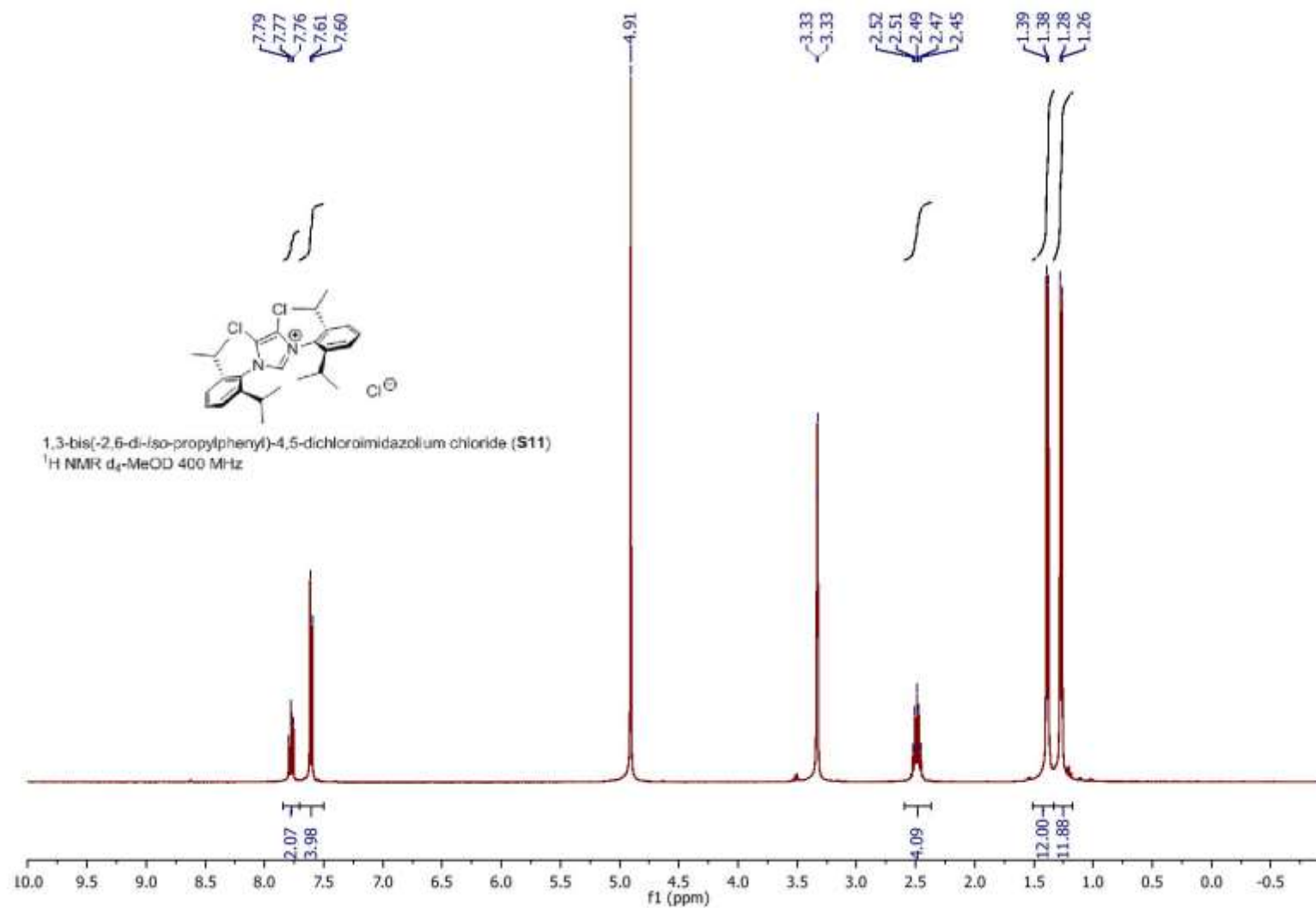


Figure S60. ¹H NMR spectra of compound **S11**.

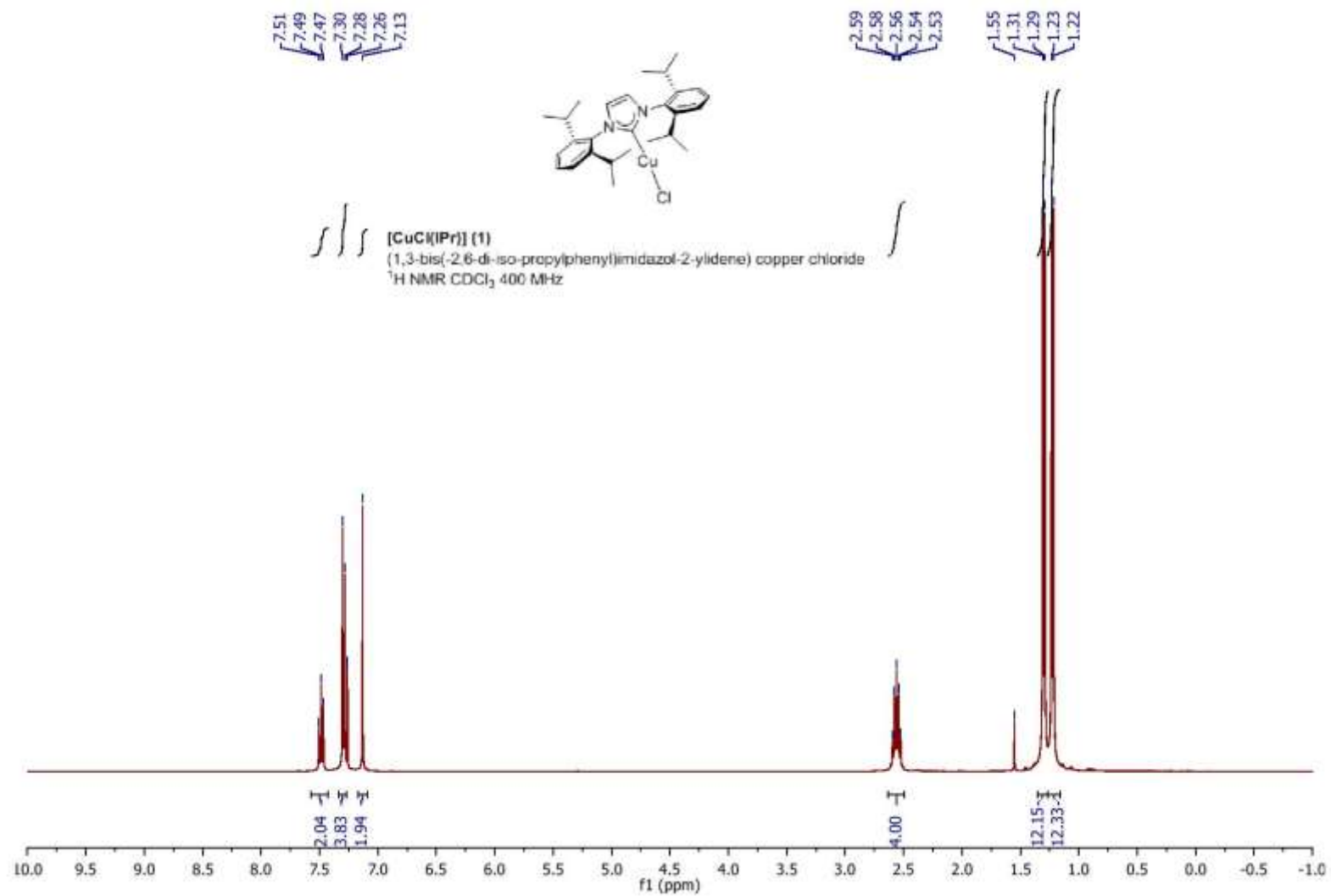


Figure S61. ¹H NMR spectra of complex 1.

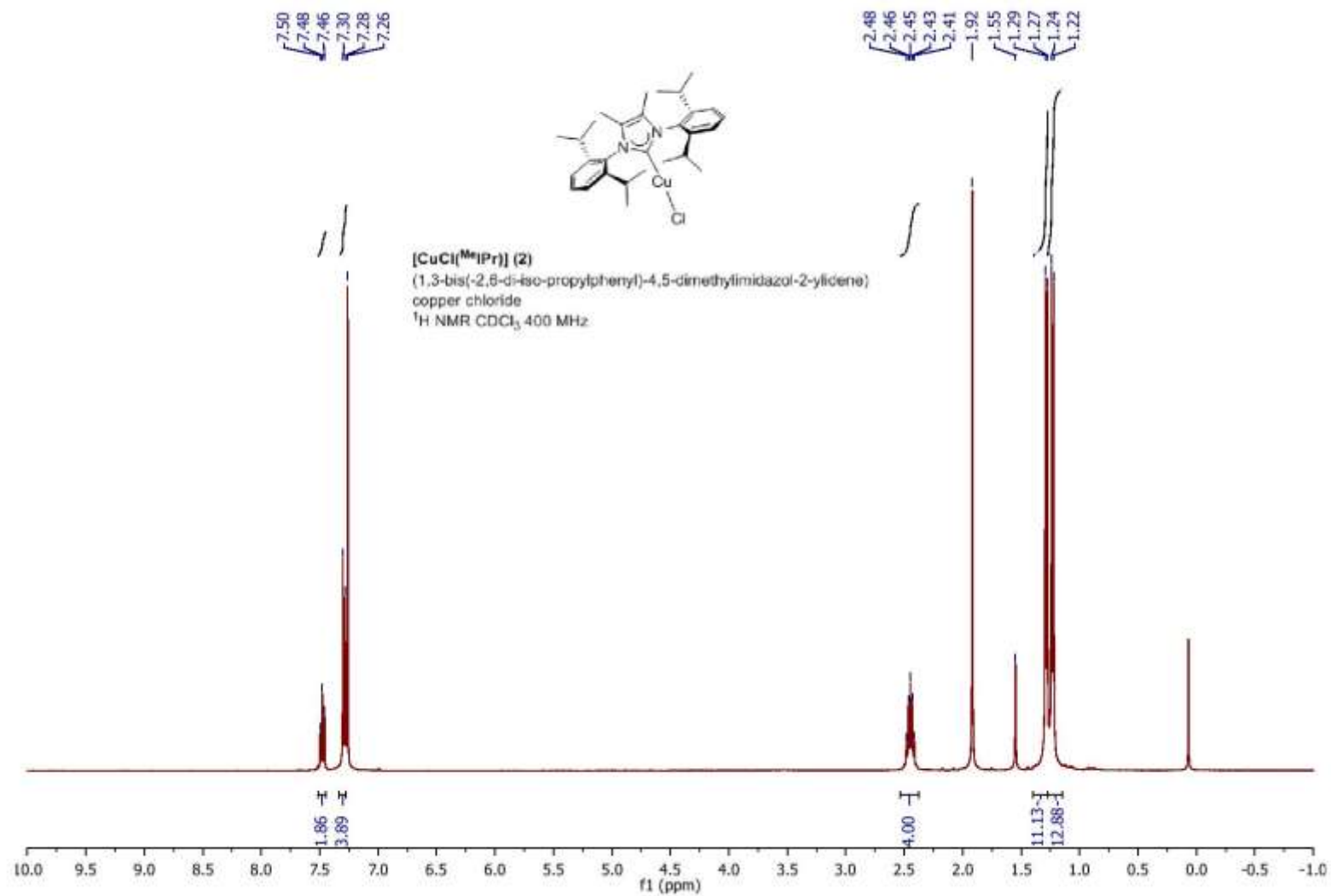


Figure S62. $^1\text{H NMR}$ spectra of complex 2.

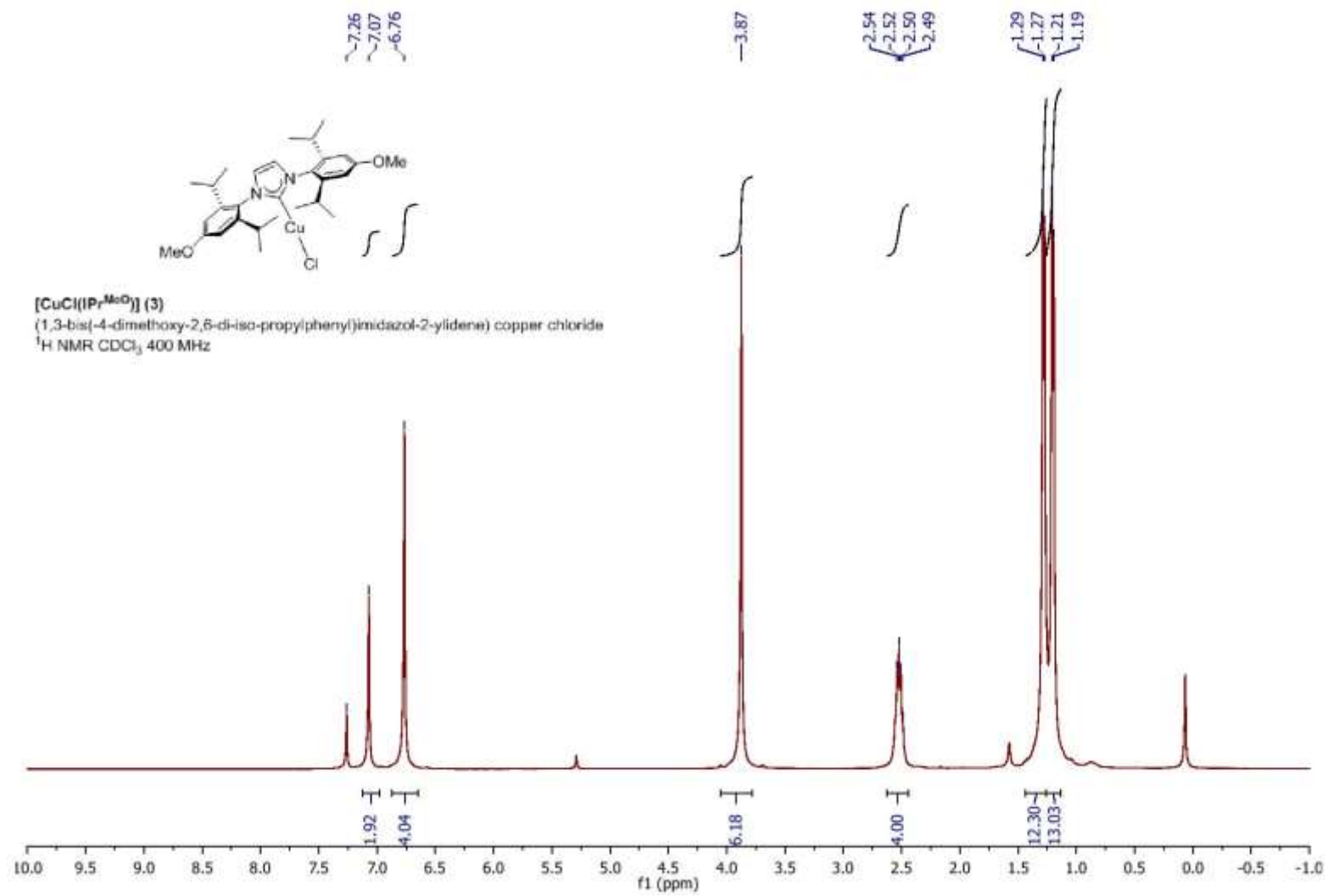


Figure S63. ¹H NMR spectra of complex **3**.

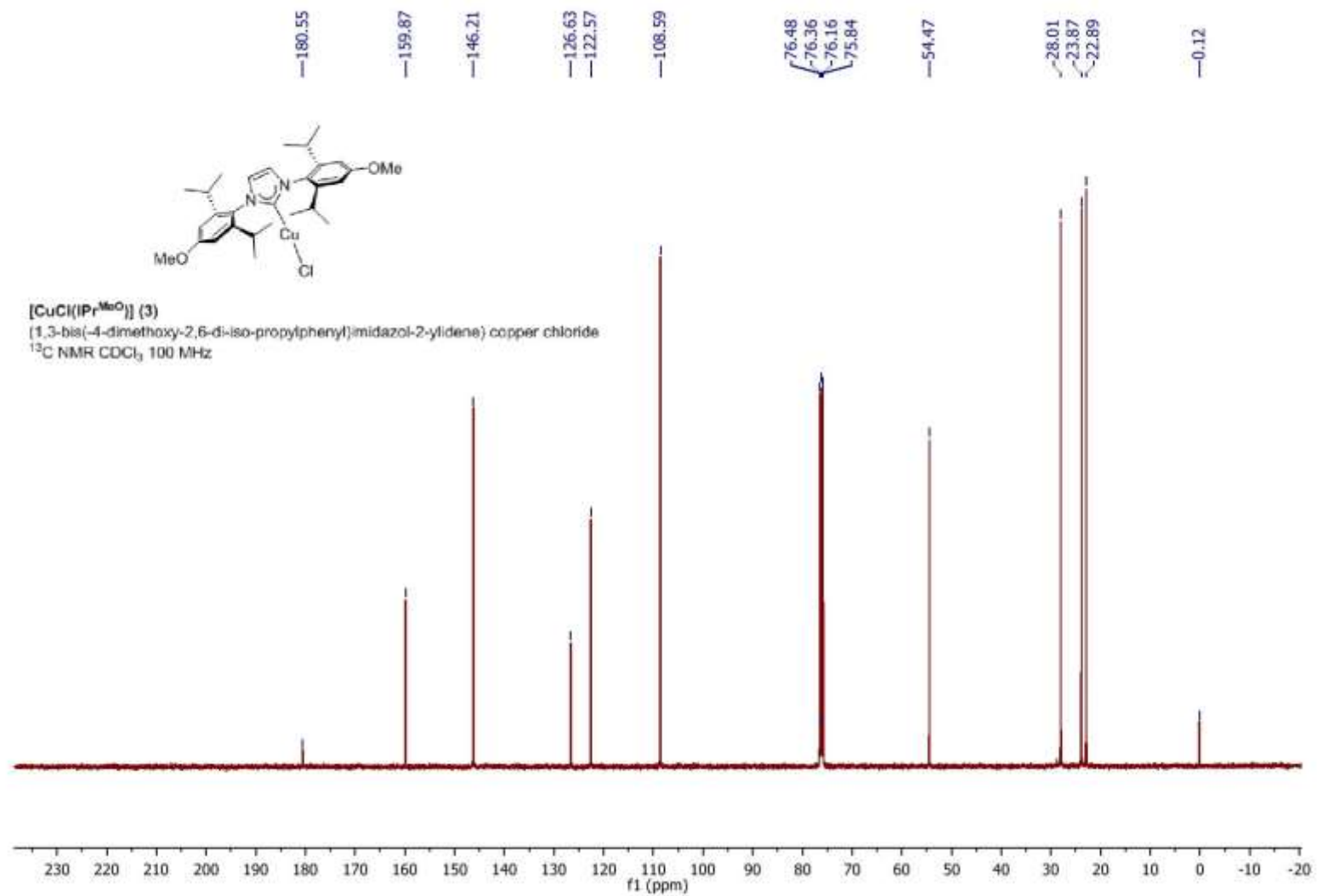


Figure S64. ¹³C NMR spectra of complex 3.

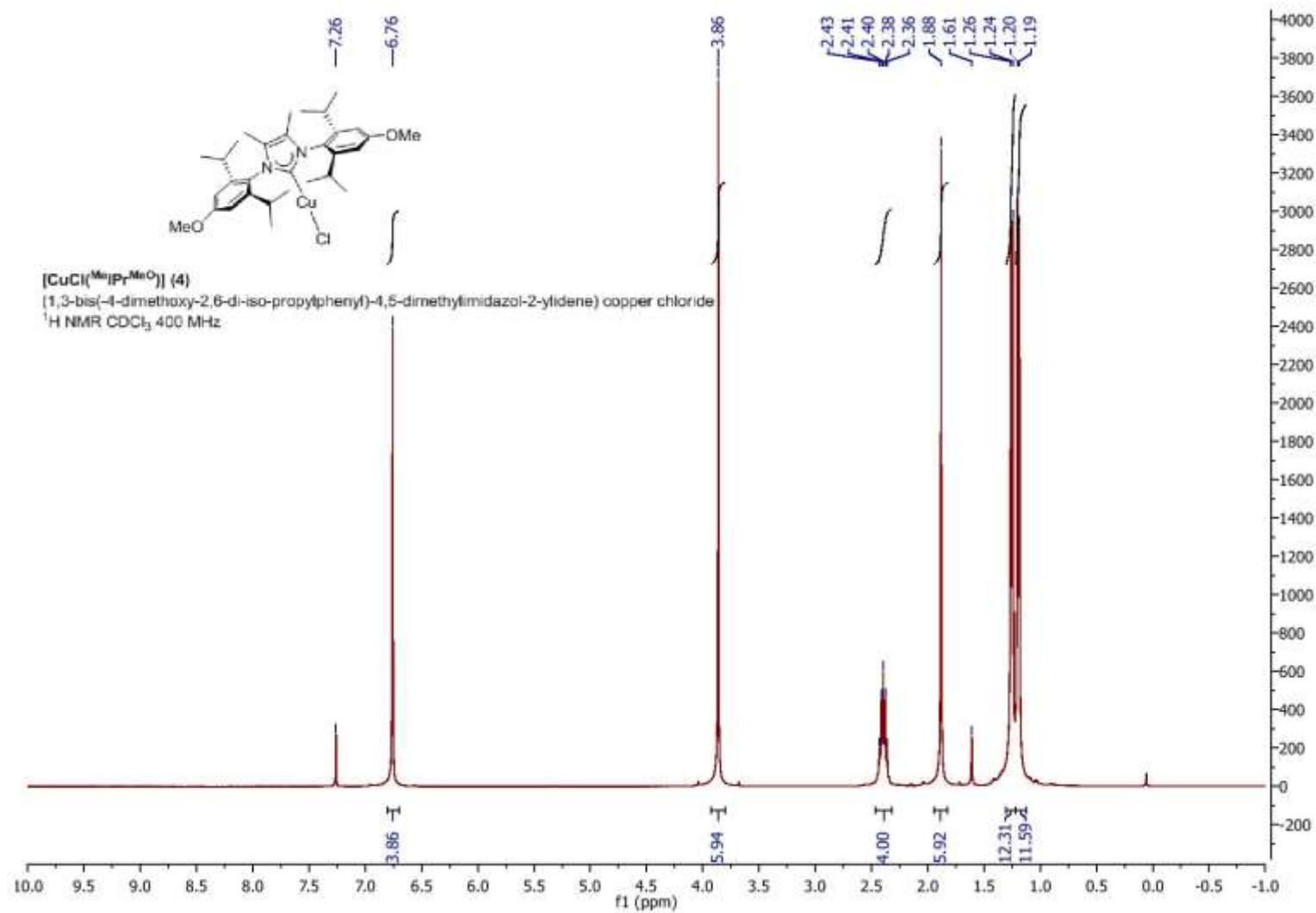


Figure S65. ¹H NMR spectra of complex 4.

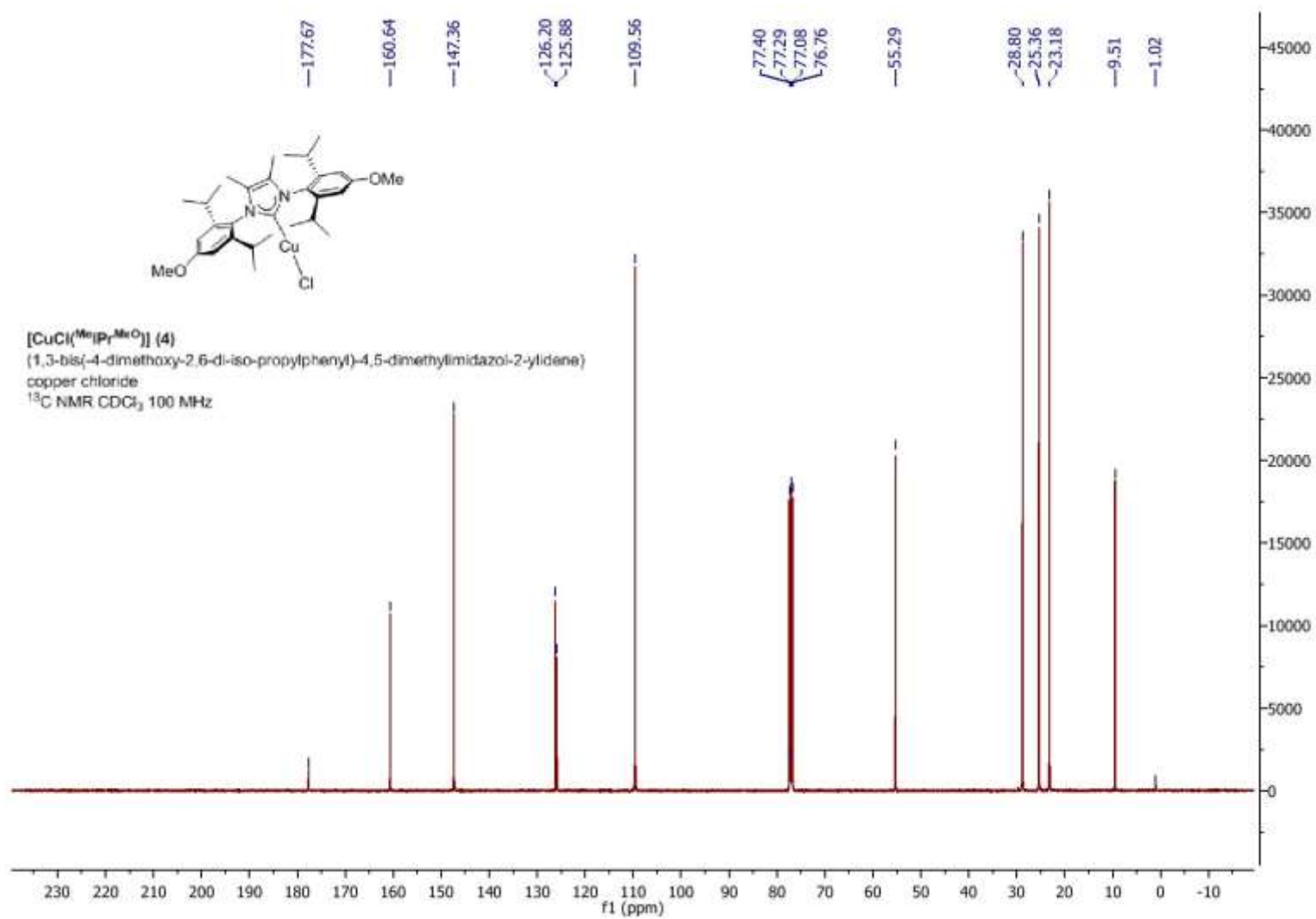


Figure S66. ¹³C NMR spectra of complex 4.

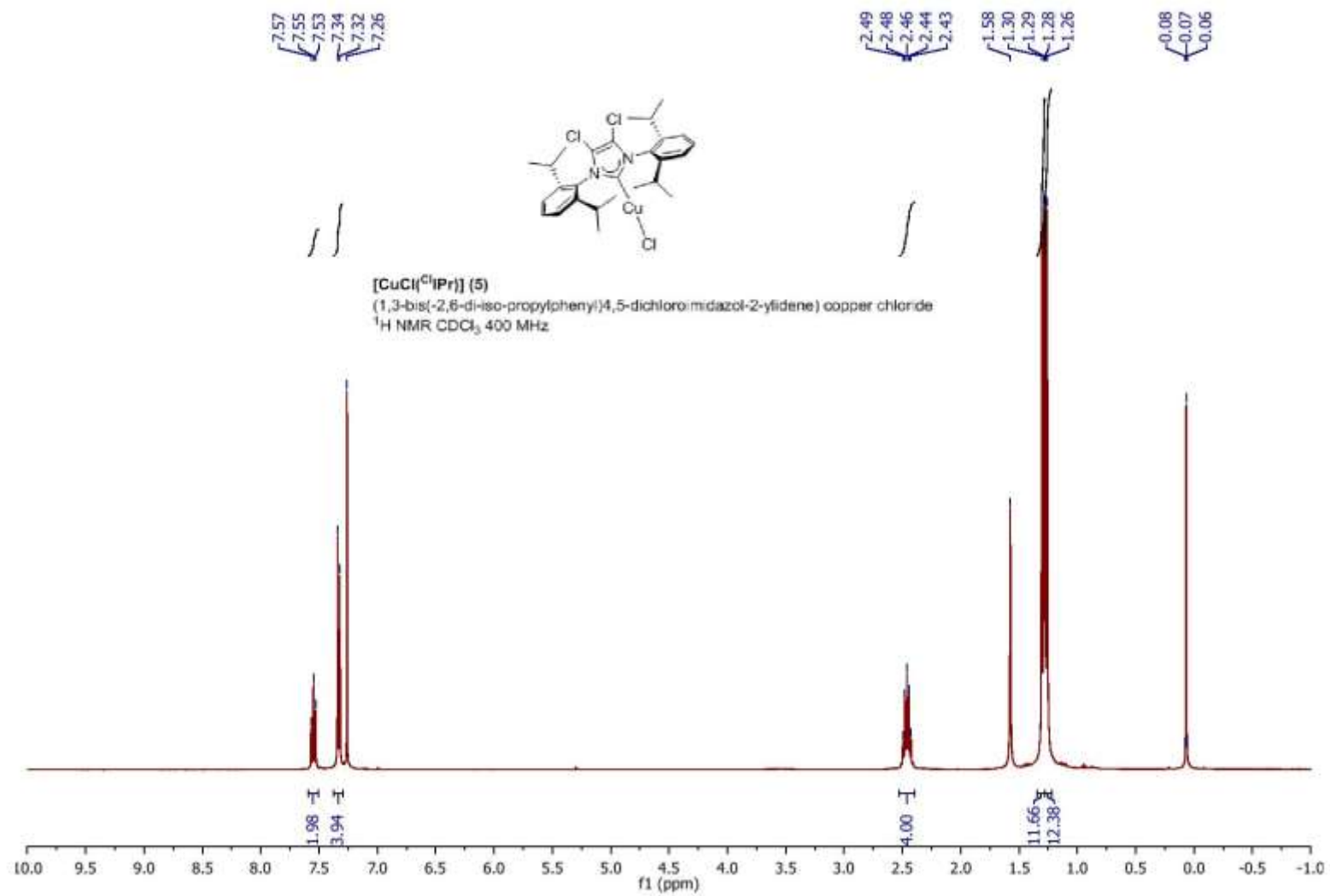


Figure S67. ¹H NMR spectra of complex 5.

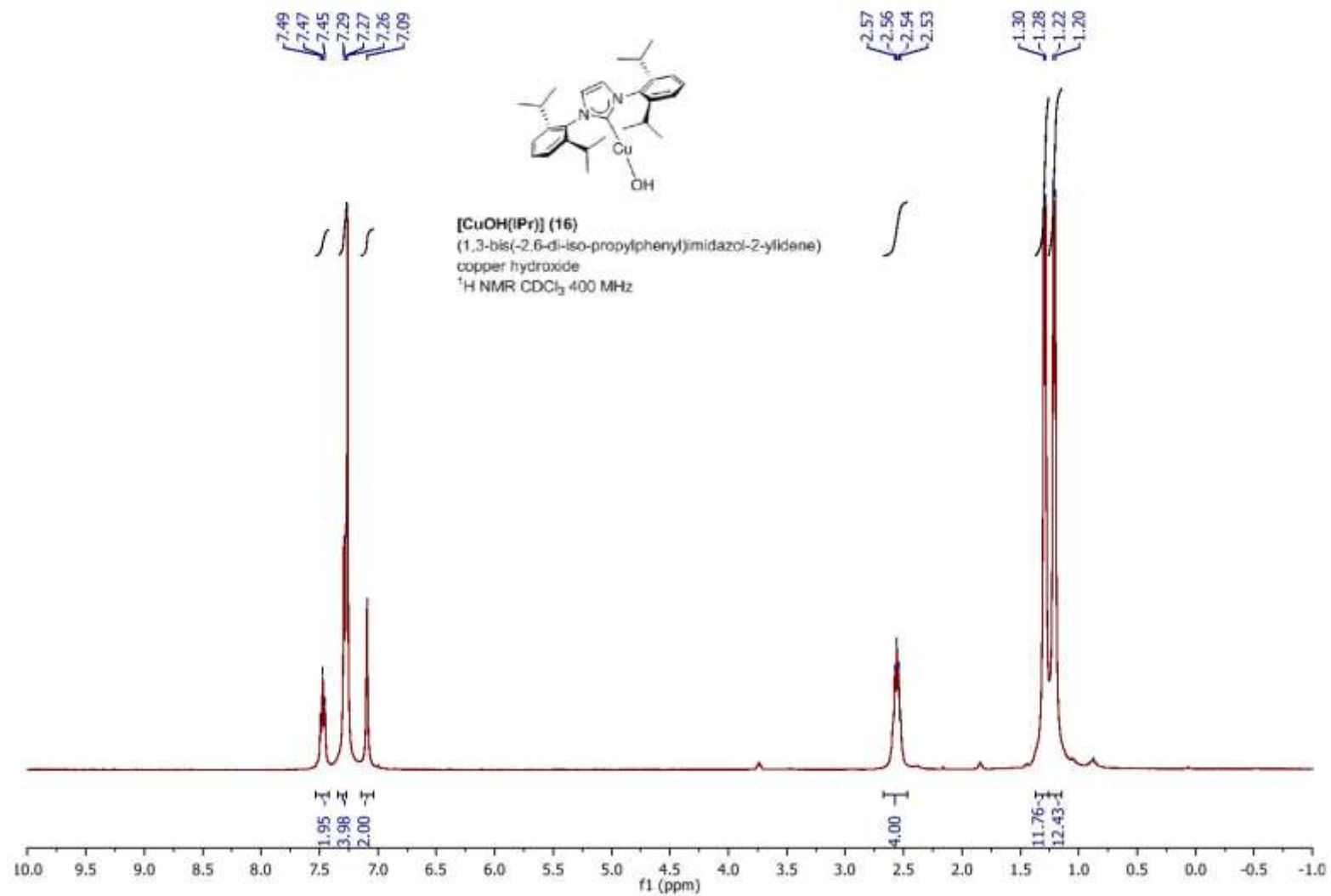


Figure S68. ¹H NMR spectra of complex **16**.

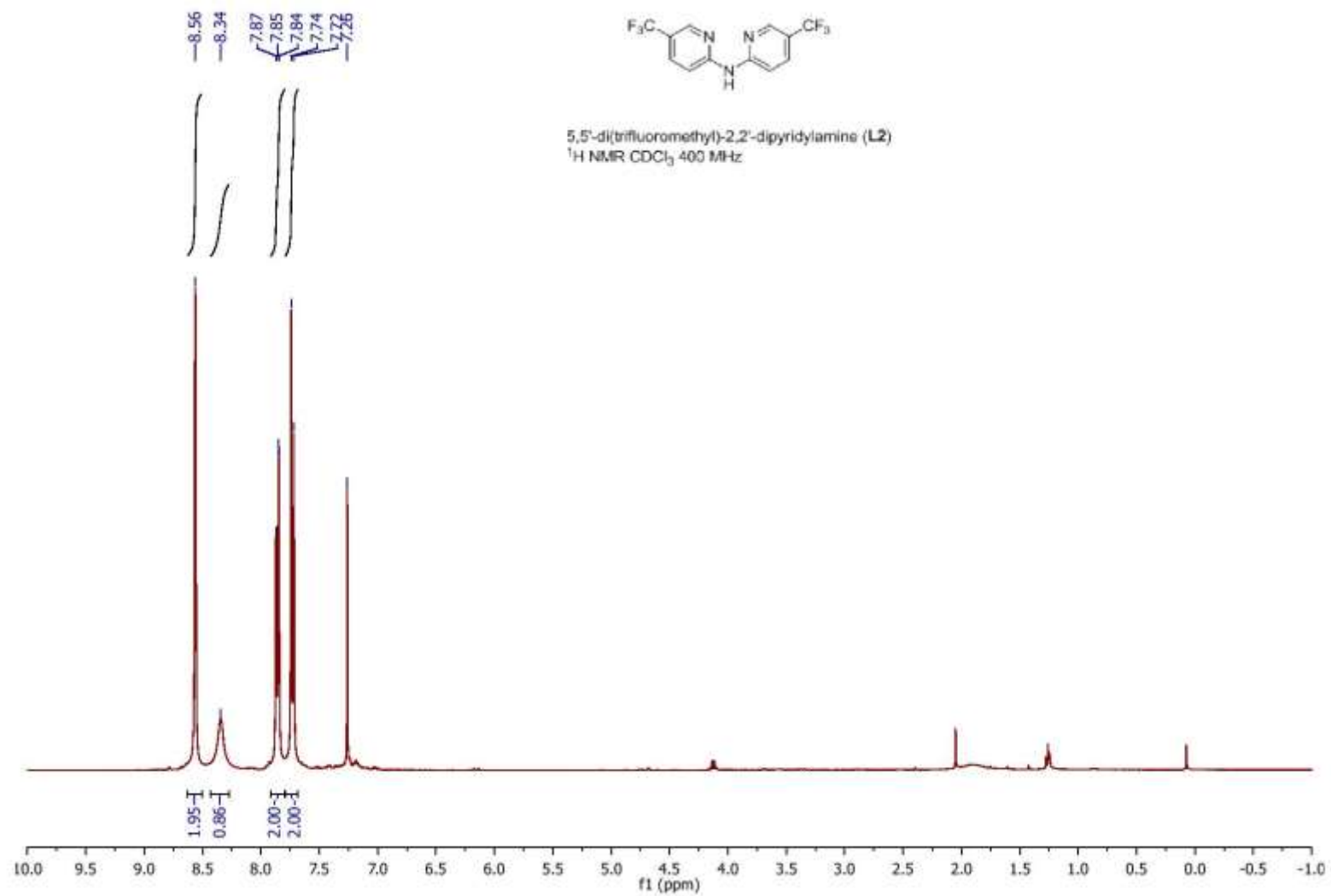


Figure S69. ¹H NMR spectra of ligand L2.

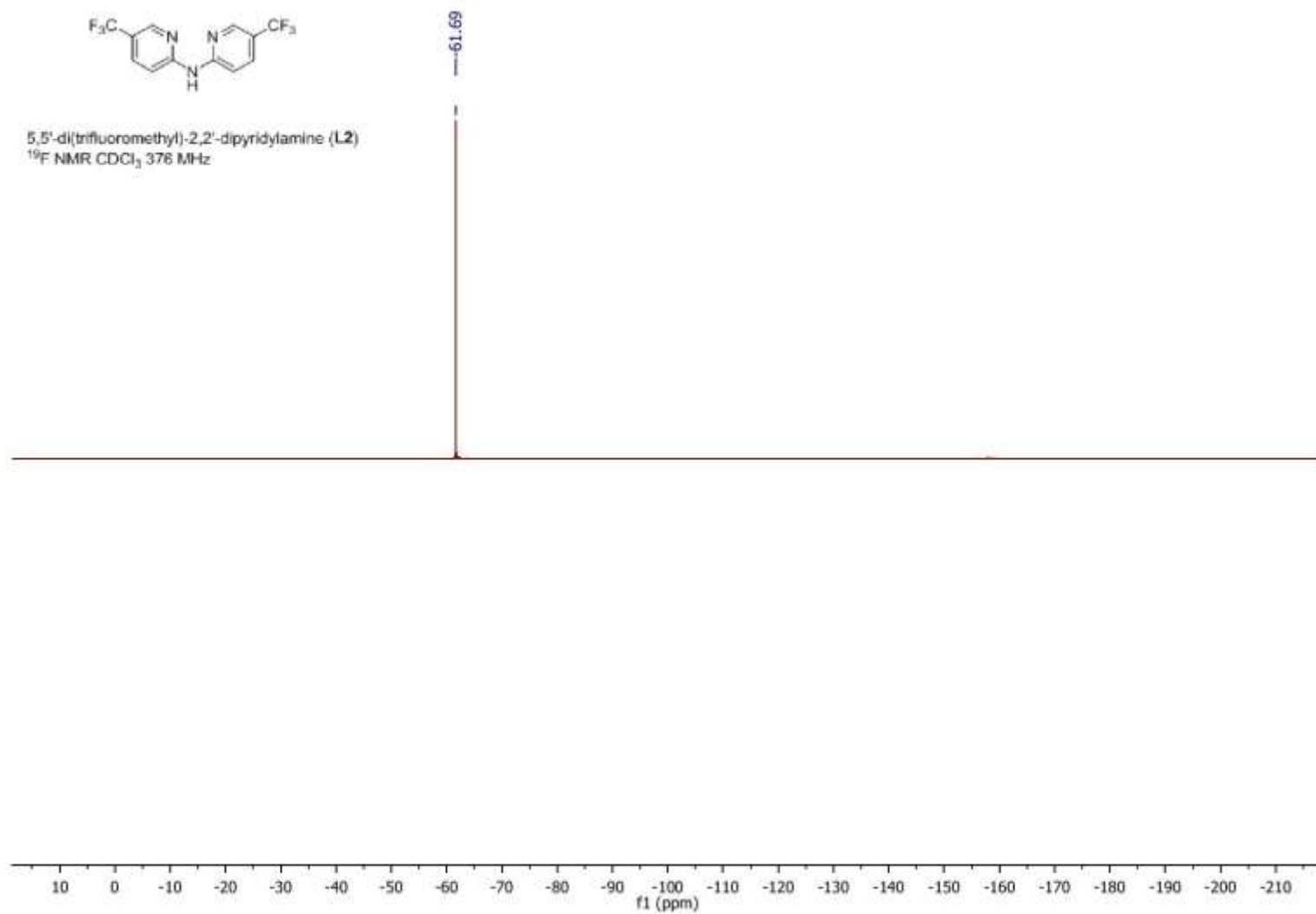


Figure S70. ^{19}F NMR spectra of ligand **L2**.

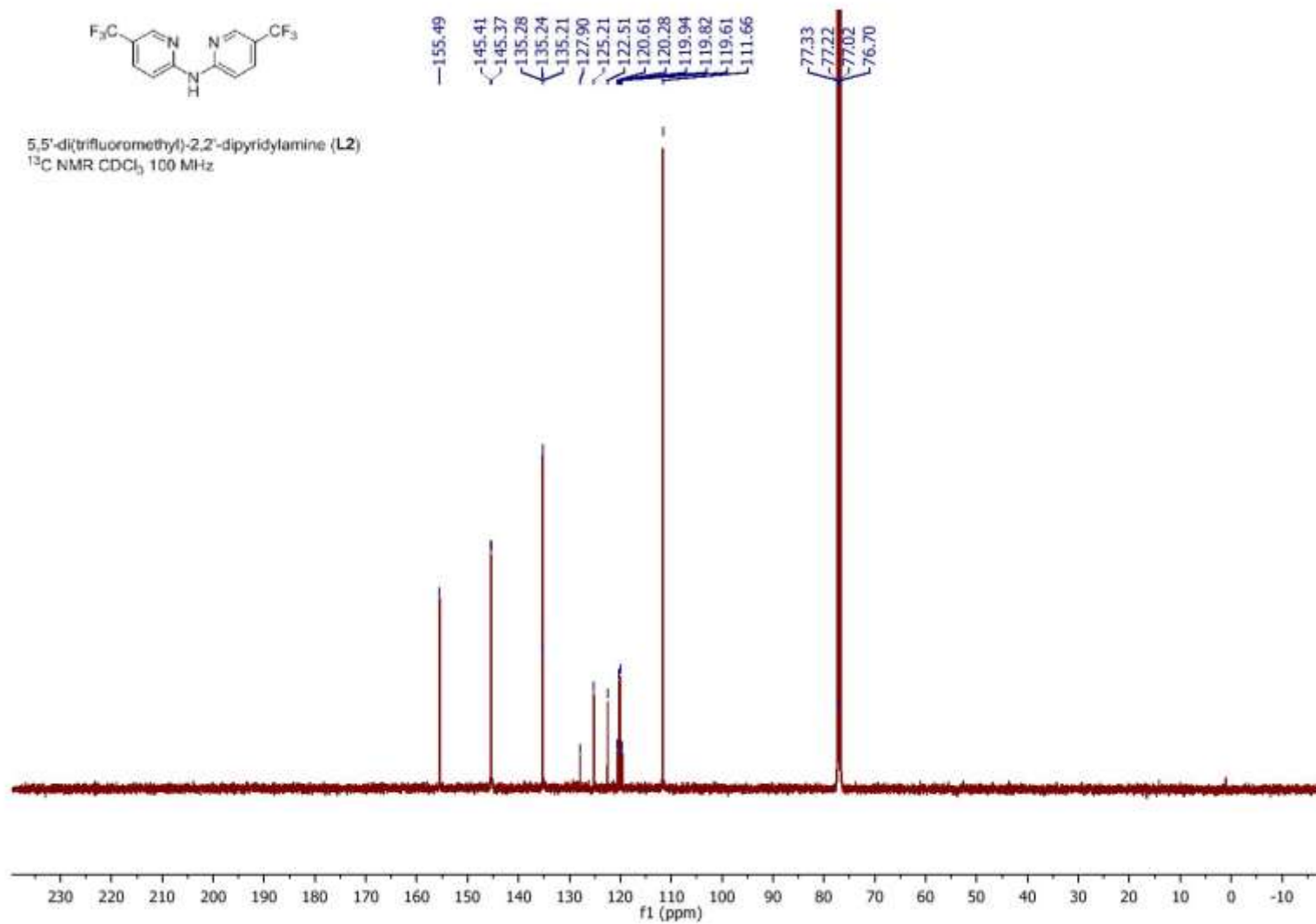


Figure S71. ^{13}C NMR spectra of ligand L2.

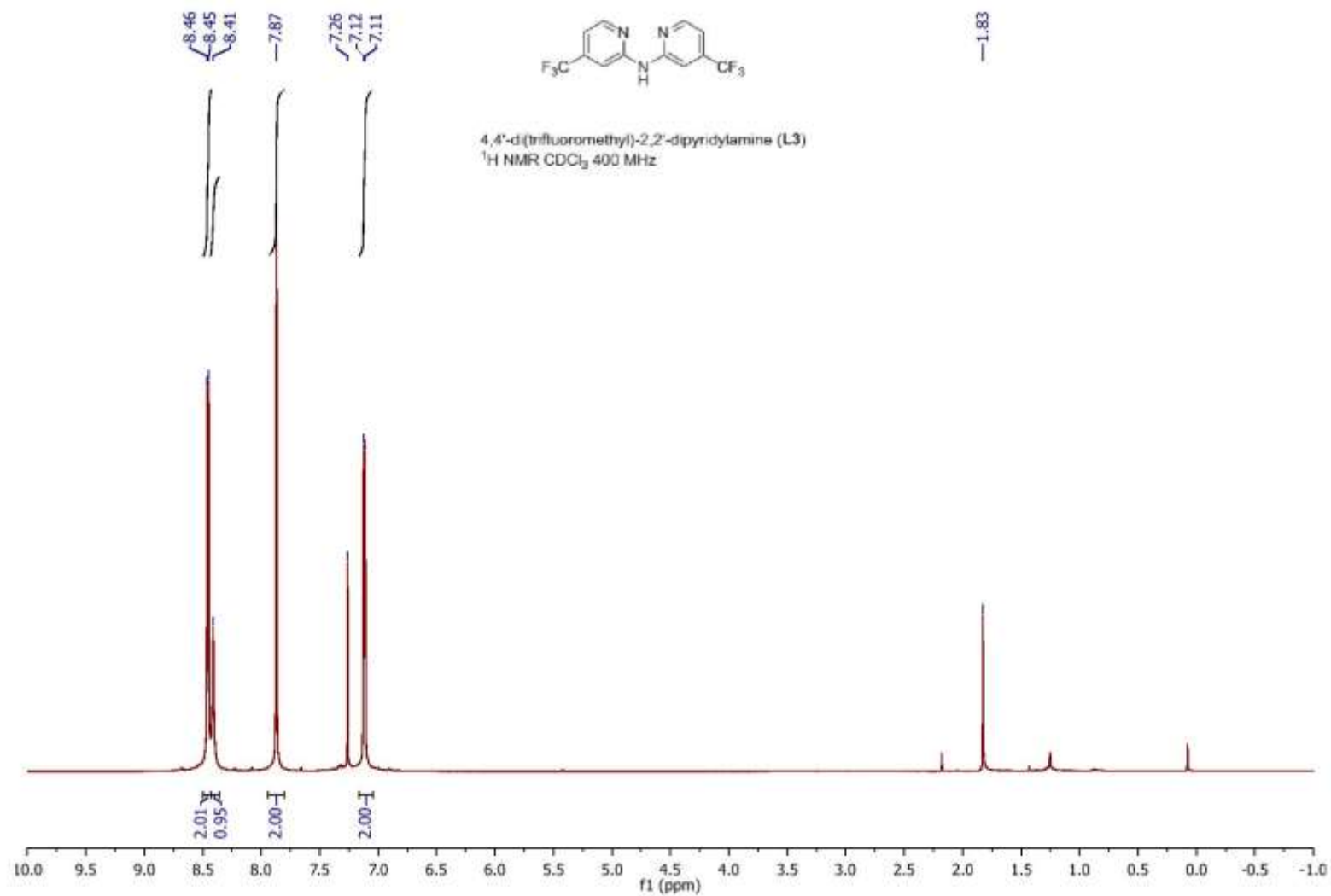


Figure S72. ¹H NMR spectra of ligand L3.

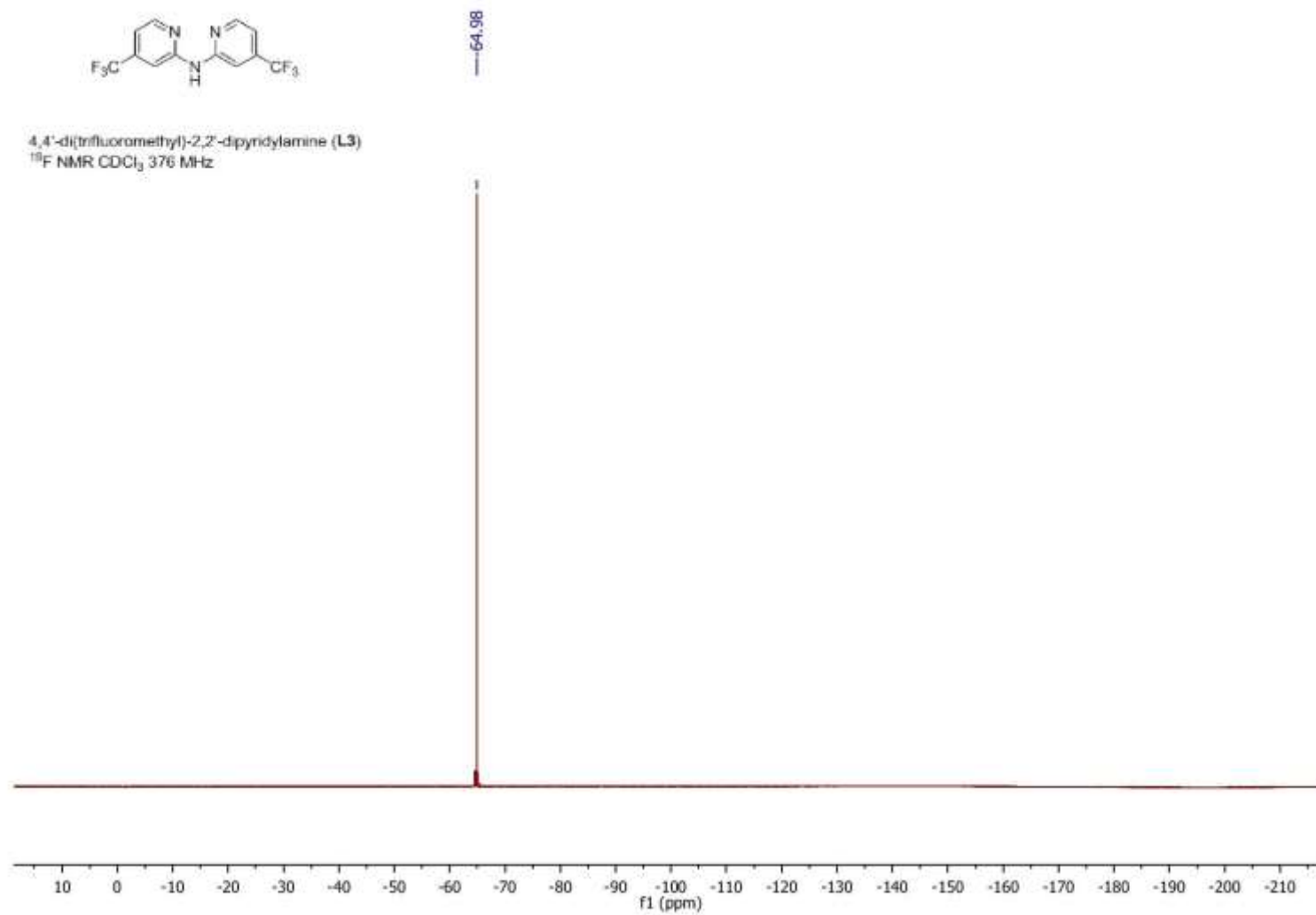


Figure S73. ^{19}F NMR spectra of ligand **L3**.

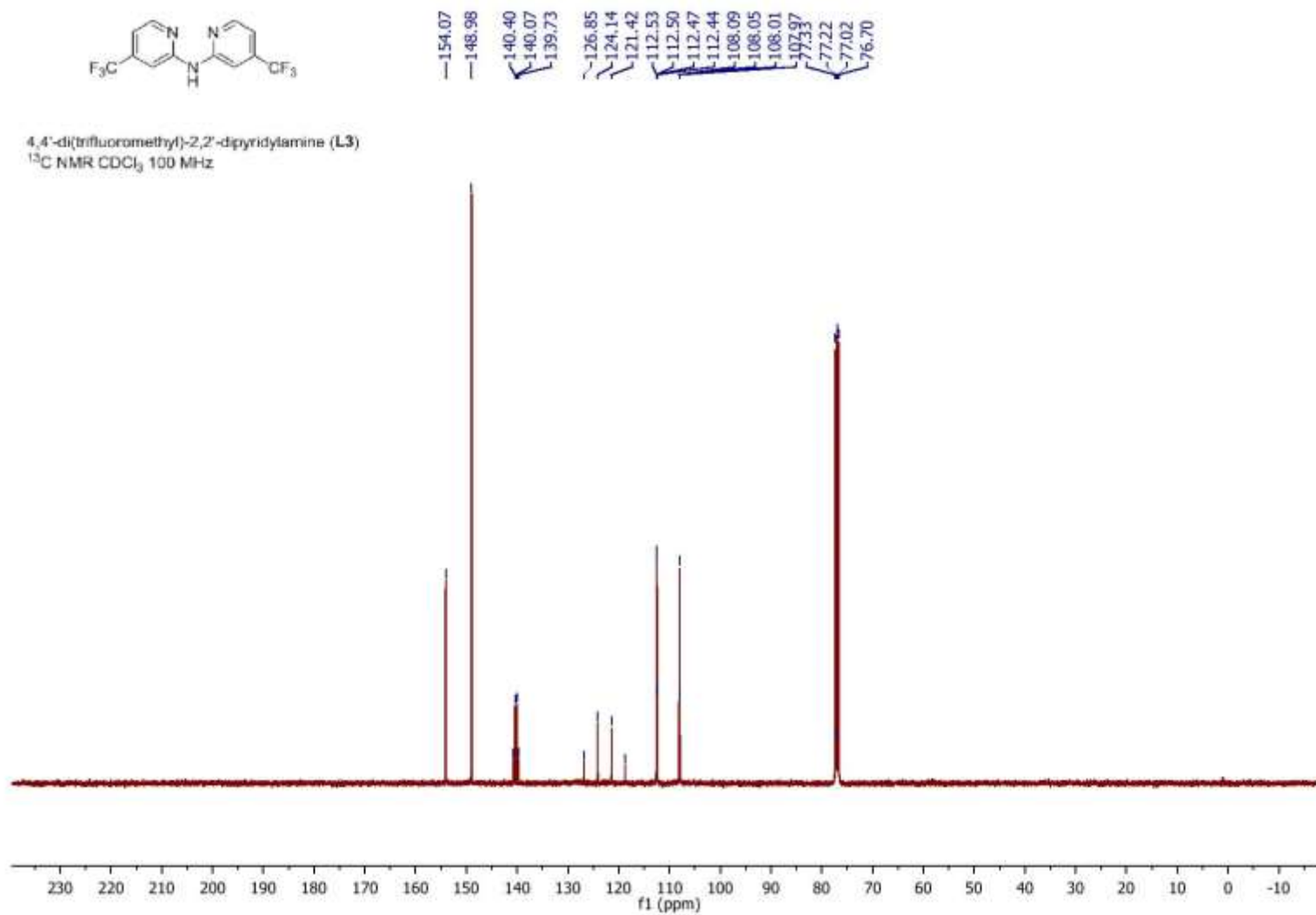


Figure S74. ¹³C NMR spectra of ligand L3.

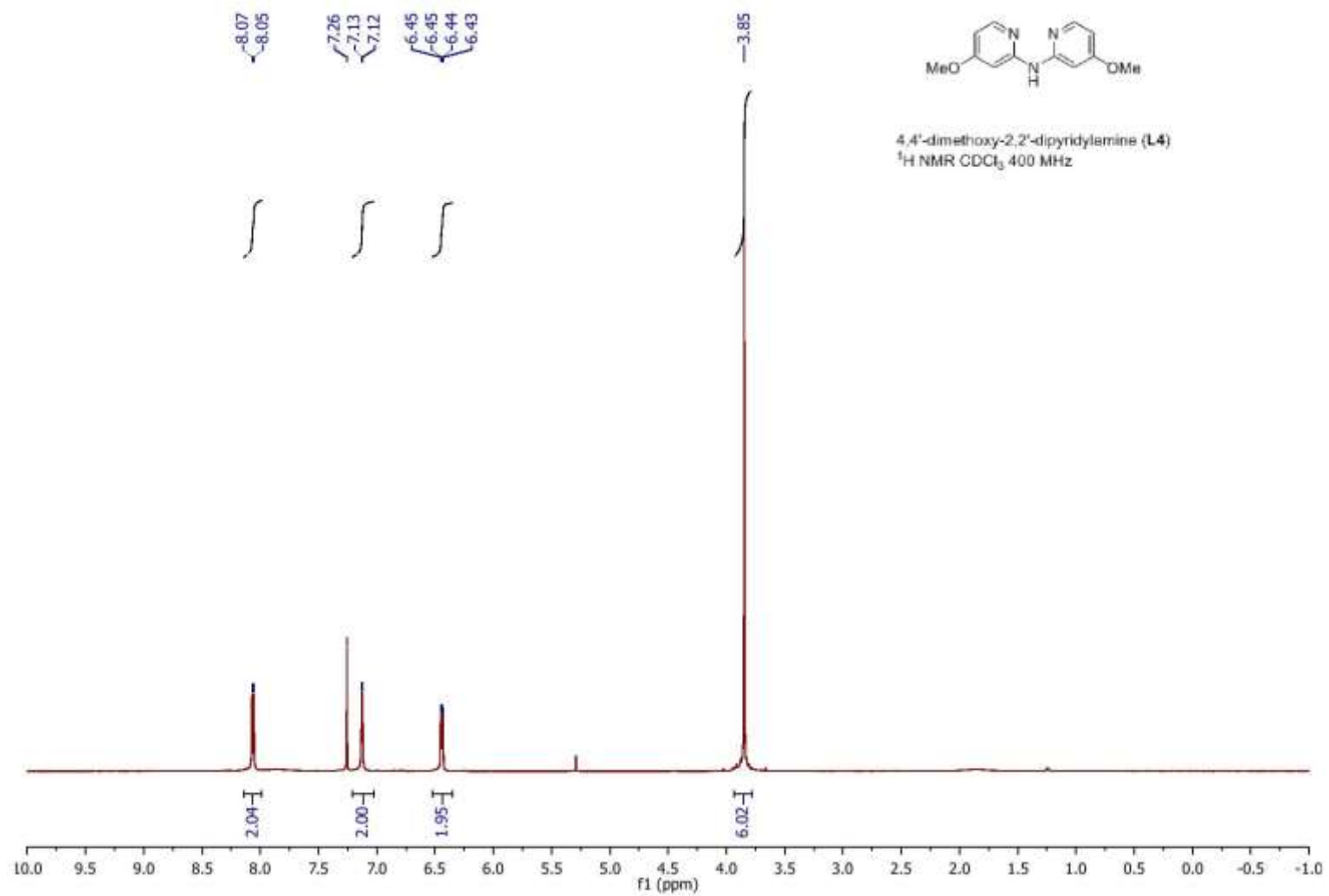


Figure S75. ¹H NMR spectra of ligand L4.

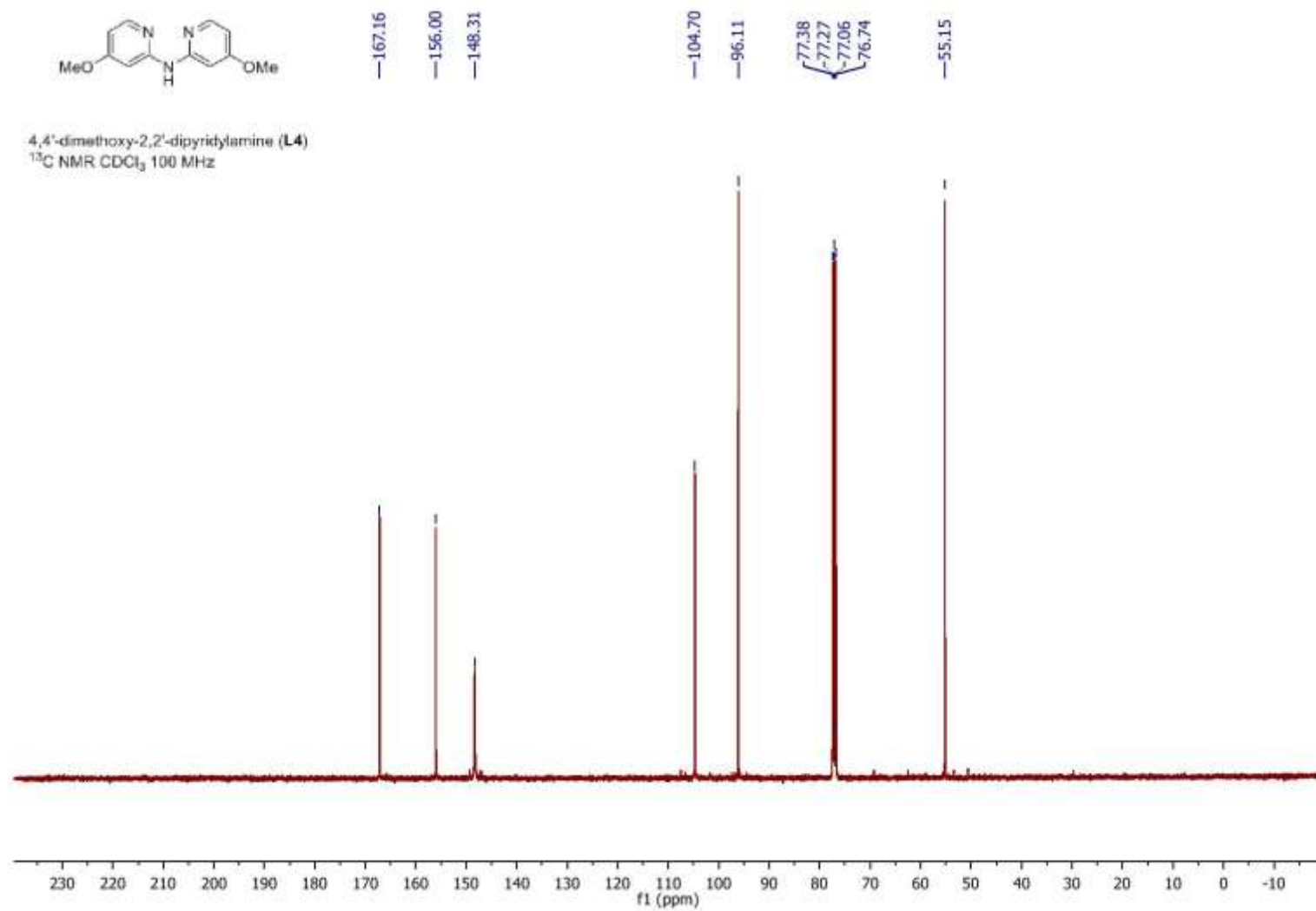


Figure S76. ^{13}C NMR spectra of ligand L4.

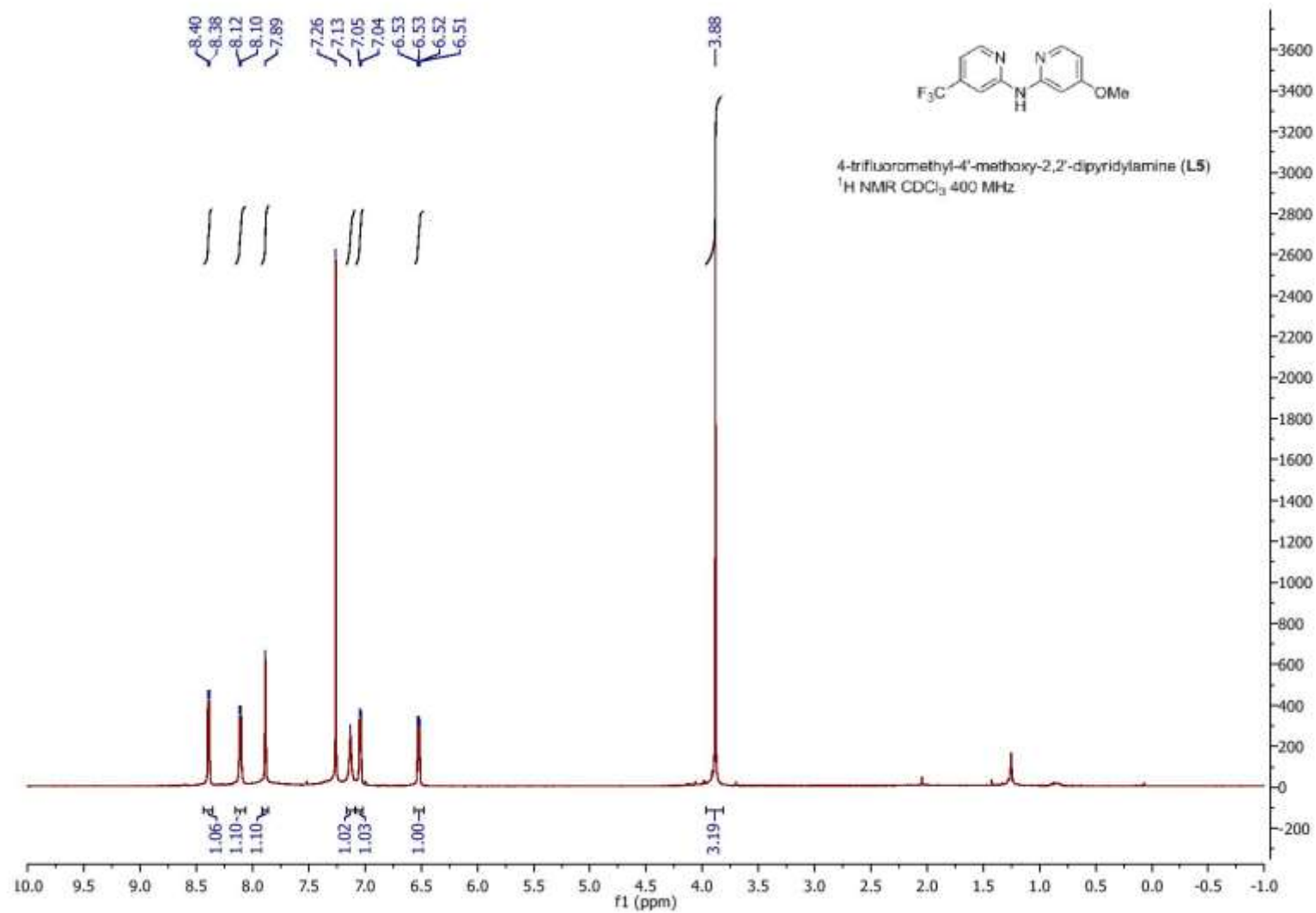


Figure S77. ¹H NMR spectra of ligand L5.

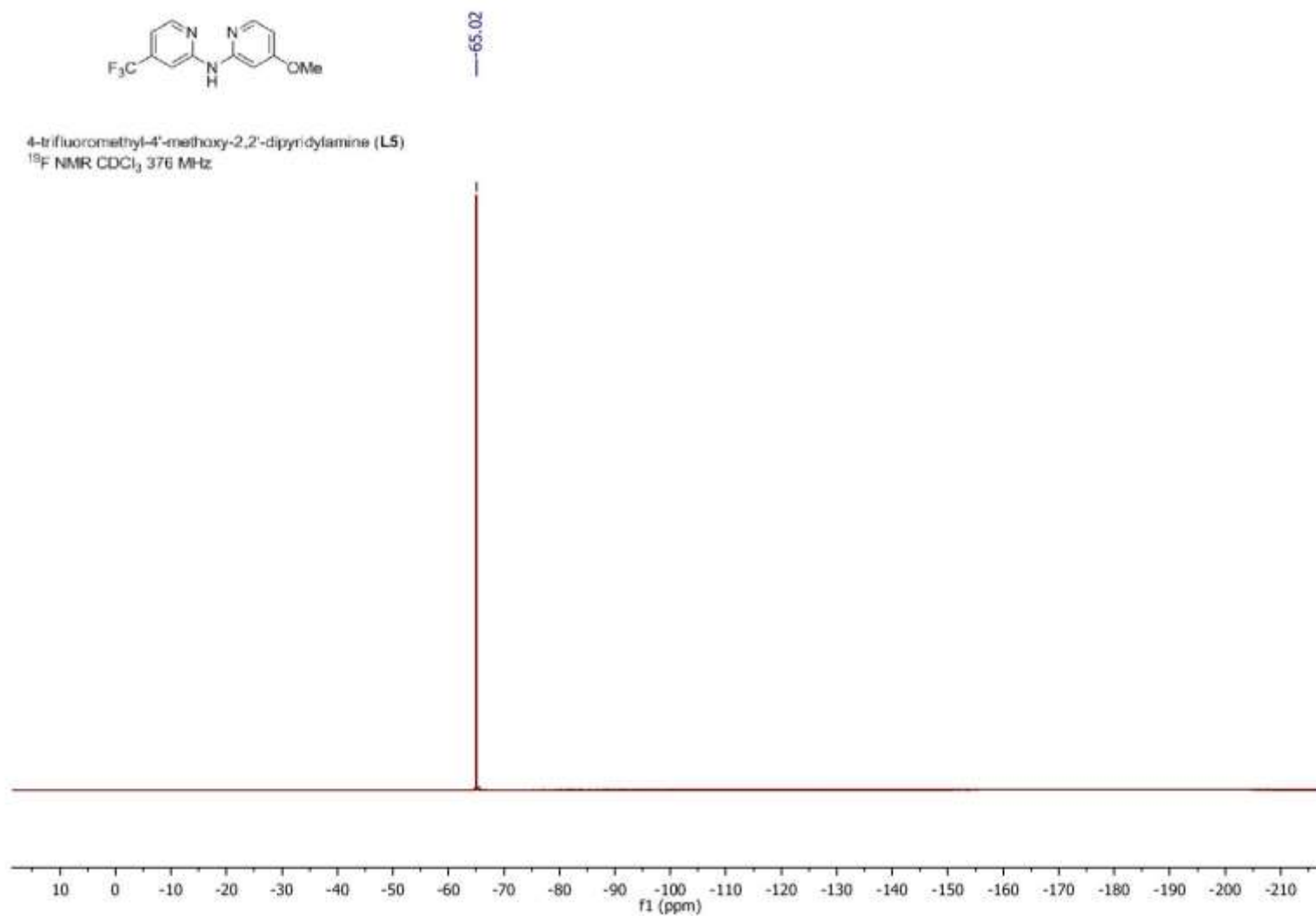


Figure S78. ^{19}F NMR spectra of ligand **L5**.

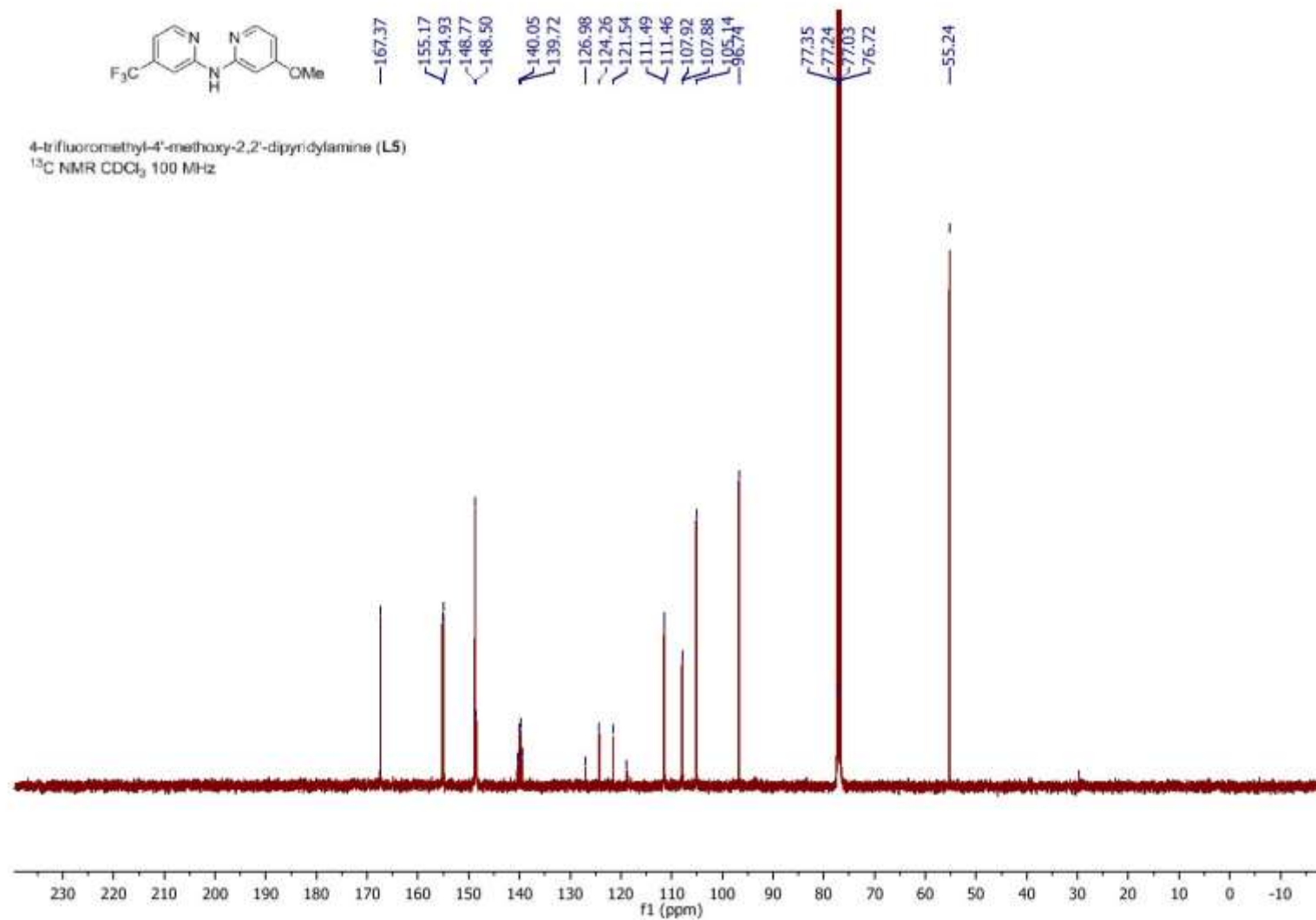


Figure S79. ¹³C NMR spectra of ligand **L5**.

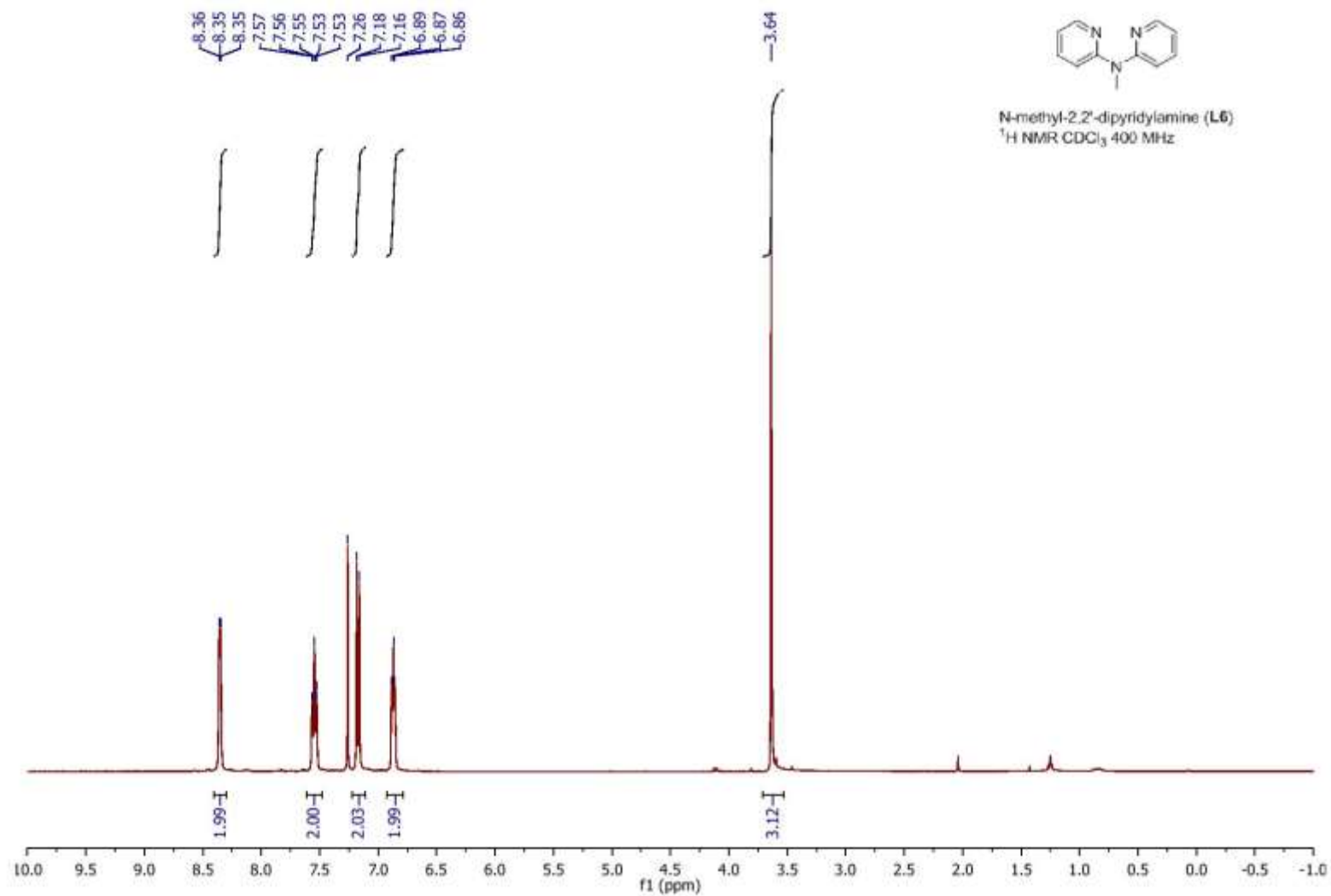


Figure S80. ¹H NMR spectra of ligand L6.

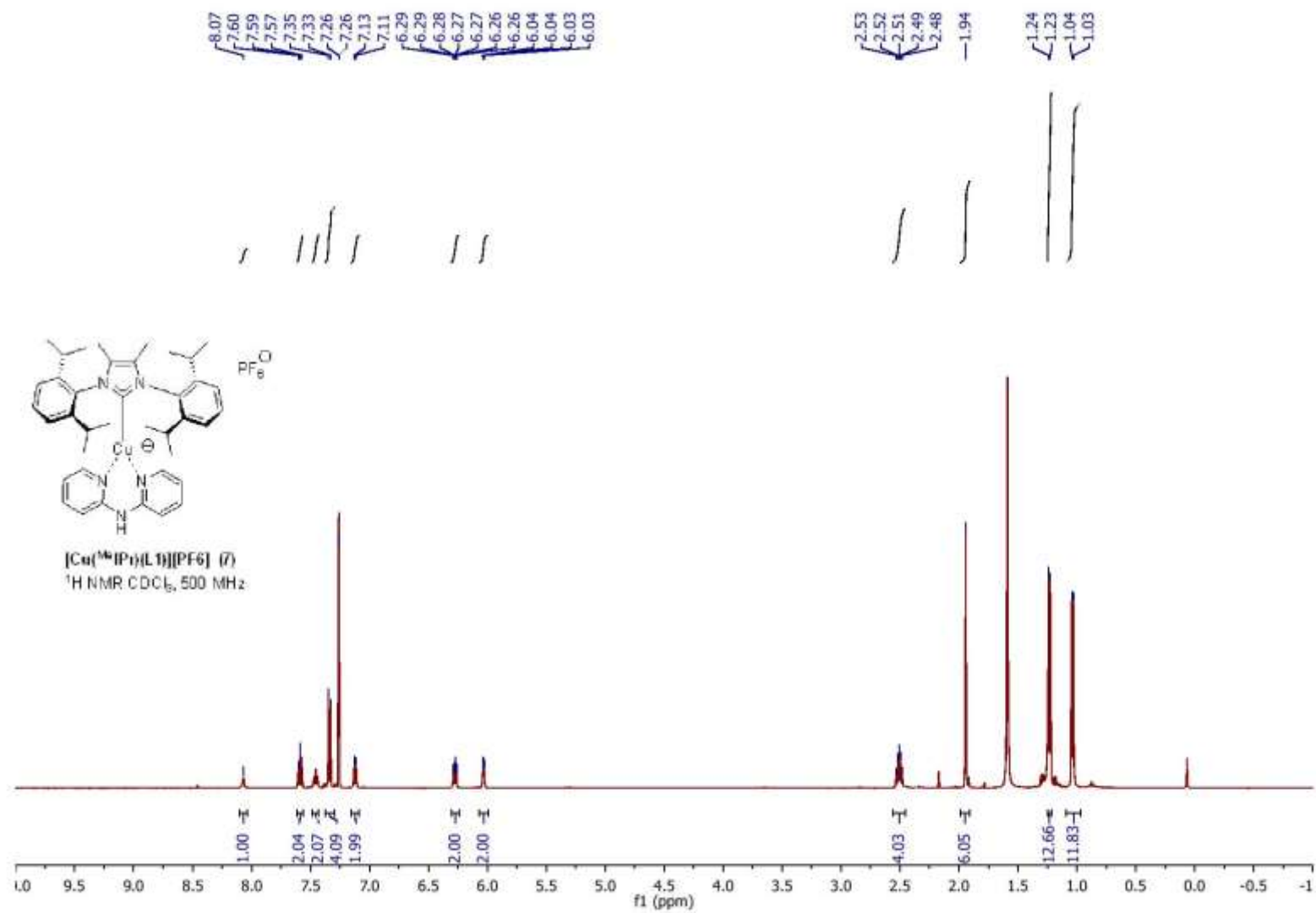


Figure S81. $^1\text{H NMR}$ spectra of complex 7.

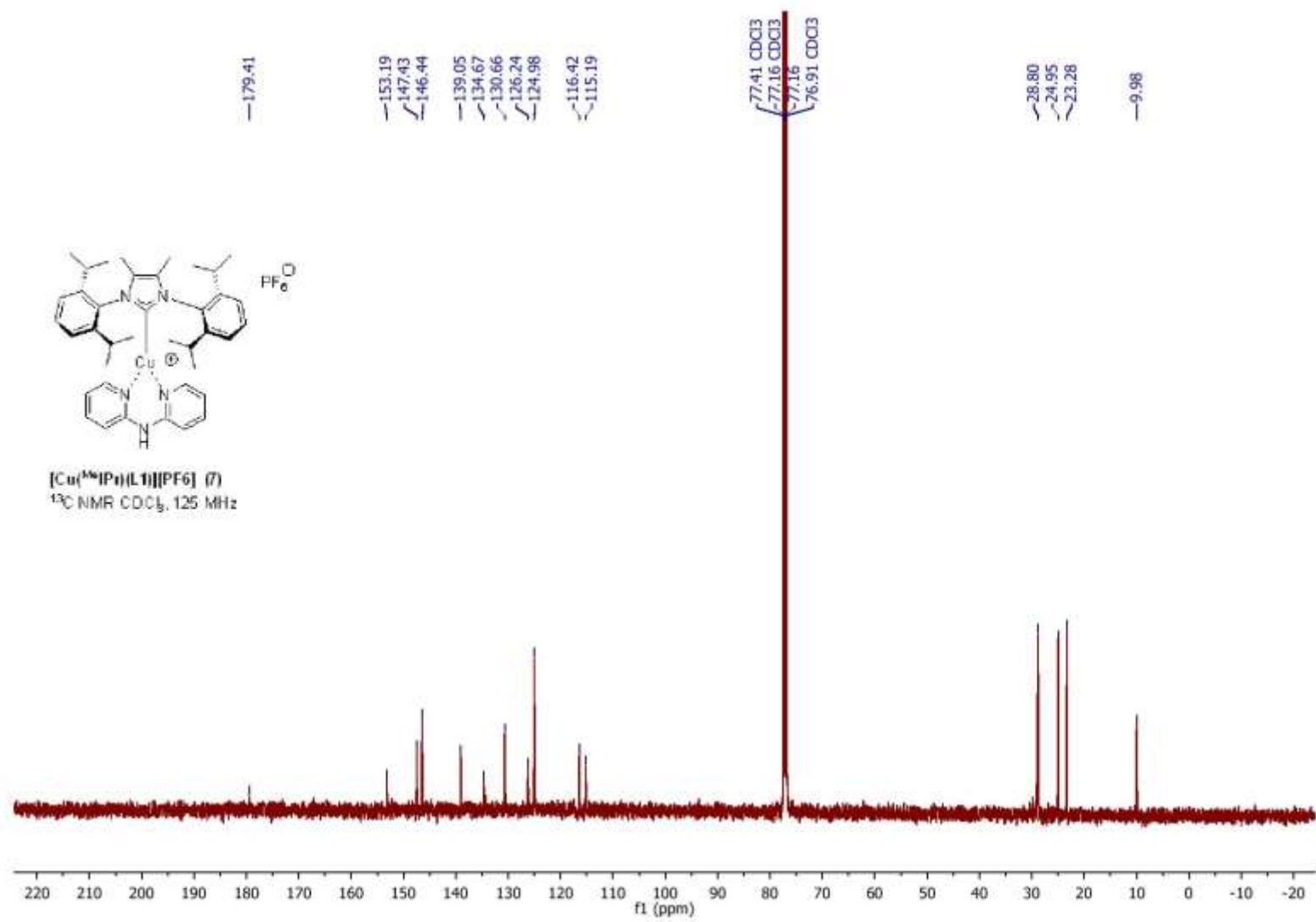


Figure S82. ^{13}C NMR spectra of complex 7.

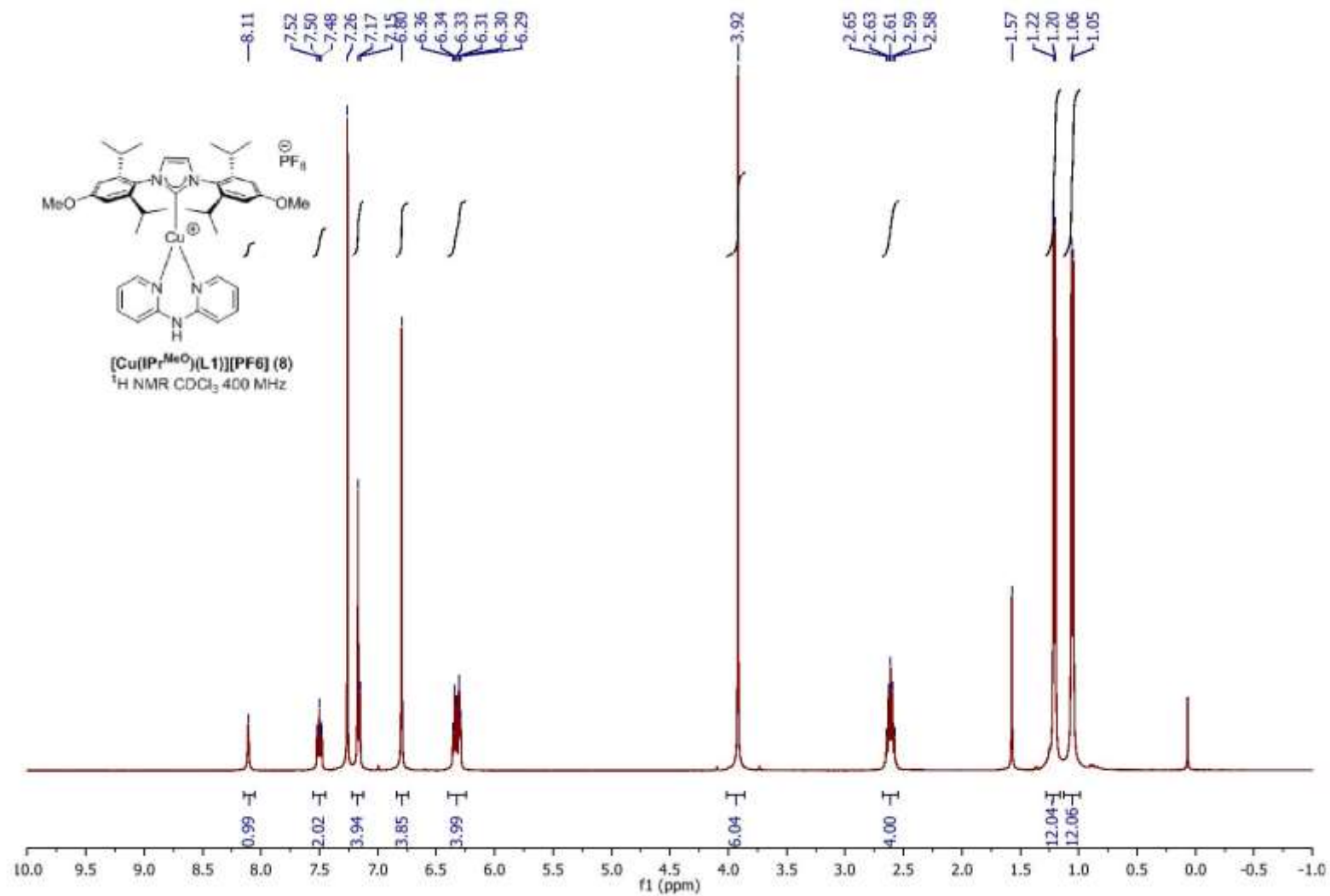


Figure S83. ^1H NMR spectra of complex **8**.

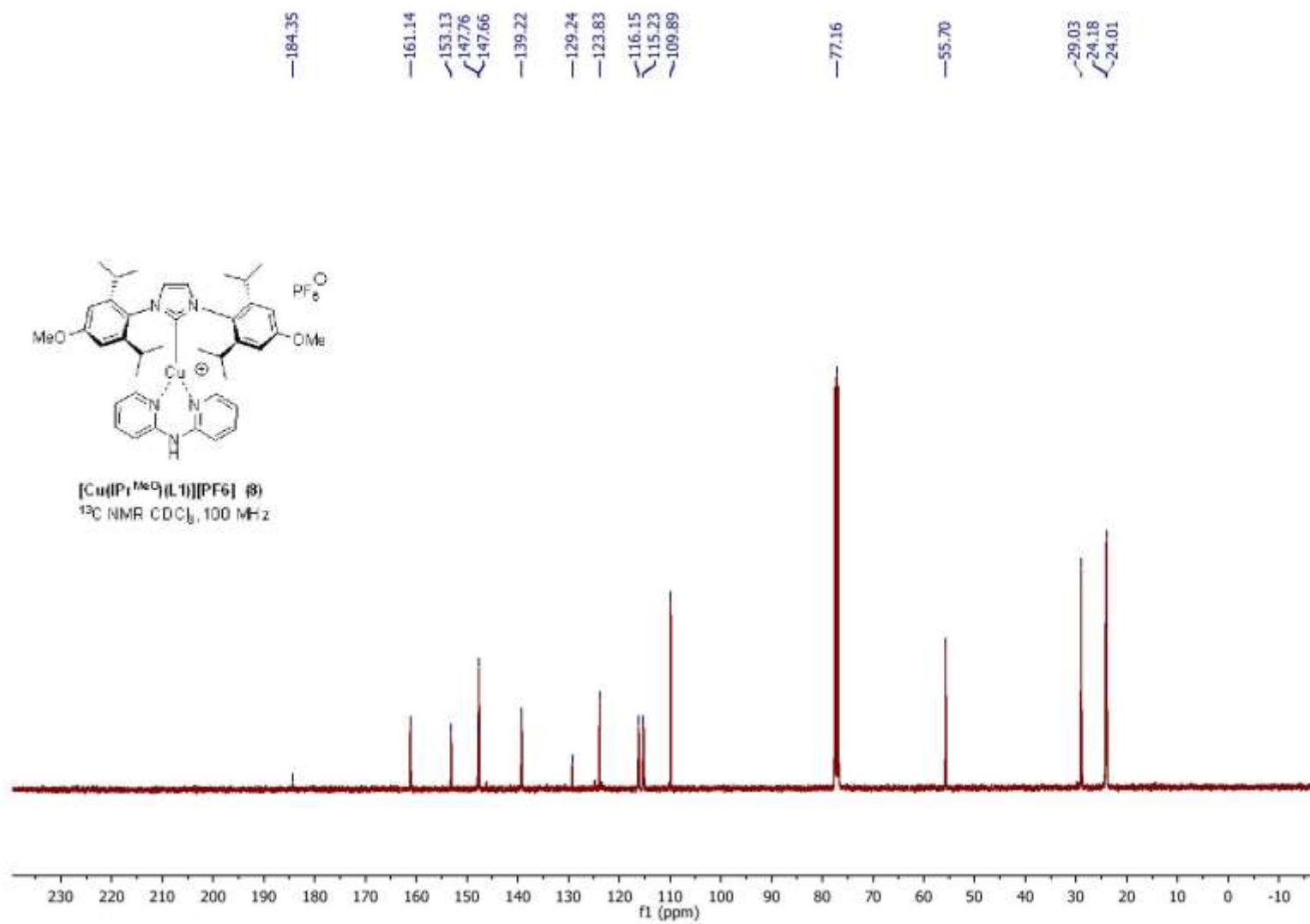


Figure S84. ^{13}C NMR spectra of complex 8.

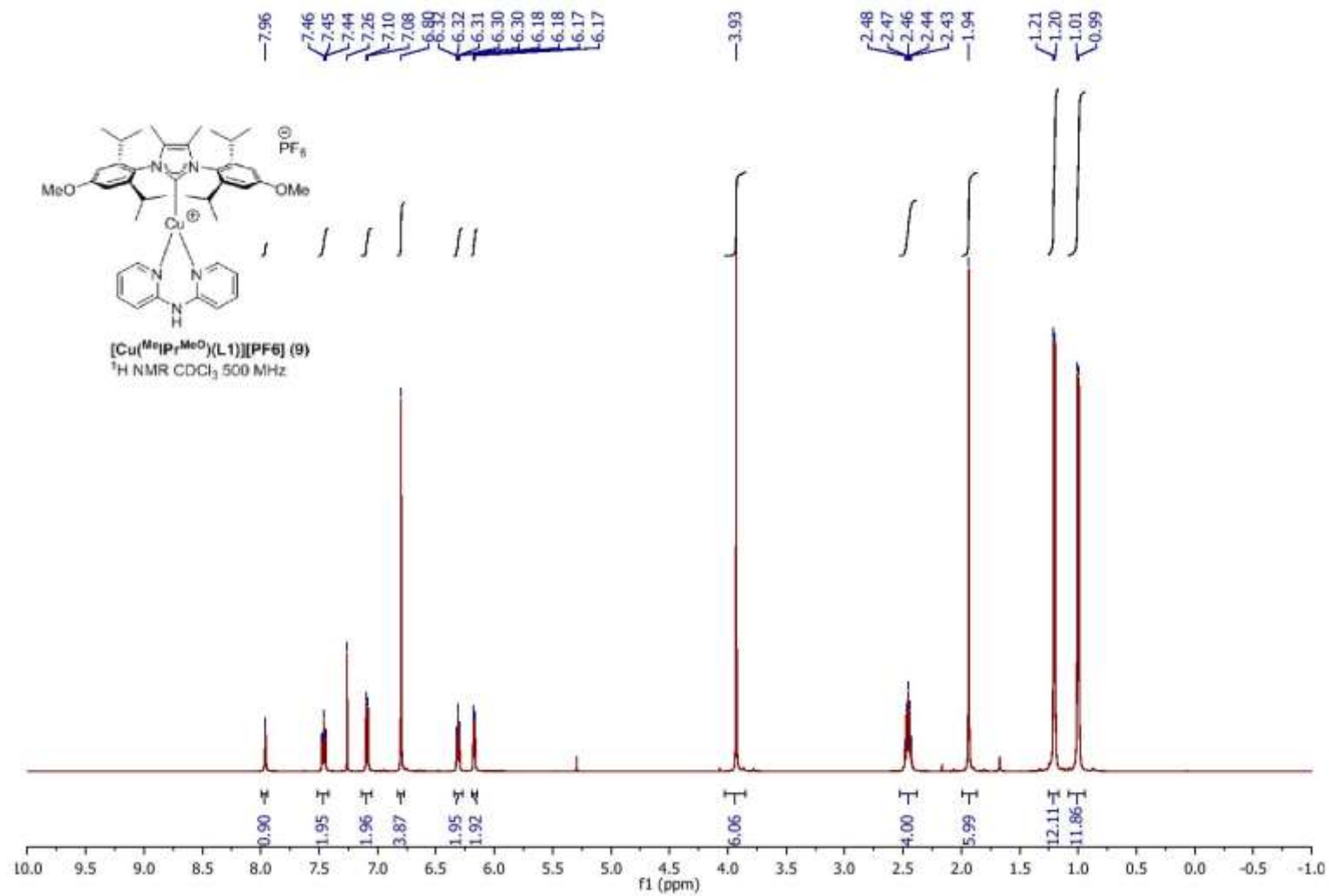


Figure S85. $^1\text{H NMR}$ spectra of complex **9**.

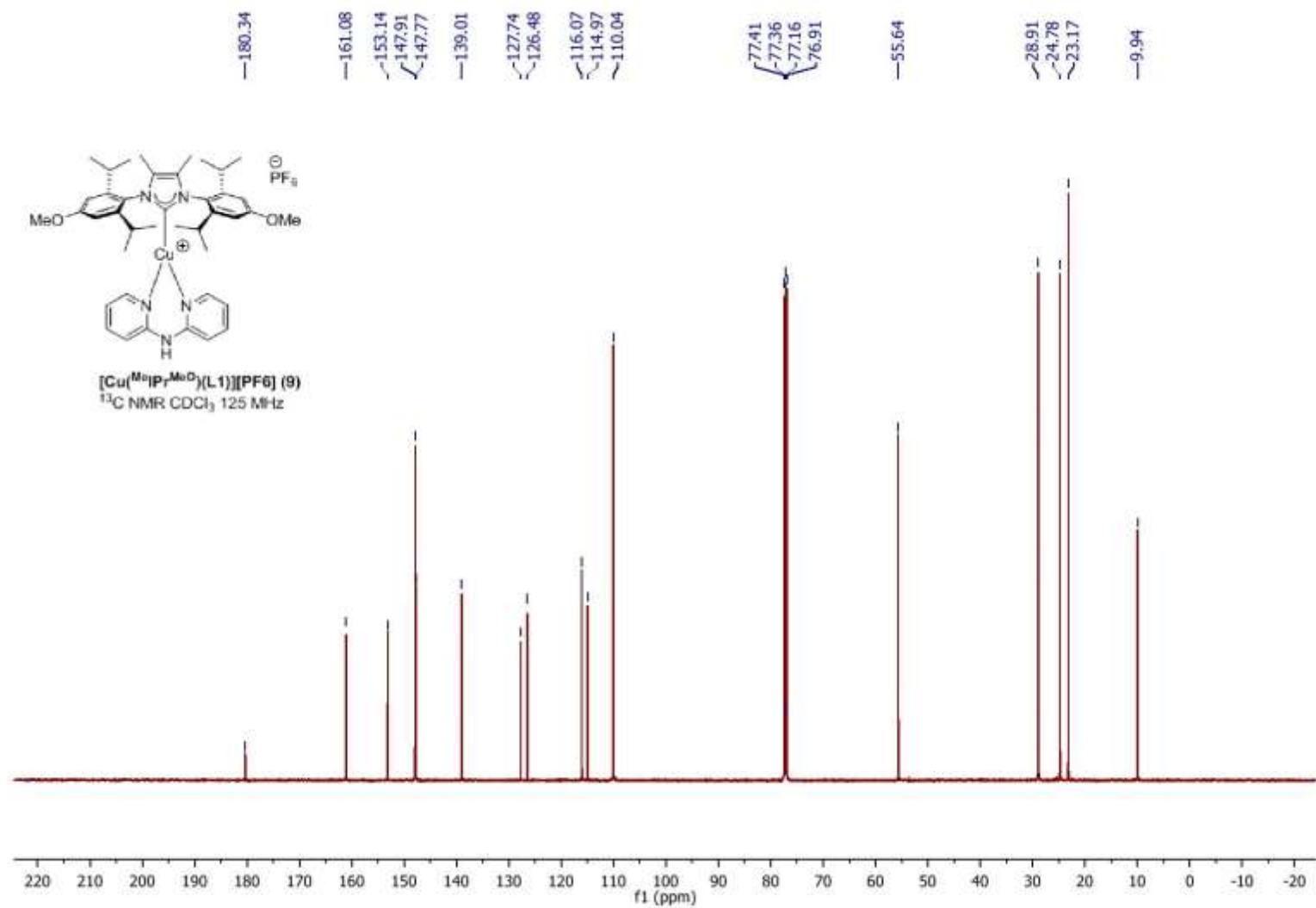


Figure S86. ^{13}C NMR spectra of complex **9**.

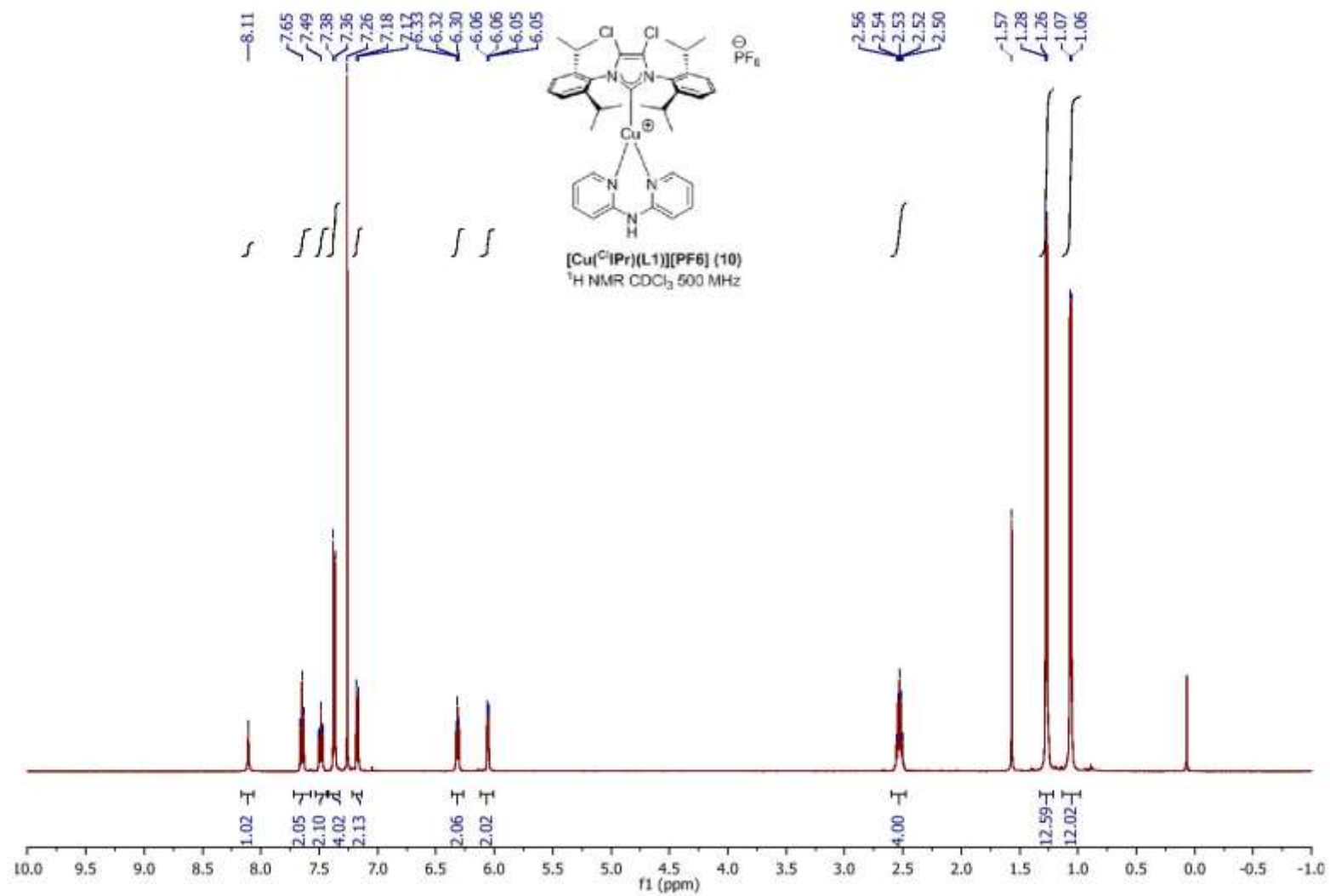


Figure S87. ¹H NMR spectra of complex 10.

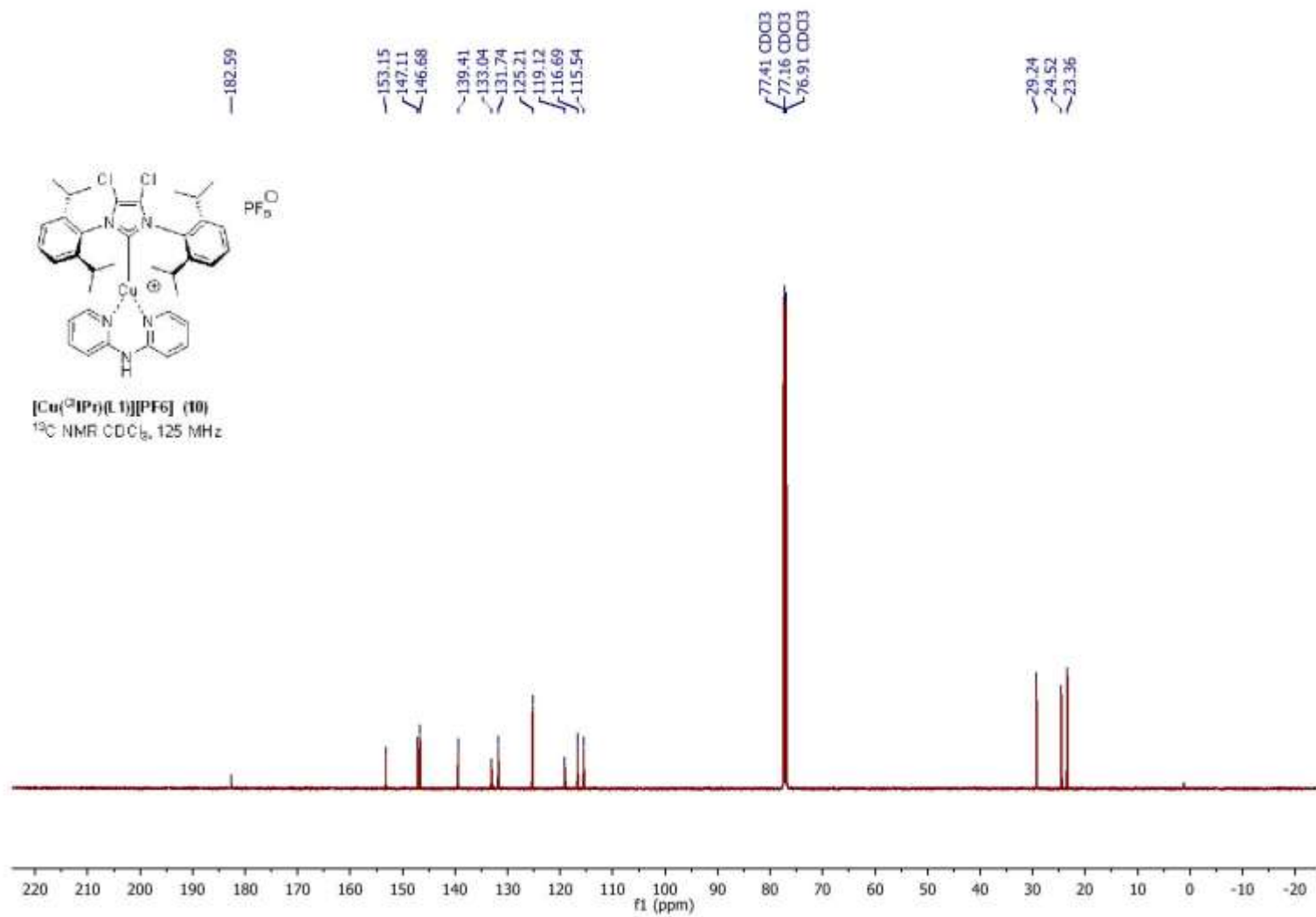


Figure S88. ^{13}C NMR spectra of complex 10.

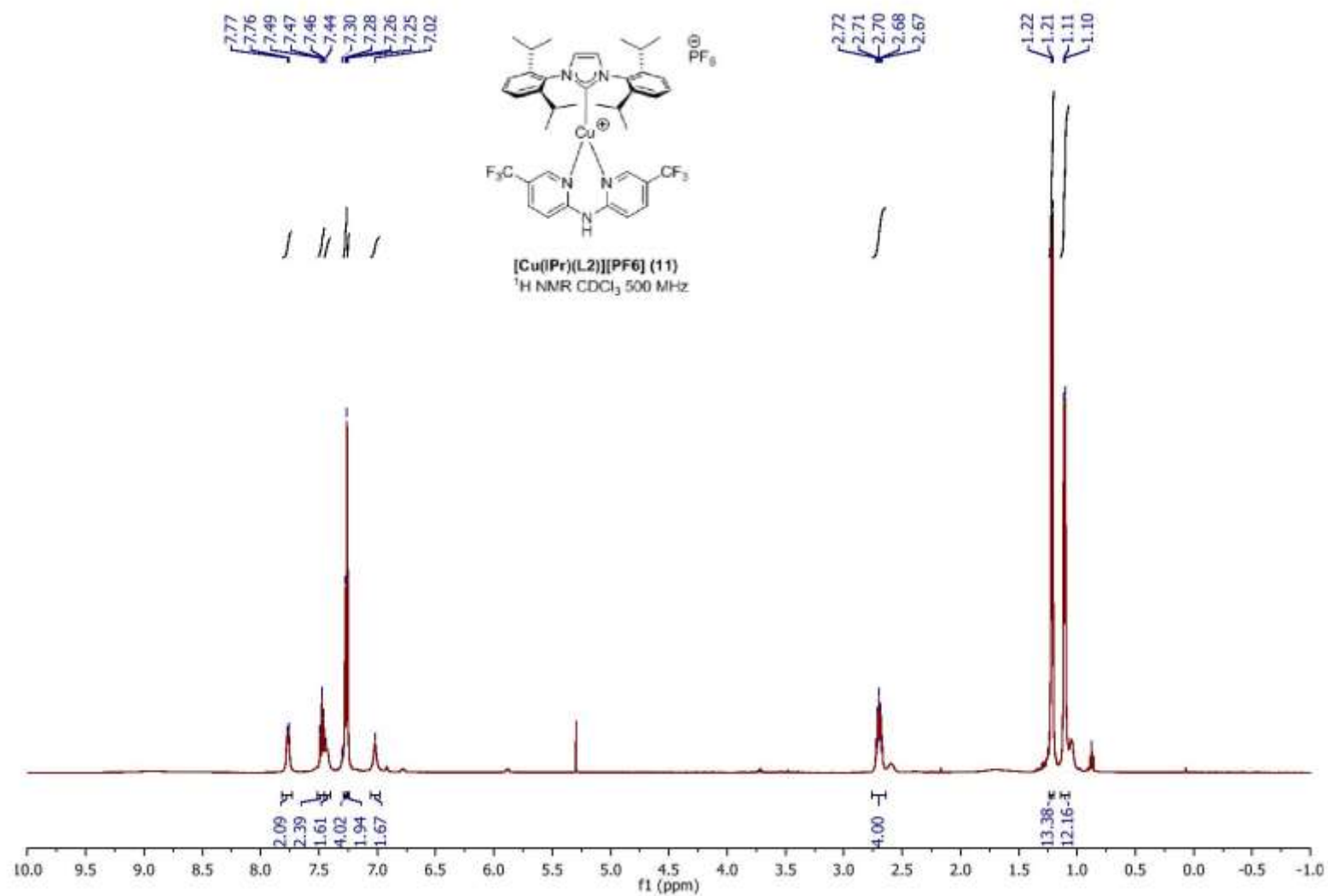


Figure S89. $^1\text{H NMR}$ spectra of complex 11.

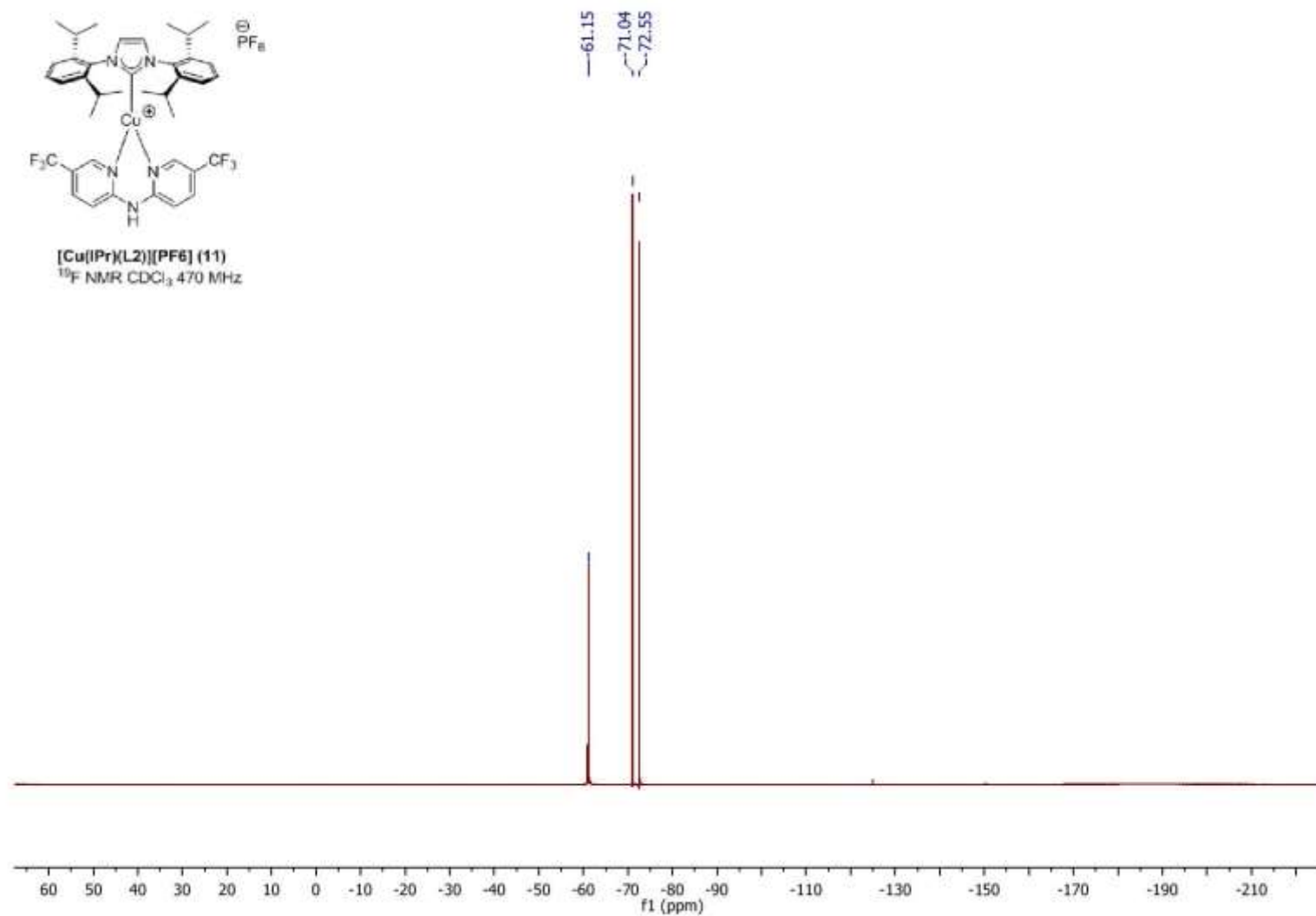


Figure S90. ¹⁹F NMR spectra of complex 11.

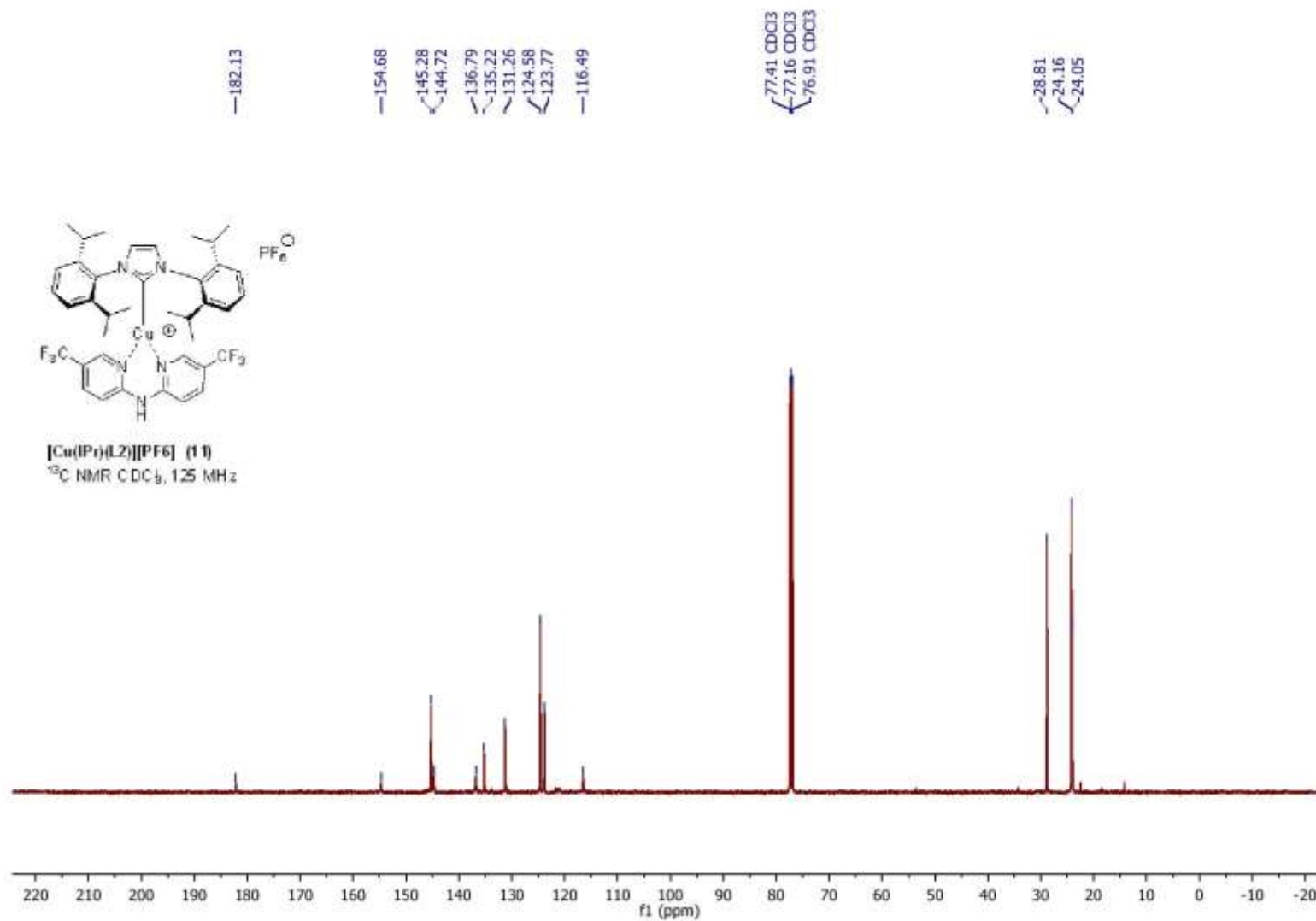


Figure S91. ^{13}C NMR spectra of complex **11**.

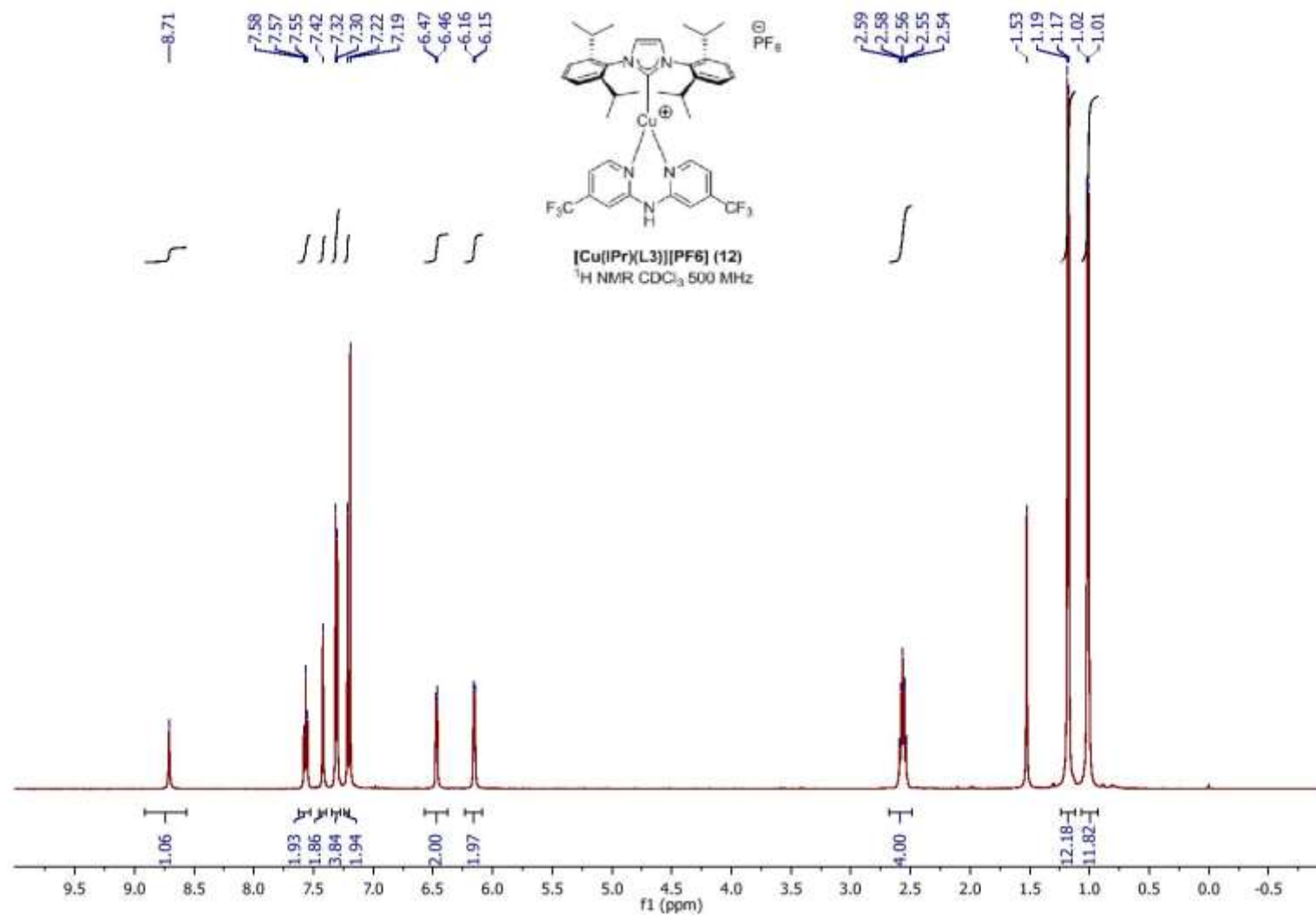


Figure S92. ¹H NMR spectra of complex 12.

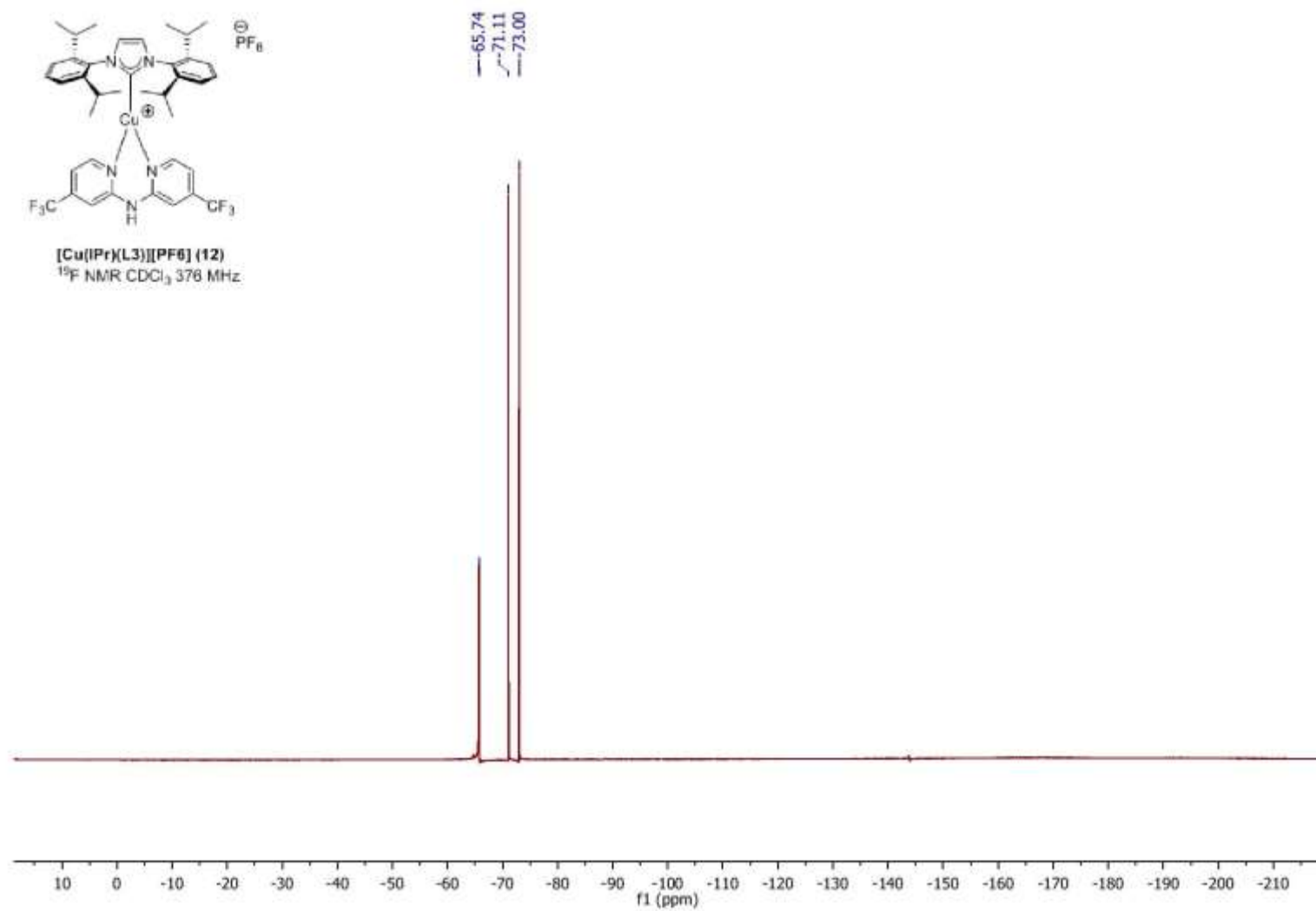


Figure S93. ¹⁹F NMR spectra of complex 12.

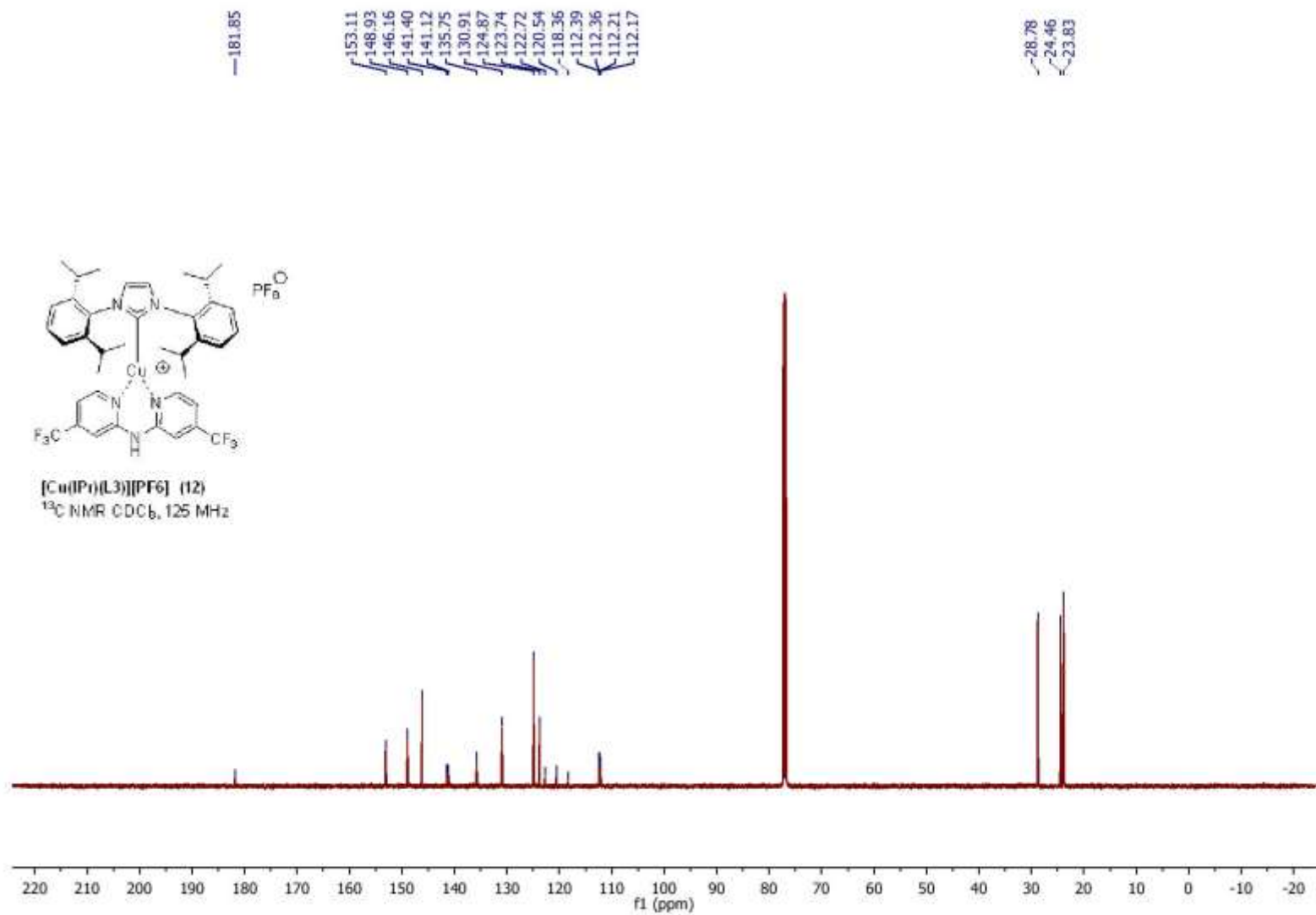


Figure S94. ^{13}C NMR spectra of complex **12**.

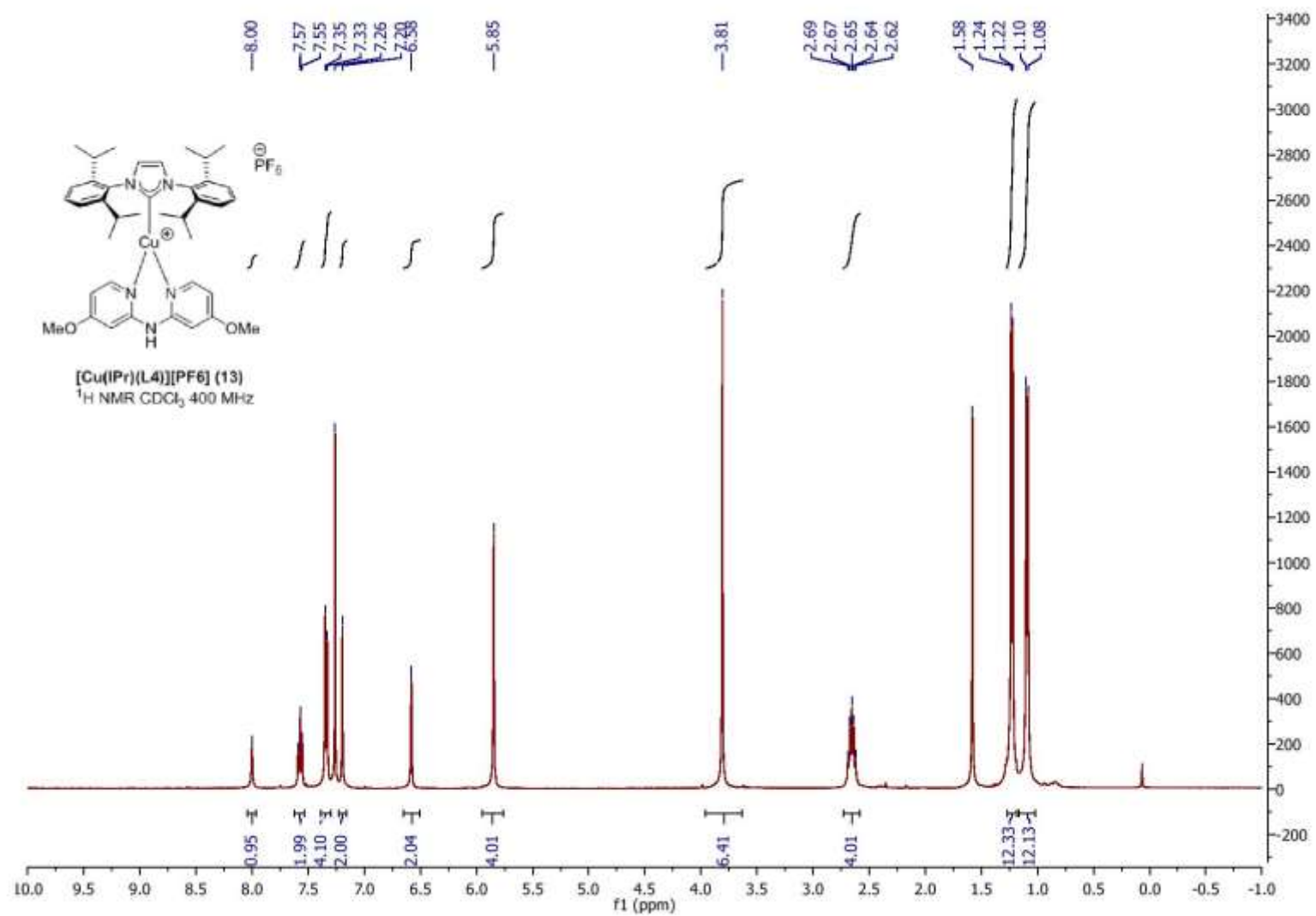


Figure S95. ^1H NMR spectra of complex 13.

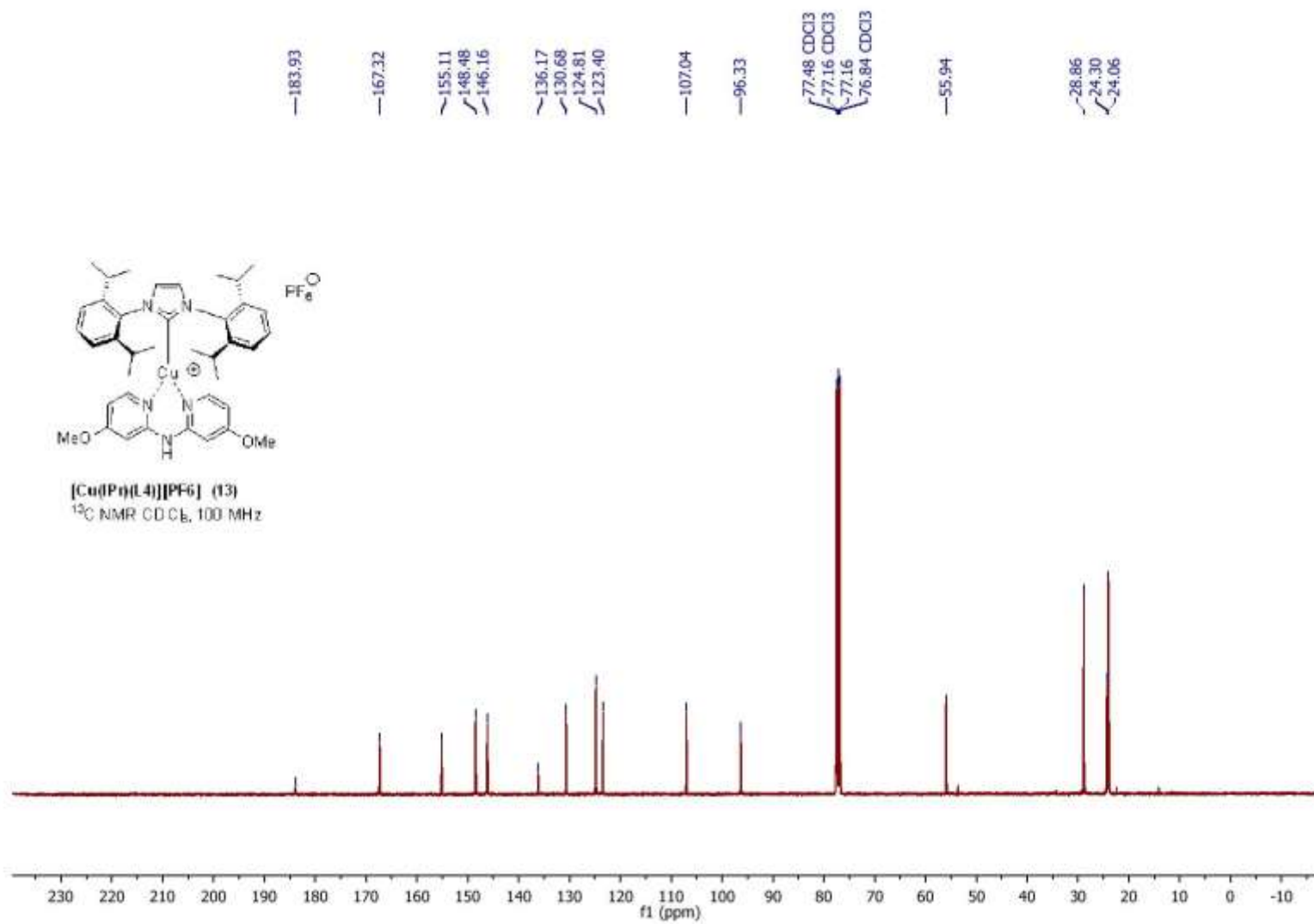


Figure S96. ^{13}C NMR spectra of complex 13.

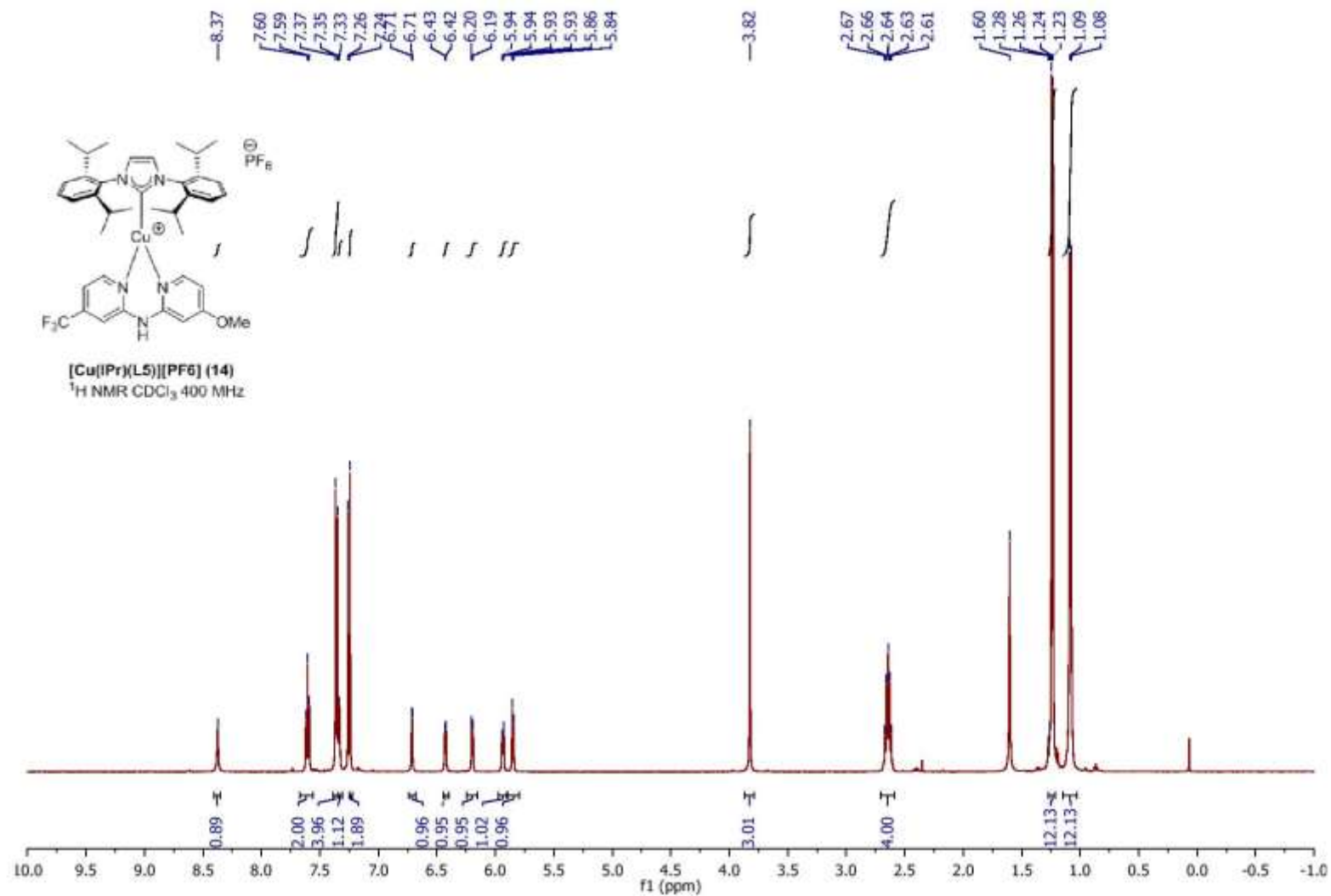


Figure S97. ¹H NMR spectra of complex 14.

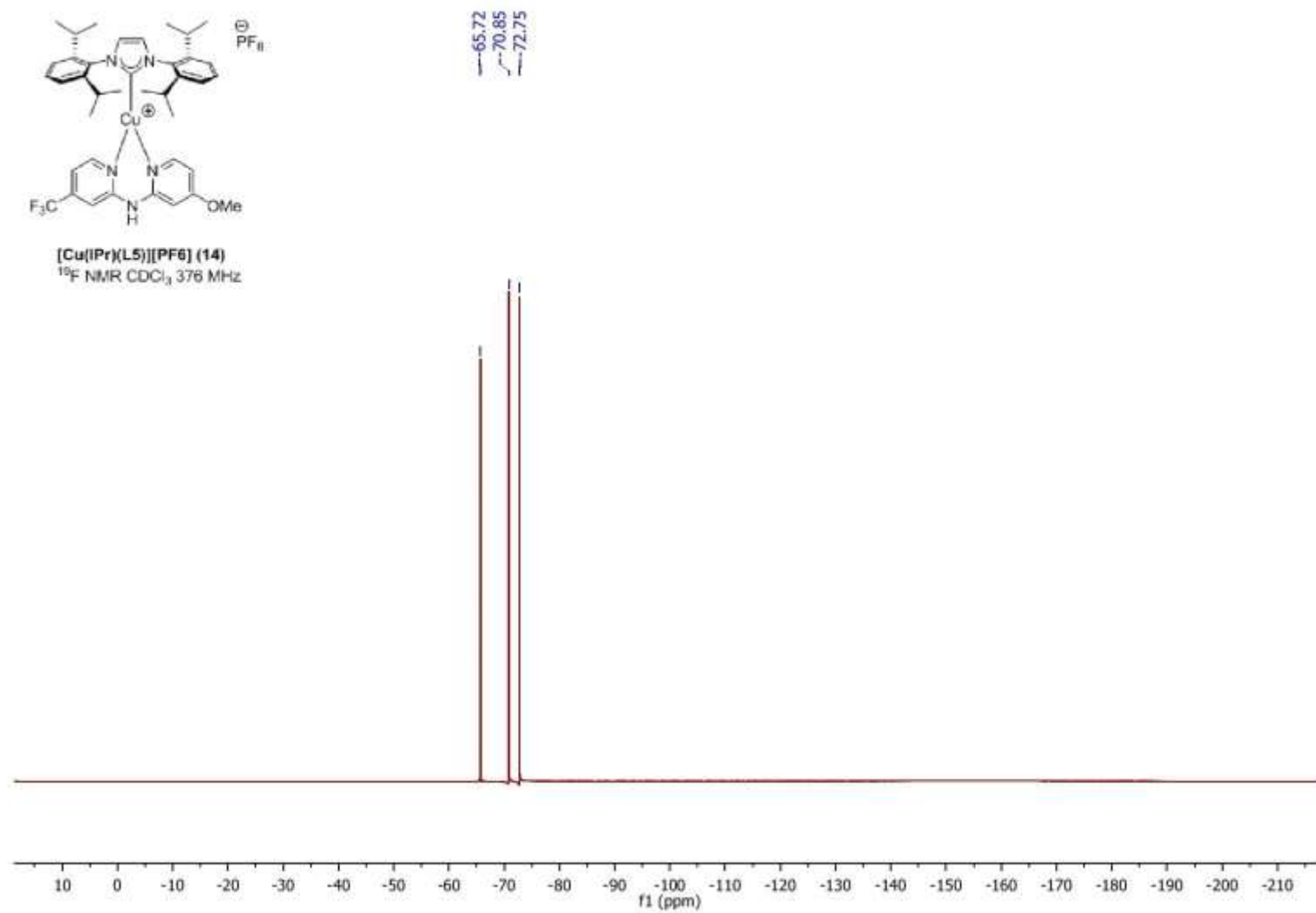


Figure S98. ¹⁹F NMR spectra of complex **14**.

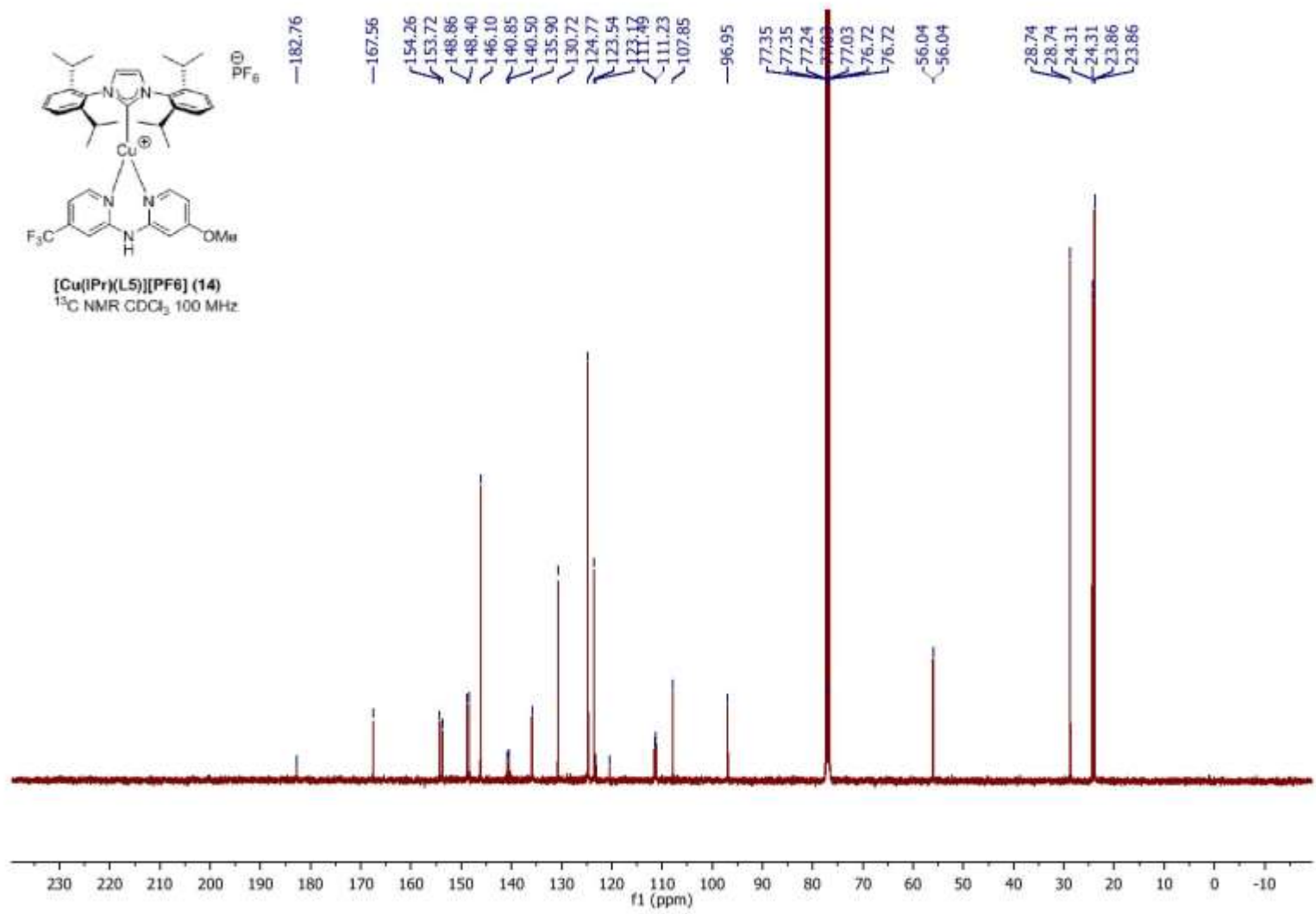


Figure S99. ^{13}C NMR spectra of complex 14.

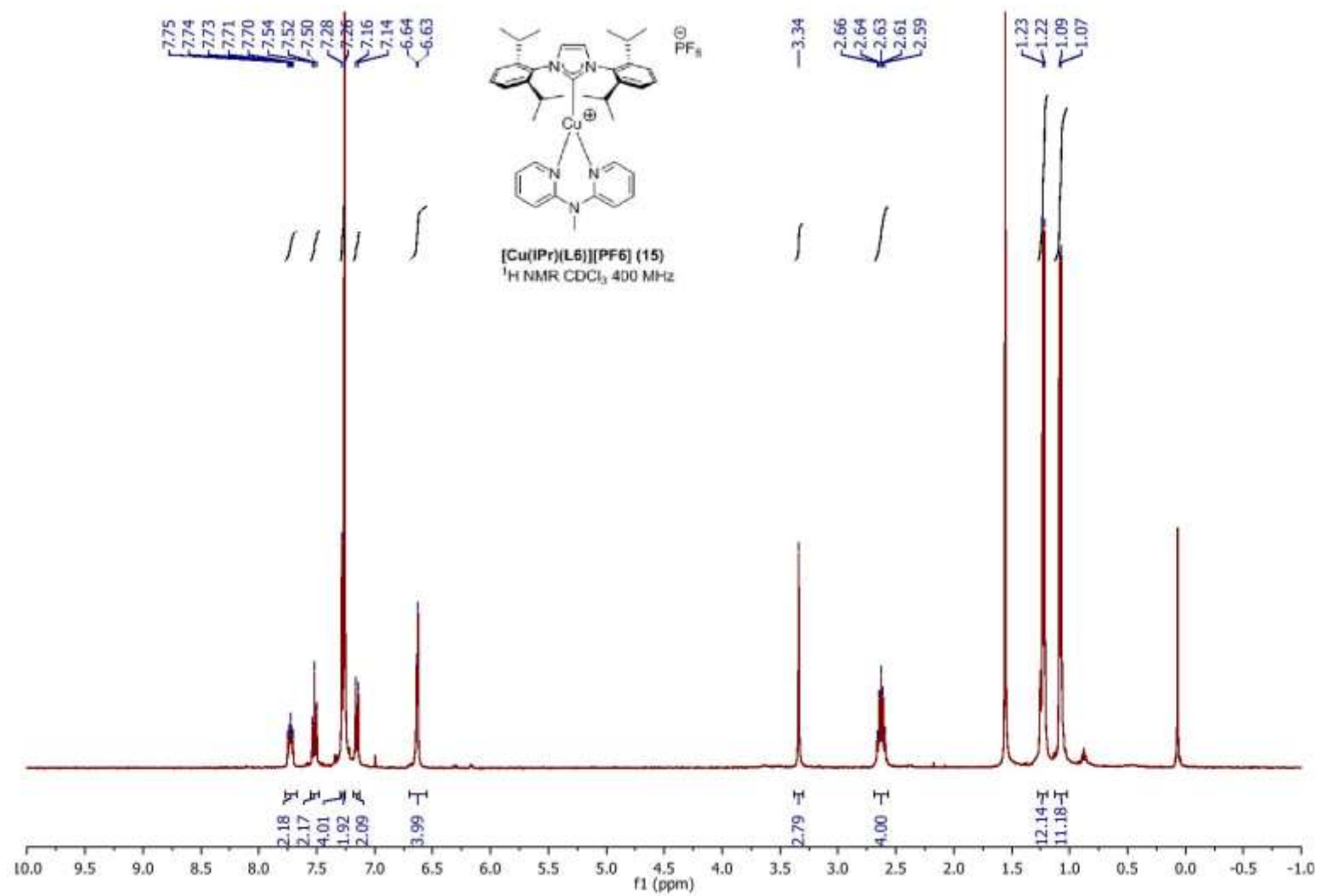


Figure S100. ^1H NMR spectra of complex **15**.

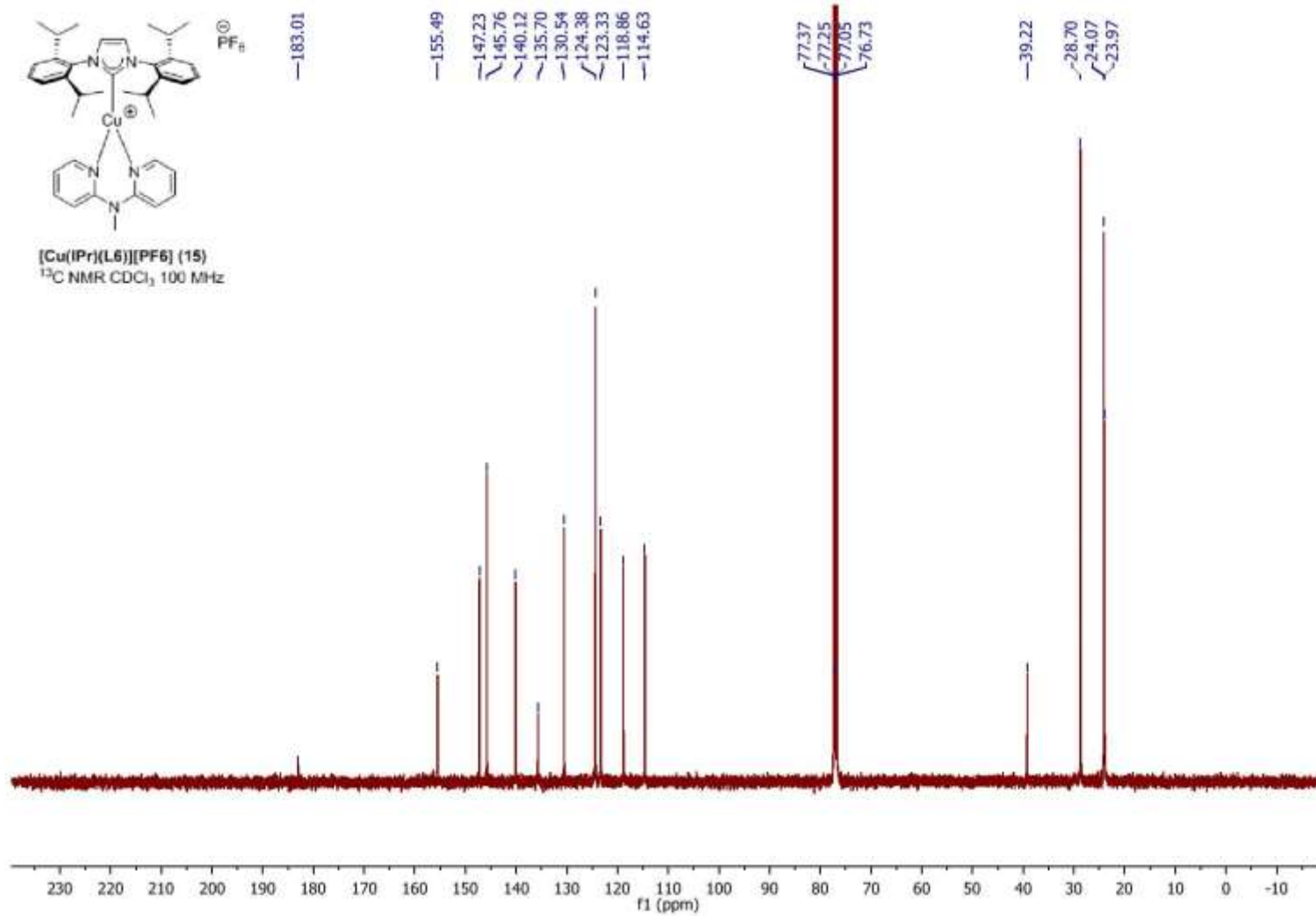


Figure S101. ^{13}C NMR spectra of complex 15.

Part 10: Calculated XYZ coordinates for complexes **6-15** at S₀, S₁ and T₁ states.

Calculated XYZ coordinates for complex **6** at S₀ state

88

IPr-L1_modify.out Energy: -1197464.5849833

Cu	0.00153	0.63284	-0.45436
N	1.44226	2.08850	-0.86689
N	-1.48482	2.02240	-0.93900
N	1.08788	-1.89201	0.65627
N	-1.05460	-1.86502	0.73156
N	-0.07194	3.89362	-0.54307
H	-0.09812	4.89573	-0.41780
C	-2.43099	-1.45660	0.60978
C	0.01300	-1.12536	0.30828
C	-2.95806	-0.58704	1.58056
C	-3.18218	-1.95731	-0.47322
C	-0.65502	-3.05093	1.33488
H	-1.36679	-3.75658	1.73285
C	-4.29941	-0.20513	1.43584
H	-4.74322	0.47051	2.16023
C	0.70209	-3.06972	1.28445
H	1.42175	-3.79497	1.62948
C	-5.07307	-0.68631	0.38201
H	-6.11393	-0.38773	0.29581
C	-4.52107	-1.55444	-0.56222
H	-5.13917	-1.91793	-1.37573
C	-2.13030	-0.06427	2.74942
H	-1.14248	-0.53195	2.70626
C	2.46289	-1.51958	0.44096
C	3.11382	-0.76822	1.43680

C	3.08623	-1.92799	-0.75387
C	5.10421	-0.82217	0.03815
H	6.14539	-0.55397	-0.11700
C	4.42819	-1.56365	-0.93190
H	4.94832	-1.85633	-1.83782
C	2.40115	-0.30499	2.70247
H	1.43744	-0.81987	2.75790
C	2.31643	-2.65322	-1.85156
H	1.41463	-3.08490	-1.40575
C	1.21918	3.40819	-0.73979
C	2.71548	1.67841	-1.07663
H	2.84440	0.61028	-1.18152
C	2.26849	4.35074	-0.77741
H	2.05426	5.40967	-0.66768
C	3.56603	3.90737	-0.97351
H	4.38394	4.62036	-1.00790
C	-1.32455	3.35249	-0.82637
C	-3.66789	3.74845	-1.22926
H	-4.50933	4.42591	-1.33648
C	-2.40511	4.24958	-0.95832
H	-2.24112	5.31866	-0.86095
C	3.80029	2.53589	-1.13808
H	4.79566	2.13910	-1.29764
C	-3.83621	2.36504	-1.37123
H	-4.80324	1.92412	-1.58112
C	2.10551	1.20698	2.63670
H	1.57961	1.53182	3.54080
H	1.48137	1.44722	1.77104
H	3.03297	1.78462	2.55577

C	4.45204	-0.42307	1.20400
H	4.98897	0.16330	1.94260
C	3.11020	-3.80769	-2.48639
H	3.47040	-4.51033	-1.72826
H	3.97586	-3.44611	-3.05108
H	2.47325	-4.35714	-3.18698
C	-2.75760	-0.44783	4.10325
H	-2.10853	-0.12612	4.92452
H	-2.89915	-1.53048	4.18357
H	-3.73312	0.02901	4.24559
C	-1.91484	1.45800	2.64486
H	-1.41199	1.71930	1.70919
H	-1.29735	1.81157	3.47722
H	-2.86817	1.99652	2.67884
C	-2.54017	-2.82946	-1.54799
H	-1.70650	-3.37148	-1.08955
C	3.18537	-0.66487	3.97774
H	3.40364	-1.73668	4.02280
H	2.60239	-0.39671	4.86493
H	4.13646	-0.12540	4.03478
C	1.86023	-1.63873	-2.92172
H	2.72513	-1.16411	-3.39855
H	1.23990	-0.85113	-2.48003
H	1.27242	-2.13632	-3.69989
C	-3.49446	-3.88095	-2.13682
H	-3.96669	-4.48029	-1.35198
H	-2.94030	-4.55647	-2.79602
H	-4.28709	-3.42328	-2.73822
C	-2.72426	1.55485	-1.21703

H	-2.80444	0.47928	-1.29327
C	-1.94874	-1.93880	-2.66198
H	-2.74143	-1.37359	-3.16549
H	-1.44079	-2.55133	-3.41432
H	-1.22254	-1.22625	-2.25783

Calculated XYZ coordinates for complex **6** at S₁ state

88

IPr-L1_modify_td.out Energy: -1197050.9390119

Cu	0.46910	0.70082	0.45722
N	-1.09798	1.72156	1.16564
N	1.60046	2.16019	0.66668
N	-1.06581	-1.73109	-0.68542
N	1.05938	-1.92566	-0.52233
N	-0.15635	3.74292	0.39619
H	-0.36136	4.71270	0.20825
C	2.43715	-1.59605	-0.26418
C	0.03370	-1.10355	-0.21422
C	3.16217	-0.95716	-1.28173
C	2.97562	-1.92261	0.99084
C	0.61736	-3.05386	-1.18422
H	1.29596	-3.82244	-1.51775
C	4.49794	-0.65569	-1.00975
H	5.09623	-0.15145	-1.76139
C	-0.72691	-2.92620	-1.29436
H	-1.46903	-3.56384	-1.74749
C	5.06995	-0.97993	0.21409
H	6.11163	-0.74042	0.40197
C	4.31595	-1.59829	1.20690
H	4.77837	-1.82841	2.16090
C	2.53734	-0.56849	-2.61375
H	1.55240	-1.04132	-2.68551
C	-2.39607	-1.18871	-0.62628
C	-2.70975	-0.12691	-1.48429
C	-3.30605	-1.75360	0.28553

C	-4.89956	-0.07734	-0.44753
H	-5.88703	0.36641	-0.36974
C	-4.56928	-1.16731	0.35436
H	-5.31163	-1.56274	1.03843
C	-1.76390	0.35660	-2.57596
H	-0.79342	-0.13066	-2.44152
C	-2.92652	-2.94794	1.15905
H	-2.30311	-3.61424	0.55380
C	-1.18614	3.05187	0.95971
C	-2.10671	1.06999	1.77850
H	-1.94700	0.01267	1.93744
C	-2.38234	3.73548	1.28752
H	-2.45732	4.80014	1.09399
C	-3.41450	3.05006	1.88131
H	-4.32643	3.57520	2.14615
C	1.22157	3.45074	0.37795
C	3.50795	4.14257	0.05335
H	4.23117	4.90723	-0.19631
C	2.12823	4.42917	0.05564
H	1.77302	5.42965	-0.17479
C	-3.27490	1.68114	2.16272
H	-4.05751	1.11048	2.64496
C	3.90626	2.85848	0.46331
H	4.95679	2.60403	0.55882
C	-1.51526	1.86806	-2.52826
H	-0.81744	2.15687	-3.31962
H	-1.08167	2.17696	-1.57367
H	-2.43912	2.43589	-2.67704
C	-3.98648	0.42902	-1.36153

H	-4.27524	1.25434	-2.00494
C	-4.13594	-3.77138	1.61323
H	-4.77787	-4.04874	0.77221
H	-4.74417	-3.23167	2.34653
H	-3.79297	-4.69112	2.09493
C	3.36408	-1.07810	-3.80209
H	2.83702	-0.87672	-4.73923
H	3.53941	-2.15574	-3.73251
H	4.33720	-0.58113	-3.86121
C	2.32504	0.95126	-2.69836
H	1.66315	1.31778	-1.90599
H	1.87729	1.21413	-3.66186
H	3.27153	1.49128	-2.59983
C	2.13306	-2.55359	2.08912
H	1.23096	-2.97221	1.63027
C	-2.29586	-0.07285	-3.95244
H	-2.44616	-1.15559	-4.00173
H	-1.58822	0.21139	-4.73709
H	-3.25420	0.40897	-4.17188
C	-2.08417	-2.53234	2.37687
H	-2.65726	-1.87137	3.03699
H	-1.15923	-2.02254	2.08732
H	-1.80325	-3.41607	2.95798
C	2.85285	-3.70703	2.79873
H	3.21253	-4.45212	2.08357
H	2.16775	-4.20176	3.49321
H	3.70904	-3.35567	3.38267
C	2.97224	1.90893	0.78090
H	3.25014	0.92127	1.12725

C	1.68748	-1.48402	3.09906
H	2.55219	-1.01780	3.58185
H	1.05870	-1.92671	3.87770
H	1.10919	-0.68558	2.61784

Calculated XYZ coordinates for complex **6** at T₁ state

88

IPr-L1_modify_triplet.out Energy: -1197395.7268946

Cu	0.38781	0.63643	0.51065
N	-1.09635	1.66356	1.29495
N	1.64209	1.98859	0.87646
N	-1.23911	-1.55055	-0.95947
N	0.84141	-1.98356	-0.62029
N	0.02334	3.73725	0.91271
H	-0.11353	4.73649	0.84731
C	2.22120	-1.80819	-0.22819
C	-0.12635	-1.07189	-0.34172
C	3.09918	-1.20683	-1.15251
C	2.61021	-2.23390	1.05776
C	0.35247	-3.01490	-1.40620
H	0.97876	-3.82810	-1.73708
C	4.43074	-1.04680	-0.74809
H	5.14083	-0.57956	-1.42219
C	-0.96020	-2.73547	-1.62852
H	-1.71161	-3.25518	-2.20096
C	4.85371	-1.46311	0.51405
H	5.89058	-1.32738	0.80684
C	3.95263	-2.04086	1.40983
H	4.29844	-2.34624	2.39180
C	2.63579	-0.69939	-2.51421
H	1.61609	-1.05631	-2.68796
C	-2.51709	-0.87765	-0.97004
C	-2.62744	0.31082	-1.71430
C	-3.58196	-1.44272	-0.23272

C	-4.91374	0.48195	-0.90726
H	-5.85571	1.02111	-0.87219
C	-4.78419	-0.72739	-0.22075
H	-5.63403	-1.11241	0.33011
C	-1.52002	0.82072	-2.63366
H	-0.61966	0.22445	-2.46225
C	-3.43212	-2.76841	0.52105
H	-2.84463	-3.44350	-0.11010
C	-1.09610	3.03643	1.27402
C	-2.20386	1.01035	1.74128
H	-2.12128	-0.06557	1.75961
C	-2.27751	3.74587	1.60741
H	-2.27385	4.83058	1.54654
C	-3.39797	3.06651	2.02887
H	-4.29708	3.61208	2.29511
C	1.34404	3.33733	0.76275
C	3.68276	3.89876	0.49924
H	4.46401	4.62930	0.32807
C	2.34236	4.28256	0.52599
H	2.06348	5.32646	0.40467
C	-3.35508	1.64884	2.12549
H	-4.20476	1.07249	2.46873
C	3.99526	2.53098	0.76975
H	5.02311	2.19116	0.83535
C	-1.14056	2.28680	-2.36191
H	-0.31798	2.58864	-3.01782
H	-0.81881	2.43276	-1.32811
H	-1.97997	2.96459	-2.54733
C	-3.85386	0.98771	-1.65295

H	-3.98153	1.91099	-2.20860
C	-4.77131	-3.47633	0.78479
H	-5.36348	-3.57977	-0.12976
H	-5.37599	-2.94276	1.52605
H	-4.58472	-4.47838	1.18268
C	3.50539	-1.24477	-3.66229
H	3.09132	-0.93311	-4.62653
H	3.54965	-2.33854	-3.64596
H	4.53105	-0.86609	-3.60783
C	2.58843	0.84219	-2.53526
H	1.92033	1.23571	-1.76227
H	2.23175	1.19607	-3.50820
H	3.57849	1.27209	-2.35542
C	1.61684	-2.83432	2.04554
H	0.70874	-3.10050	1.49495
C	-1.92378	0.61880	-4.10883
H	-2.15952	-0.42998	-4.31684
H	-1.10794	0.92542	-4.77205
H	-2.80626	1.21632	-4.36093
C	-2.65273	-2.60661	1.84383
H	-3.19699	-1.95695	2.53831
H	-1.65420	-2.18739	1.68681
H	-2.52969	-3.58055	2.32882
C	2.14266	-4.12388	2.70184
H	2.44566	-4.85878	1.94951
H	1.36088	-4.57200	3.32337
H	3.00326	-3.92972	3.34983
C	2.98495	1.63406	0.96163
H	3.17614	0.58728	1.16295

C	1.22235	-1.79411	3.11417
H	2.09698	-1.47085	3.68832
H	0.49225	-2.21672	3.81211
H	0.77473	-0.89988	2.66384

Calculated XYZ coordinates for complex 7 at S₀ state

94

diMe-IPr_L1_modify.out Energy: -1246824.3140770

Cu	0.00006	0.88541	0.45195
N	-1.46290	2.35857	0.72585
N	1.46319	2.35833	0.72598
N	-1.06901	-1.74064	-0.39288
N	1.06884	-1.74067	-0.39313
N	0.00032	4.13352	0.12390
H	0.00042	5.10902	-0.13848
C	2.44144	-1.32764	-0.27681
C	-0.00004	-0.94738	-0.09996
C	3.02714	-0.63559	-1.35186
C	3.13974	-1.65494	0.90173
C	0.68215	-2.99956	-0.86817
C	4.36750	-0.24942	-1.21253
H	4.85316	0.29609	-2.01553
C	-0.68247	-2.99954	-0.86801
C	5.08733	-0.55970	-0.06007
H	6.12854	-0.26132	0.02333
C	4.48010	-1.25586	0.98689
H	5.05508	-1.48652	1.87744
C	2.25081	-0.29588	-2.61864
H	1.27549	-0.78794	-2.56049
C	-2.44158	-1.32761	-0.27619
C	-3.02766	-0.63582	-1.35119
C	-3.13949	-1.65470	0.90264
C	-5.08745	-0.55978	-0.05877
H	-6.12864	-0.26144	0.02489

C	-4.47985	-1.25566	0.98815
H	-5.05452	-1.48615	1.87894
C	-2.25169	-0.29624	-2.61823
H	-1.27641	-0.78841	-2.56037
C	-2.44026	-2.34055	2.07046
H	-1.56520	-2.86818	1.67688
C	-1.27242	3.65613	0.43053
C	-2.71939	1.95562	1.02770
H	-2.82303	0.90503	1.26162
C	-2.33871	4.57907	0.39253
H	-2.15001	5.62012	0.14768
C	-3.61938	4.14154	0.68816
H	-4.45029	4.83986	0.66638
C	1.27293	3.65598	0.43090
C	3.61983	4.14114	0.68946
H	4.45080	4.83939	0.66815
C	2.33929	4.57884	0.39349
H	2.15076	5.61997	0.14885
C	-3.81941	2.79624	1.02394
H	-4.80083	2.40516	1.26365
C	3.81963	2.79573	1.02496
H	4.80094	2.40451	1.26491
C	-1.99121	1.21969	-2.71557
H	-1.41521	1.45056	-3.61795
H	-1.42803	1.57529	-1.84791
H	-2.93219	1.77904	-2.76081
C	-4.36800	-0.24971	-1.21153
H	-4.85395	0.29559	-2.01450
C	-3.31946	-3.38310	2.78064

H	-3.72989	-4.11097	2.07296
H	-4.15734	-2.91965	3.31179
H	-2.72697	-3.92608	3.52393
C	2.95381	-0.82464	-3.88277
H	2.33162	-0.64037	-4.76485
H	3.13905	-1.90178	-3.81525
H	3.91657	-0.33010	-4.04900
C	1.99047	1.22007	-2.71591
H	1.42767	1.57574	-1.84803
H	1.41413	1.45097	-3.61806
H	2.93148	1.77933	-2.76156
C	2.44089	-2.34107	2.06962
H	1.56590	-2.86889	1.67613
C	-2.95511	-0.82490	-3.88217
H	-3.14051	-1.90201	-3.81458
H	-2.33311	-0.64075	-4.76440
H	-3.91782	-0.33020	-4.04817
C	-1.92410	-1.27842	3.06398
H	-2.75940	-0.71163	3.49076
H	-1.24803	-0.57340	2.56863
H	-1.37803	-1.75119	3.88704
C	3.32046	-3.38341	2.77961
H	3.73103	-4.11111	2.07184
H	2.72821	-3.92664	3.52291
H	4.15826	-2.91976	3.31071
C	2.71955	1.95520	1.02814
H	2.82302	0.90455	1.26183
C	1.92459	-1.27914	3.06329
H	2.75980	-0.71219	3.49002

H	1.37873	-1.75212	3.88638
H	1.24828	-0.57424	2.56810
C	1.67685	-4.04111	-1.25495
H	2.29969	-4.33307	-0.40216
H	1.16909	-4.93285	-1.62727
H	2.34941	-3.67633	-2.03871
C	-1.67730	-4.04109	-1.25447
H	-1.16967	-4.93271	-1.62723
H	-2.29968	-4.33325	-0.40141
H	-2.35029	-3.67620	-2.03780

Calculated XYZ coordinates for complex 7 at S₁ state

94

diMe-IPr_L1_optS1.out Energy: -1246394.3777653

Cu	0.96629	-0.44190	-0.37453
N	2.05911	-0.94448	1.21678
N	2.45158	-0.49286	-1.49636
N	-1.63221	0.41985	1.07822
N	-1.70080	0.32913	-1.05153
N	3.94263	0.10429	0.25849
H	4.86900	0.44818	0.46223
C	-1.29892	0.12768	-2.41699
C	-0.90815	0.04940	0.00350
C	-0.71964	1.20520	-3.10482
C	-1.51842	-1.13256	-2.99490
C	-2.91405	0.87808	-0.65529
C	-0.35142	0.98421	-4.43272
H	0.11610	1.78354	-4.99819
C	-2.86612	0.94900	0.70338
C	-0.56638	-0.24693	-5.04006
H	-0.27763	-0.39472	-6.07572
C	-1.13860	-1.29612	-4.32823
H	-1.28689	-2.25412	-4.81613
C	-0.47201	2.55462	-2.44715
H	-0.99534	2.56939	-1.48508
C	-1.18202	0.31426	2.43628
C	-0.31489	1.29773	2.92579
C	-1.65146	-0.76441	3.20559
C	-0.27082	0.07169	5.01540
H	0.09516	-0.02954	6.03235

C	-1.17200	-0.86343	4.51139
H	-1.50440	-1.67505	5.14954
C	0.07428	2.52406	2.11207
H	-0.41552	2.45997	1.13534
C	-2.62696	-1.78747	2.63102
H	-3.23873	-1.27973	1.87863
C	3.34106	-0.53111	1.30299
C	1.50480	-1.61886	2.24435
H	0.48522	-1.94325	2.09257
C	4.05831	-0.71017	2.51065
H	5.07862	-0.34873	2.58154
C	3.46631	-1.36977	3.56058
H	4.01832	-1.51946	4.48275
C	3.67673	0.00850	-1.12191
C	4.34842	0.33731	-3.41345
H	5.07937	0.66570	-4.14004
C	4.60979	0.43673	-2.03203
H	5.55596	0.83552	-1.67706
C	2.16004	-1.86624	3.42591
H	1.66228	-2.40252	4.22294
C	3.14294	-0.27098	-3.80344
H	2.91624	-0.43821	-4.85136
C	1.58438	2.60073	1.85676
H	1.82588	3.50502	1.29020
H	1.93831	1.74112	1.28244
H	2.14788	2.63152	2.79526
C	0.14664	1.14162	4.23589
H	0.82998	1.87446	4.65419
C	-3.58974	-2.35050	3.68220

H	-4.07588	-1.55269	4.25170
H	-3.08106	-3.01280	4.38997
H	-4.36812	-2.94163	3.19153
C	-1.03580	3.71068	-3.28468
H	-0.93593	4.65326	-2.73865
H	-2.09477	3.56082	-3.51616
H	-0.49982	3.82360	-4.23195
C	1.02401	2.76113	-2.16264
H	1.41947	1.99494	-1.48771
H	1.18843	3.73905	-1.69941
H	1.61370	2.71279	-3.08333
C	-2.09847	-2.29208	-2.20037
H	-2.50931	-1.89507	-1.26591
C	-0.43482	3.80465	2.79078
H	-1.51312	3.75978	2.97101
H	-0.22953	4.67453	2.15972
H	0.05699	3.96882	3.75495
C	-1.89795	-2.92749	1.90212
H	-1.23737	-3.47292	2.58558
H	-1.30320	-2.55644	1.06066
H	-2.62309	-3.64257	1.50110
C	-3.24665	-2.99303	-2.93714
H	-4.02480	-2.28201	-3.22974
H	-3.69956	-3.74958	-2.28968
H	-2.89885	-3.50224	-3.84113
C	2.23692	-0.68838	-2.86534
H	1.31054	-1.17682	-3.14106
C	-0.98890	-3.28927	-1.83320
H	-0.54024	-3.72529	-2.73147

H	-1.38850	-4.10453	-1.22234
H	-0.18366	-2.80756	-1.26530
C	-3.96053	1.26671	-1.63961
H	-4.27044	0.40653	-2.24107
H	-4.83932	1.65894	-1.12610
H	-3.59336	2.03528	-2.32630
C	-3.83200	1.48942	1.70013
H	-4.71247	1.88691	1.19348
H	-4.16202	0.72156	2.40609
H	-3.37892	2.29820	2.28124

Calculated XYZ coordinates for complex 7 at T₁ state

94

diMe-IPr_L1_modify_triplet.out Energy: -1246754.2397181

Cu	-0.50534	0.83400	0.38789
N	-1.94692	2.03568	0.68206
N	0.81174	2.23547	0.83026
N	-0.66068	-1.86790	-0.44167
N	1.43689	-1.41467	-0.51732
N	-0.63440	3.75656	-0.24163
H	-0.67479	4.69018	-0.63008
C	2.69854	-0.73445	-0.38339
C	0.24082	-0.89583	-0.13728
C	3.05932	0.20127	-1.36730
C	3.51091	-1.05324	0.72493
C	1.28511	-2.69393	-1.07024
C	4.26709	0.88863	-1.18060
H	4.57752	1.63122	-1.90897
C	-0.04964	-2.98489	-1.01283
C	5.07878	0.62364	-0.08066
H	6.01237	1.16468	0.04337
C	4.71226	-0.34672	0.85513
H	5.37197	-0.55314	1.69060
C	2.21565	0.44343	-2.61462
H	1.36204	-0.24126	-2.58705
C	-2.07514	-1.69941	-0.22495
C	-2.85230	-1.13447	-1.25820
C	-2.61414	-2.11455	1.01028
C	-4.79306	-1.42100	0.18209
H	-5.86214	-1.31394	0.34028

C	-3.99632	-1.97203	1.18687
H	-4.45266	-2.28178	2.12137
C	-2.25139	-0.68249	-2.58482
H	-1.18165	-0.91432	-2.57239
C	-1.73016	-2.62693	2.14065
H	-0.73872	-2.84115	1.72943
C	-1.88383	3.33480	0.26762
C	-3.15272	1.56968	1.17218
H	-3.14958	0.55196	1.53885
C	-2.98582	4.16793	0.26946
H	-2.87940	5.19764	-0.05724
C	-4.24141	3.66236	0.68577
H	-5.12296	4.29203	0.66413
C	0.56395	3.51520	0.44708
C	2.72303	4.23025	1.26260
H	3.46577	5.00683	1.40893
C	1.49214	4.53202	0.65908
H	1.25188	5.54458	0.35140
C	-4.29805	2.34273	1.15425
H	-5.22585	1.91298	1.51713
C	2.95411	2.92026	1.69079
H	3.87832	2.63453	2.17912
C	-2.38787	0.84172	-2.77340
H	-1.92265	1.14794	-3.71609
H	-1.90335	1.39096	-1.95962
H	-3.43910	1.14672	-2.80020
C	-4.22569	-0.99436	-1.01754
H	-4.85822	-0.55142	-1.77998
C	-2.25717	-3.92973	2.76764

H	-2.40092	-4.70739	2.01048
H	-3.21299	-3.77881	3.27948
H	-1.54477	-4.30322	3.51021
C	3.01772	0.12327	-3.89194
H	2.37606	0.21647	-4.77433
H	3.42082	-0.89455	-3.86841
H	3.85959	0.81166	-4.01888
C	1.64749	1.87359	-2.66260
H	0.98211	2.06255	-1.81709
H	1.07312	2.02104	-3.58330
H	2.44722	2.62170	-2.64047
C	3.08391	-2.10285	1.75112
H	2.45970	-2.83941	1.23458
C	-2.87450	-1.44050	-3.77366
H	-2.77655	-2.52455	-3.65738
H	-2.37924	-1.15187	-4.70641
H	-3.94016	-1.21215	-3.87868
C	-1.55788	-1.52603	3.20791
H	-2.52038	-1.26558	3.66089
H	-1.13429	-0.61313	2.77127
H	-0.88556	-1.86066	4.00414
C	4.26941	-2.86901	2.36095
H	4.93372	-3.26566	1.58660
H	3.90041	-3.70833	2.95872
H	4.86533	-2.23673	3.02742
C	1.97819	1.96024	1.47985
H	2.11147	0.93690	1.79099
C	2.20840	-1.48562	2.86141
H	2.76538	-0.72730	3.42326

H	1.89098	-2.25912	3.56874
H	1.30712	-1.02130	2.44985
C	2.44244	-3.46564	-1.60728
H	3.18902	-3.67019	-0.83295
H	2.10402	-4.42014	-2.01456
H	2.94571	-2.91079	-2.40627
C	-0.82812	-4.19033	-1.41651
H	-0.16782	-4.94576	-1.84600
H	-1.34120	-4.63303	-0.55569
H	-1.59244	-3.93987	-2.15903

Calculated XYZ coordinates for complex **8** at S₀ state

96

diOMe-IPr_L1_modify.out Energy: -1341208.1427582

Cu	0.00832	0.62758	-0.46242
N	1.45025	2.06684	-0.93543
N	-1.46939	1.99748	-1.03354
N	1.08476	-1.79655	0.85675
N	-1.06128	-1.78297	0.88276
N	-0.06259	3.88743	-0.70877
H	-0.09005	4.89263	-0.61325
C	-2.43335	-1.39374	0.68879
C	0.01128	-1.07030	0.42646
C	-3.00478	-0.45950	1.57676
C	-3.14702	-1.94986	-0.38620
C	-0.66575	-2.91496	1.58469
C	-4.32261	-0.07010	1.34647
H	-4.81063	0.65560	1.98796
C	0.69254	-2.92553	1.56524
C	-5.05710	-0.60026	0.27865
C	-4.47534	-1.54306	-0.57750
H	-5.03989	-1.95460	-1.40326
C	-2.22818	0.13084	2.74910
H	-1.24857	-0.35469	2.78716
C	2.45699	-1.42781	0.62791
C	3.09687	-0.58557	1.56184
C	3.10056	-1.90413	-0.52496
C	5.08174	-0.67057	0.15733
C	4.43106	-1.51740	-0.74686
H	4.93895	-1.86530	-1.63681

C	2.37601	-0.04871	2.79411
H	1.43620	-0.59879	2.90258
C	2.36102	-2.73151	-1.57046
H	1.44593	-3.11679	-1.11061
C	1.23044	3.39028	-0.84894
C	2.72771	1.64468	-1.08275
H	2.85032	0.57344	-1.15515
C	2.28694	4.32555	-0.87266
H	2.07610	5.38827	-0.79810
C	3.58863	3.86918	-1.00114
H	4.41230	4.57620	-1.01649
C	-1.31643	3.33046	-0.94786
C	-3.67454	3.70070	-1.28553
H	-4.52540	4.36915	-1.37311
C	-2.40792	4.21675	-1.06576
H	-2.25038	5.28864	-0.99056
C	3.82151	2.49247	-1.11770
H	4.82178	2.08580	-1.21016
C	-3.83648	2.31377	-1.39754
H	-4.80884	1.86264	-1.55517
C	2.01360	1.43874	2.60970
H	1.49314	1.81642	3.49624
H	1.36032	1.57936	1.74376
H	2.91327	2.04502	2.45674
C	4.41381	-0.21456	1.30173
H	4.95136	0.44542	1.97348
C	3.16890	-3.94438	-2.06300
H	3.49344	-4.57349	-1.22800
H	4.05960	-3.64288	-2.62435

H	2.55532	-4.55487	-2.73343
C	-2.93166	-0.14685	4.09114
H	-2.32020	0.22208	4.92140
H	-3.09833	-1.21873	4.23895
H	-3.90371	0.35414	4.14574
C	-1.97994	1.63882	2.55214
H	-1.42481	1.82679	1.62891
H	-1.39947	2.04034	3.38938
H	-2.92420	2.19135	2.49796
C	-2.47447	-2.89048	-1.38137
H	-1.64031	-3.38024	-0.86872
C	3.18492	-0.26845	4.08518
H	3.45552	-1.32157	4.21190
H	2.59488	0.04051	4.95430
H	4.10914	0.31871	4.09041
C	1.93699	-1.82662	-2.74617
H	2.81484	-1.40353	-3.24735
H	1.31059	-0.99821	-2.39740
H	1.36528	-2.39710	-3.48538
C	-3.40133	-4.00085	-1.90178
H	-3.87374	-4.54800	-1.07979
H	-2.82674	-4.71366	-2.50160
H	-4.19341	-3.60438	-2.54638
C	-2.71243	1.51608	-1.26802
H	-2.78402	0.43878	-1.32607
C	-1.87929	-2.07474	-2.54910
H	-2.67206	-1.56065	-3.10457
H	-1.34824	-2.73129	-3.24648
H	-1.17236	-1.32190	-2.18563

O	6.35295	-0.20983	-0.00017
O	-6.32308	-0.11864	0.14236
C	-7.17332	-0.67873	-0.85897
H	-7.30270	-1.75764	-0.71105
H	-8.13466	-0.17779	-0.74376
H	-6.78259	-0.48963	-1.86716
C	7.13439	-0.69536	-1.09269
H	8.11420	-0.22990	-0.98458
H	7.24052	-1.78602	-1.04978
H	6.69705	-0.40478	-2.05649
H	-1.38122	-3.59332	2.02160
H	1.41001	-3.61502	1.98089

Calculated XYZ coordinates for complex **8** at S₁ state

96

diOMe-IPr_L1_modify_td.out Energy: -1340746.0585967

Cu	-0.30389	0.70694	0.44301
N	-1.37197	2.19601	0.76368
N	1.31447	1.63725	1.18984
N	-1.02143	-1.72868	-0.83536
N	1.11972	-1.75276	-0.80546
N	0.44373	3.69772	0.44636
H	0.68587	4.65954	0.26143
C	2.48540	-1.37795	-0.56949
C	0.05056	-1.05242	-0.36946
C	3.03859	-0.34696	-1.34622
C	3.20219	-2.04926	0.42967
C	0.71775	-2.84902	-1.54824
C	4.33118	0.05980	-1.04347
H	4.81254	0.85581	-1.60206
C	-0.63732	-2.83695	-1.56297
C	5.05766	-0.55622	-0.02261
C	4.50427	-1.62106	0.69317
H	5.08146	-2.12326	1.45831
C	2.30225	0.26827	-2.52872
H	1.31582	-0.20061	-2.60113
C	-2.37358	-1.28397	-0.63055
C	-2.95946	-0.44635	-1.60003
C	-3.05248	-1.70239	0.52027
C	-4.97876	-0.45409	-0.25781
C	-4.37033	-1.27471	0.69453
H	-4.90934	-1.58076	1.58268

C	-2.20082	0.03356	-2.82788
H	-1.19870	-0.40732	-2.80533
C	-2.37835	-2.54917	1.58953
H	-1.44312	-2.94039	1.17584
C	-0.94835	3.47737	0.50187
C	-2.74720	2.00212	0.93057
H	-3.05378	1.01723	1.25916
C	-1.82014	4.50578	0.25293
H	-1.42886	5.49662	0.04066
C	-3.21285	4.27824	0.29469
H	-3.91080	5.08073	0.09690
C	1.45351	2.96502	1.00020
C	3.68714	2.86835	1.90089
H	4.62252	3.35381	2.15905
C	2.67540	3.59946	1.32345
H	2.78920	4.66223	1.13919
C	-3.65118	3.00089	0.67585
H	-4.70820	2.78584	0.79471
C	3.49454	1.50601	2.17118
H	4.25839	0.89902	2.63910
C	-2.03135	1.55991	-2.81401
H	-1.43356	1.87882	-3.67361
H	-1.53613	1.90524	-1.90134
H	-2.99818	2.06945	-2.86779
C	-4.26883	-0.04490	-1.39102
H	-4.76979	0.61318	-2.09279
C	-3.22552	-3.75872	2.00393
H	-3.51281	-4.35898	1.13583
H	-4.14017	-3.45748	2.52413

H	-2.65666	-4.39558	2.68767
C	3.04658	-0.04218	-3.83640
H	2.46987	0.31774	-4.69374
H	3.20612	-1.11768	-3.95809
H	4.02524	0.44732	-3.86261
C	2.07730	1.77598	-2.36759
H	1.44149	1.99894	-1.50719
H	1.58570	2.17989	-3.25760
H	3.02360	2.31041	-2.23458
C	2.57601	-3.19358	1.22281
H	1.92495	-3.74960	0.54009
C	-2.87571	-0.44239	-4.12136
H	-2.99042	-1.53061	-4.13540
H	-2.27766	-0.14929	-4.98957
H	-3.86963	0.00120	-4.23747
C	-2.01842	-1.68311	2.80646
H	-2.91606	-1.25645	3.26532
H	-1.36165	-0.84994	2.52903
H	-1.49973	-2.27947	3.56330
C	3.60434	-4.19191	1.76383
H	4.28566	-4.53660	0.98075
H	3.08985	-5.06501	2.17456
H	4.20158	-3.76222	2.57514
C	2.30086	0.94168	1.78832
H	2.10964	-0.11268	1.93220
C	1.68946	-2.67375	2.36710
H	2.28857	-2.12573	3.10333
H	1.21238	-3.51142	2.88520
H	0.89557	-2.01315	2.00409

O	-6.23832	0.01282	-0.16274
O	6.29347	-0.05791	0.19501
C	7.11728	-0.66894	1.17275
H	7.30050	-1.72316	0.93669
H	8.06029	-0.12477	1.14921
H	6.67478	-0.58616	2.17302
C	-7.02140	-0.34453	0.96421
H	-7.98788	0.13497	0.81699
H	-7.15975	-1.42995	1.02348
H	-6.56929	0.02571	1.89173
H	1.43223	-3.52478	-1.99051
H	-1.35665	-3.49865	-2.01815

Calculated XYZ coordinates for complex **8** at T₁ state

96

diOMe-IPr_L1_modify_triplet.out Energy: -1341139.9592799

Cu	0.35538	0.63684	-0.51014
N	1.50354	2.06951	-0.93109
N	-1.19502	1.51853	-1.35394
N	1.00713	-1.78648	0.88805
N	-1.13360	-1.61400	1.02937
N	-0.24949	3.68163	-0.99842
H	-0.46782	4.66708	-0.94810
C	-2.48024	-1.12046	0.88222
C	-0.04263	-1.03917	0.45887
C	-2.83214	0.06817	1.55419
C	-3.37881	-1.83162	0.06428
C	-0.76351	-2.69650	1.81769
C	-4.10393	0.58604	1.32086
H	-4.43124	1.50108	1.80216
C	0.58900	-2.81137	1.72199
C	-5.00436	-0.06756	0.47205
C	-4.65227	-1.28412	-0.12849
H	-5.36306	-1.80625	-0.75301
C	-1.91324	0.74299	2.57056
H	-0.96451	0.19887	2.59616
C	2.37666	-1.45755	0.57362
C	3.09901	-0.64903	1.48203
C	2.93689	-1.95355	-0.61682
C	5.00820	-0.82731	-0.01655
C	4.26771	-1.62134	-0.90290
H	4.71392	-1.98070	-1.82080

C	2.46405	-0.07184	2.74286
H	1.47083	-0.51616	2.86156
C	2.12064	-2.77473	-1.60861
H	1.20701	-3.10347	-1.10344
C	1.09763	3.39072	-0.82771
C	2.87154	1.82312	-0.97928
H	3.14731	0.79228	-1.16326
C	2.01267	4.41309	-0.57773
H	1.64904	5.43177	-0.46667
C	3.37928	4.13728	-0.51984
H	4.09585	4.92851	-0.33587
C	-1.30179	2.88749	-1.36918
C	-3.57896	2.72042	-2.17850
H	-4.51282	3.18686	-2.47353
C	-2.52663	3.49449	-1.74498
H	-2.61006	4.57705	-1.70748
C	3.80473	2.79676	-0.77041
H	4.85690	2.53482	-0.80078
C	-3.42025	1.30997	-2.24584
H	-4.21216	0.66053	-2.59633
C	2.26934	1.45199	2.60870
H	1.77939	1.85039	3.50322
H	1.65323	1.70313	1.73975
H	3.22806	1.96472	2.48500
C	4.41873	-0.34882	1.16346
H	5.01863	0.28244	1.80923
C	2.85682	-4.04113	-2.08164
H	3.18142	-4.65303	-1.23422
H	3.74033	-3.80018	-2.68181

H	2.19392	-4.64673	-2.70787
C	-2.52434	0.65200	3.98401
H	-1.82890	1.06036	4.72491
H	-2.74554	-0.38527	4.25564
H	-3.45742	1.22112	4.04872
C	-1.58598	2.20149	2.20591
H	-1.07442	2.26867	1.24320
H	-0.93257	2.64213	2.96552
H	-2.49116	2.81395	2.14294
C	-2.97884	-3.14603	-0.61335
H	-2.34546	-3.69855	0.08860
C	3.27135	-0.42161	4.00658
H	3.41135	-1.50303	4.10478
H	2.74818	-0.06110	4.89818
H	4.26130	0.04531	3.99327
C	1.69646	-1.90228	-2.80794
H	2.57132	-1.52406	-3.34712
H	1.10605	-1.03569	-2.48672
H	1.08600	-2.48068	-3.50898
C	-4.17290	-4.05871	-0.93684
H	-4.81074	-4.21566	-0.06152
H	-3.81000	-5.03474	-1.27317
H	-4.79179	-3.65092	-1.74374
C	-2.23364	0.77176	-1.81641
H	-2.07010	-0.29491	-1.80159
C	-2.13458	-2.90782	-1.88407
H	-2.71818	-2.37504	-2.64340
H	-1.82389	-3.86517	-2.31559
H	-1.22954	-2.32944	-1.67474

O	6.29147	-0.44378	-0.22081
O	-6.20105	0.55098	0.30168
C	-7.20306	-0.07805	-0.49783
H	-7.48364	-1.05523	-0.08650
H	-8.06474	0.58889	-0.46892
H	-6.86807	-0.19617	-1.53613
C	6.97880	-0.89565	-1.39063
H	7.98311	-0.47847	-1.31994
H	7.03793	-1.99023	-1.41574
H	6.49265	-0.52628	-2.30186
H	-1.49166	-3.26832	2.37040
H	1.28413	-3.50406	2.16924

Calculated XYZ coordinates for complex **9** at S₀ state

102

diOMe-diMe-IPr_L1_modify.out Energy: -1390567.7528573

Cu	-0.00006	0.85706	-0.47813
N	1.45801	2.32832	-0.80031
N	-1.45813	2.32815	-0.80045
N	1.07020	-1.70711	0.53630
N	-1.07008	-1.70713	0.53623
N	-0.00016	4.11897	-0.23398
H	-0.00024	5.09418	0.02877
C	-2.43819	-1.29583	0.38325
C	0.00007	-0.93766	0.18924
C	-3.03582	-0.52756	1.40351
C	-3.13115	-1.67318	-0.77766
C	-0.68238	-2.93031	1.09642
C	-4.35334	-0.11417	1.21801
H	-4.85780	0.49545	1.95982
C	0.68249	-2.93028	1.09647
C	-5.06454	-0.46407	0.06314
C	-4.45978	-1.24900	-0.92543
H	-5.00452	-1.52160	-1.81959
C	-2.27664	-0.12739	2.66370
H	-1.31463	-0.64864	2.65753
C	2.43832	-1.29589	0.38319
C	3.03607	-0.52773	1.40347
C	3.13114	-1.67312	-0.77783
C	5.06462	-0.46409	0.06288
C	4.45975	-1.24889	-0.92572
H	5.00437	-1.52135	-1.81999

C	2.27695	-0.12762	2.66372
H	1.31494	-0.64887	2.65757
C	2.43562	-2.43817	-1.89824
H	1.55957	-2.93604	-1.46996
C	1.27482	3.62519	-0.49735
C	2.71928	1.90898	-1.05450
H	2.81297	0.85968	-1.29811
C	2.35322	4.53064	-0.40692
H	2.17146	5.57181	-0.15712
C	3.63881	4.07359	-0.64712
H	4.47972	4.75639	-0.57505
C	-1.27506	3.62505	-0.49749
C	-3.63908	4.07331	-0.64756
H	-4.48004	4.75605	-0.57560
C	-2.35355	4.53043	-0.40721
H	-2.17188	5.57161	-0.15740
C	3.83302	2.72873	-0.98828
H	4.82003	2.32132	-1.17227
C	-3.83315	2.72843	-0.98871
H	-4.82012	2.32093	-1.17281
C	1.97491	1.38357	2.67005
H	1.41507	1.65673	3.57076
H	1.37918	1.66531	1.79728
H	2.90014	1.96988	2.65205
C	4.35356	-0.11434	1.21789
H	4.85811	0.49519	1.95971
C	3.31569	-3.52740	-2.53269
H	3.71856	-4.20831	-1.77577
H	4.15907	-3.10210	-3.08728

H	2.72718	-4.11629	-3.24360
C	-3.02202	-0.55322	3.94209
H	-2.41492	-0.32880	4.82542
H	-3.23686	-1.62698	3.93904
H	-3.97368	-0.02281	4.05064
C	-1.97463	1.38381	2.67000
H	-1.37891	1.66557	1.79722
H	-1.41478	1.65699	3.57070
H	-2.89988	1.97009	2.65200
C	-2.43574	-2.43837	-1.89805
H	-1.55974	-2.93631	-1.46976
C	3.02241	-0.55352	3.94204
H	3.23718	-1.62728	3.93893
H	2.41539	-0.32909	4.82542
H	3.97411	-0.02317	4.05052
C	1.92085	-1.44571	-2.96215
H	2.75596	-0.90944	-3.42699
H	1.24635	-0.70795	-2.51466
H	1.37364	-1.97261	-3.75079
C	-3.31596	-3.52749	-2.53245
H	-3.71887	-4.20835	-1.77550
H	-2.72754	-4.11645	-3.24339
H	-4.15932	-3.10209	-3.08700
C	-2.71936	1.90875	-1.05478
H	-2.81296	0.85943	-1.29835
C	-1.92089	-1.44599	-2.96199
H	-2.75596	-0.90968	-3.42685
H	-1.37372	-1.97297	-3.75062
H	-1.24632	-0.70825	-2.51456

C	-1.67830	-3.94151	1.55414
H	-2.31206	-4.27822	0.72627
H	-1.17186	-4.81324	1.97297
H	-2.34031	-3.52683	2.32190
C	1.67842	-3.94144	1.55430
H	1.17196	-4.81325	1.97295
H	2.31237	-4.27801	0.72653
H	2.34024	-3.52678	2.32224
O	6.33172	0.02908	-0.01700
O	-6.33165	0.02907	-0.01666
C	-7.15734	-0.36047	-1.11459
H	-7.28346	-1.44938	-1.14898
H	-8.12394	0.11231	-0.93955
H	-6.74644	-0.00714	-2.06913
C	7.15727	-0.36027	-1.11511
H	8.12388	0.11250	-0.94012
H	7.28341	-1.44917	-1.14969
H	6.74622	-0.00679	-2.06953

Calculated XYZ coordinates for complex **9** at S₁ state

102

diOMe-diMe-IPr_L1_modify_td.out Energy: -1390089.5611302

Cu	-0.27607	0.90417	0.50002
N	-1.43595	2.31086	0.88704
N	1.33494	2.11943	0.64569
N	-0.95658	-1.59914	-0.58856
N	1.17317	-1.68827	-0.49844
N	-0.00364	3.86088	-0.20720
H	0.03388	4.77638	-0.62988
C	2.54738	-1.37755	-0.23704
C	0.12420	-0.90676	-0.17510
C	3.29121	-0.71962	-1.23299
C	3.09681	-1.76308	0.98762
C	0.75391	-2.87002	-1.10912
C	4.60573	-0.39299	-0.93828
H	5.23041	0.12773	-1.65508
C	-0.60464	-2.81010	-1.17024
C	5.17024	-0.71831	0.29990
C	4.42522	-1.41408	1.25179
H	4.86568	-1.69072	2.20171
C	2.67522	-0.36033	-2.57857
H	1.85486	-1.06275	-2.76614
C	-2.29186	-1.08803	-0.45587
C	-2.78913	-0.22106	-1.45034
C	-3.05584	-1.48733	0.64767
C	-4.86021	-0.11091	-0.19507
C	-4.35411	-0.99120	0.76357
H	-4.95557	-1.28117	1.61621

C	-1.97314	0.16535	-2.67601
H	-0.97818	-0.28281	-2.58116
C	-2.48429	-2.39744	1.72481
H	-1.57225	-2.85801	1.33133
C	-1.26944	3.56328	0.34501
C	-2.68033	2.03199	1.46362
H	-2.77520	1.07432	1.95718
C	-2.28487	4.47894	0.26288
H	-2.09264	5.45015	-0.18395
C	-3.56713	4.16191	0.76459
H	-4.37636	4.87729	0.70764
C	1.21890	3.36934	0.15402
C	3.59922	3.68511	0.35419
H	4.48514	4.29779	0.22245
C	2.37057	4.16732	-0.03408
H	2.26635	5.16092	-0.45639
C	-3.72596	2.91596	1.38763
H	-4.67381	2.63579	1.83578
C	3.69493	2.41540	0.93943
H	4.63969	2.00514	1.27152
C	-1.78364	1.68407	-2.78325
H	-1.15549	1.92356	-3.64697
H	-1.30873	2.09799	-1.88940
H	-2.74085	2.19858	-2.91061
C	-4.07743	0.26335	-1.29170
H	-4.50920	0.95100	-2.01090
C	-3.43880	-3.53581	2.10519
H	-3.76503	-4.09584	1.22360
H	-4.33303	-3.16464	2.61558

H	-2.94015	-4.23041	2.78742
C	3.66682	-0.50310	-3.73879
H	3.14083	-0.39479	-4.69161
H	4.16080	-1.47911	-3.72951
H	4.44134	0.26958	-3.70890
C	2.07005	1.05179	-2.55261
H	1.25113	1.12381	-1.83313
H	1.67372	1.31293	-3.53867
H	2.82677	1.79448	-2.27693
C	2.27261	-2.49328	2.03835
H	1.39999	-2.92737	1.53872
C	-2.61048	-0.39886	-3.95421
H	-2.73852	-1.48387	-3.89535
H	-1.98229	-0.17564	-4.82193
H	-3.59595	0.04403	-4.12990
C	-2.08344	-1.57710	2.96013
H	-2.95394	-1.07951	3.40018
H	-1.34601	-0.80738	2.70713
H	-1.64206	-2.22399	3.72453
C	3.03813	-3.64871	2.69366
H	3.46137	-4.32442	1.94444
H	2.36490	-4.22743	3.33265
H	3.85580	-3.29105	3.32755
C	2.54012	1.67483	1.05251
H	2.56108	0.67424	1.46345
C	1.75148	-1.50889	3.09664
H	2.58159	-1.01416	3.61276
H	1.15090	-2.03247	3.84643
H	1.12071	-0.73528	2.64626

C	1.72464	-3.90986	-1.54782
H	2.30612	-4.28798	-0.70111
H	1.19920	-4.75023	-2.00366
H	2.43178	-3.50928	-2.28109
C	-1.62463	-3.76224	-1.68835
H	-1.14132	-4.62132	-2.15570
H	-2.26744	-4.12805	-0.88140
H	-2.26878	-3.28371	-2.43131
O	-6.09117	0.43182	-0.14990
O	6.44451	-0.30918	0.48041
C	7.11094	-0.65141	1.68416
H	7.17704	-1.73838	1.80575
H	8.11355	-0.23574	1.59490
H	6.61152	-0.21024	2.55509
C	-6.93917	0.11946	0.94150
H	-7.86576	0.66296	0.76328
H	-7.15129	-0.95489	0.98523
H	-6.49904	0.45021	1.88975

Calculated XYZ coordinates for complex **9** at T₁ state

102

diOMe-diMe-IPr_L1_modify_triplet.out Energy: -1390500.3299958

Cu	-0.34042	0.89307	0.50936
N	-1.56883	2.31125	0.76771
N	1.19213	2.01381	1.04128
N	-0.97719	-1.67125	-0.60215
N	1.16054	-1.54749	-0.70973
N	0.05593	3.99855	0.34412
H	0.19459	4.96463	0.08200
C	2.51587	-1.09017	-0.55519
C	0.07193	-0.88959	-0.24280
C	3.00409	-0.11479	-1.44645
C	3.29551	-1.63792	0.47850
C	0.79879	-2.72408	-1.37707
C	4.29272	0.36686	-1.23106
H	4.71887	1.13190	-1.87084
C	-0.56385	-2.80892	-1.29691
C	5.07934	-0.12333	-0.18153
C	4.59145	-1.13748	0.65390
H	5.21049	-1.53769	1.44502
C	2.18307	0.38846	-2.63047
H	1.25338	-0.18849	-2.66954
C	-2.34651	-1.32314	-0.32017
C	-3.09084	-0.64160	-1.31094
C	-2.89992	-1.70076	0.91555
C	-4.99537	-0.69459	0.20225
C	-4.24008	-1.37522	1.16554
H	-4.67833	-1.64379	2.11788

C	-2.46947	-0.20434	-2.63323
H	-1.48577	-0.67736	-2.71994
C	-2.06873	-2.38528	1.99456
H	-1.11998	-2.69561	1.54608
C	-1.27175	3.60072	0.35704
C	-2.90789	1.99006	0.94419
H	-3.09442	0.99772	1.33570
C	-2.27719	4.49254	-0.02284
H	-1.99900	5.48438	-0.37068
C	-3.61779	4.12844	0.08192
H	-4.40243	4.81995	-0.20056
C	1.18800	3.36691	0.79079
C	3.50952	3.52754	1.46619
H	4.41411	4.10914	1.60723
C	2.37406	4.12125	0.96148
H	2.36235	5.17936	0.71460
C	-3.92486	2.83963	0.61666
H	-4.95052	2.51908	0.76315
C	3.46914	2.14950	1.81488
H	4.32861	1.64065	2.23209
C	-2.24900	1.32206	-2.65684
H	-1.77803	1.62208	-3.59871
H	-1.60676	1.65052	-1.83431
H	-3.19782	1.85877	-2.55975
C	-4.41507	-0.33284	-1.02279
H	-5.02815	0.21259	-1.73123
C	-2.74510	-3.65200	2.54897
H	-2.99419	-4.35378	1.74642
H	-3.66857	-3.41867	3.08875

H	-2.07530	-4.15898	3.25102
C	2.92301	0.14890	-3.96107
H	2.28234	0.42579	-4.80485
H	3.20649	-0.90246	-4.07660
H	3.83619	0.74911	-4.02551
C	1.79227	1.86945	-2.47413
H	1.17307	2.02354	-1.58766
H	1.22640	2.20796	-3.34823
H	2.67833	2.50500	-2.37299
C	2.73808	-2.71604	1.40940
H	2.00408	-3.29631	0.84120
C	-3.30494	-0.65667	-3.84524
H	-3.48452	-1.73662	-3.83128
H	-2.78266	-0.40887	-4.77495
H	-4.27870	-0.15743	-3.87143
C	-1.73948	-1.39016	3.12586
H	-2.65226	-1.03569	3.61606
H	-1.20671	-0.51069	2.74391
H	-1.10573	-1.86140	3.88378
C	3.80673	-3.70600	1.90185
H	4.38718	-4.11847	1.07047
H	3.32847	-4.53637	2.43076
H	4.50497	-3.23782	2.60405
C	2.31350	1.45205	1.57524
H	2.24537	0.39455	1.77756
C	1.98063	-2.09924	2.60417
H	2.65218	-1.49422	3.22360
H	1.56336	-2.88976	3.23702
H	1.15169	-1.46654	2.27262

C	1.80874	-3.60295	-2.03358
H	2.51687	-4.02024	-1.31027
H	1.31463	-4.43147	-2.54431
H	2.39150	-3.04231	-2.77213
C	-1.53237	-3.82577	-1.79739
H	-1.00449	-4.64891	-2.28226
H	-2.12967	-4.23693	-0.97658
H	-2.22832	-3.38949	-2.52127
O	-6.28604	-0.31450	0.36740
O	6.30578	0.44717	-0.05604
C	7.19429	-0.02882	0.95489
H	7.42929	-1.09027	0.80981
H	8.10416	0.56216	0.84994
H	6.77481	0.12282	1.95764
C	-6.96417	-0.65327	1.57954
H	-7.97581	-0.26332	1.46874
H	-7.00410	-1.74009	1.71950
H	-6.48374	-0.18271	2.44619

Calculated XYZ coordinates for complex **10** at S₀ state

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diCl-IPr_L1_modify.out Energy: -1774253.6929515

Cu	-0.05449	1.10109	-0.44744
N	1.28093	2.70076	-0.48367
N	-1.62342	2.45022	-0.71210
N	1.18180	-1.52268	0.14702
N	-0.96554	-1.60005	0.30952
N	-0.37918	4.26924	0.17906
H	-0.48866	5.20858	0.53440
C	-2.35653	-1.22086	0.30949
C	0.06155	-0.75931	-0.01567
C	-2.85246	-0.51478	1.41779
C	-3.14488	-1.59497	-0.79694
C	-0.49447	-2.85632	0.68209
C	-4.20599	-0.15041	1.38462
H	-4.63069	0.40120	2.21752
C	0.86299	-2.81066	0.56945
C	-5.01549	-0.49890	0.30625
H	-6.06476	-0.21790	0.30677
C	-4.49277	-1.21773	-0.77151
H	-5.14372	-1.48741	-1.59565
C	-1.98835	-0.16542	2.62381
H	-0.98306	-0.56105	2.45335
C	2.52801	-1.05476	-0.06724
C	3.23802	-0.55108	1.03757
C	3.06045	-1.13771	-1.36562
C	5.10588	-0.16901	-0.47352
H	6.12376	0.17546	-0.63263

C	4.37290	-0.67861	-1.54558
H	4.82460	-0.71909	-2.53139
C	2.60586	-0.44891	2.42121
H	1.73849	-1.11641	2.44854
C	2.23729	-1.63792	-2.54586
H	1.34197	-2.13003	-2.15300
C	0.95186	3.93529	-0.06488
C	2.58674	2.44031	-0.72866
H	2.79990	1.43897	-1.07614
C	1.92522	4.93038	0.16388
H	1.62646	5.91665	0.50635
C	3.25816	4.63601	-0.07199
H	4.01888	5.39194	0.09642
C	-1.57408	3.72582	-0.29010
C	-3.92511	4.03935	-0.71830
H	-4.81406	4.66241	-0.71276
C	-2.71756	4.55092	-0.27122
H	-2.64400	5.57666	0.07760
C	3.60273	3.36138	-0.54101
H	4.62971	3.08391	-0.74600
C	-3.97618	2.71894	-1.18324
H	-4.89651	2.27295	-1.54054
C	2.08571	0.98191	2.67076
H	1.61761	1.04989	3.65857
H	1.34465	1.26965	1.91896
H	2.90689	1.70617	2.63043
C	4.54348	-0.10191	0.80180
H	5.12788	0.30232	1.62138
C	2.99030	-2.67596	-3.39577

H	3.34310	-3.51025	-2.78155
H	3.85646	-2.23765	-3.90220
H	2.32806	-3.07632	-4.17026
C	-2.52934	-0.82966	3.90500
H	-1.86111	-0.62489	4.74809
H	-2.60771	-1.91484	3.78493
H	-3.52184	-0.44744	4.16565
C	-1.84912	1.35901	2.79683
H	-1.40503	1.81650	1.90761
H	-1.20800	1.58541	3.65499
H	-2.82242	1.83079	2.96934
C	-2.53482	-2.32369	-1.99102
H	-1.71510	-2.94846	-1.62092
C	3.55479	-0.90087	3.54458
H	3.95211	-1.90195	3.35105
H	3.01779	-0.92422	4.49821
H	4.40049	-0.21586	3.66490
C	1.76681	-0.44376	-3.40137
H	2.62271	0.09338	-3.82475
H	1.18468	0.26524	-2.80135
H	1.13688	-0.78659	-4.22835
C	-3.51919	-3.26221	-2.70583
H	-3.99398	-3.95423	-2.00351
H	-2.98718	-3.85176	-3.45900
H	-4.30722	-2.70869	-3.22739
C	-2.80906	1.97518	-1.15876
H	-2.79859	0.94394	-1.48363
C	-1.92522	-1.30725	-2.98044
H	-2.70802	-0.67098	-3.40919

H	-1.42603	-1.82661	-3.80526
H	-1.18855	-0.66253	-2.49017
Cl	-1.51446	-4.13473	1.16844
Cl	2.03343	-4.01597	0.86534

Calculated XYZ coordinates for complex **10** at S₁ state

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diCl-IPr_L1_optS1.out Energy: -1773819.0850075

Cu	-1.19097	-0.38956	0.37405
N	-2.30381	-0.84098	-1.21737
N	-2.68822	-0.31800	1.47056
N	1.46197	0.24428	-1.09005
N	1.52585	0.15746	1.05771
N	-4.07749	0.41666	-0.31165
H	-4.96203	0.84807	-0.53461
C	1.09908	-0.01551	2.42217
C	0.71794	-0.06141	-0.00381
C	0.59135	1.10004	3.10413
C	1.21916	-1.29350	2.98998
C	2.76772	0.60623	0.64883
C	0.19948	0.90017	4.42892
H	-0.21042	1.73005	4.99514
C	2.72364	0.67457	-0.70704
C	0.31999	-0.34604	5.03109
H	0.01573	-0.47614	6.06471
C	0.81526	-1.43346	4.31814
H	0.88958	-2.40156	4.80289
C	0.44525	2.46756	2.45555
H	0.87876	2.42354	1.45053
C	0.98388	0.18135	-2.44503
C	0.17256	1.22596	-2.90028
C	1.36579	-0.92051	-3.22942
C	-0.00462	0.02169	-4.99468
H	-0.40073	-0.04628	-6.00306

C	0.84807	-0.97398	-4.52251
H	1.11508	-1.79549	-5.17784
C	-0.09010	2.47976	-2.07838
H	0.37380	2.35437	-1.09465
C	2.29626	-2.00242	-2.68816
H	3.02116	-1.51688	-2.02679
C	-3.53781	-0.31161	-1.33355
C	-1.80584	-1.60267	-2.21044
H	-0.82530	-2.02118	-2.03217
C	-4.25825	-0.46297	-2.53988
H	-5.23934	-0.01048	-2.63474
C	-3.72096	-1.21350	-3.56055
H	-4.27625	-1.34291	-4.48378
C	-3.85852	0.28373	1.07586
C	-4.53547	0.66184	3.35765
H	-5.24726	1.05094	4.07340
C	-4.76817	0.78490	1.97008
H	-5.67268	1.26014	1.60183
C	-2.47175	-1.82658	-3.39233
H	-2.02194	-2.43836	-4.16311
C	-3.39885	-0.04976	3.76502
H	-3.20749	-0.24121	4.81586
C	-1.58331	2.73270	-1.84249
H	-1.72068	3.65158	-1.26500
H	-2.04835	1.91491	-1.28576
H	-2.12494	2.84927	-2.78690
C	-0.33287	1.10988	-4.19853
H	-0.97311	1.89133	-4.59601
C	3.10607	-2.70012	-3.78537

H	3.61891	-1.97910	-4.42803
H	2.47631	-3.33730	-4.41504
H	3.86211	-3.34563	-3.33008
C	1.21775	3.54336	3.23179
H	1.16825	4.49781	2.69955
H	2.27023	3.27173	3.35244
H	0.79147	3.69936	4.22768
C	-1.03496	2.84929	2.30183
H	-1.58668	2.11731	1.70370
H	-1.12235	3.82553	1.81510
H	-1.53331	2.91002	3.27416
C	1.71988	-2.48880	2.19480
H	2.15662	-2.12162	1.25989
C	0.58081	3.69169	-2.74391
H	1.64847	3.51610	-2.90440
H	0.46896	4.57950	-2.11443
H	0.12564	3.91008	-3.71530
C	1.54140	-3.04092	-1.84218
H	0.80648	-3.58091	-2.44999
H	1.02465	-2.58316	-0.99190
H	2.24288	-3.77907	-1.44107
C	2.82209	-3.25957	2.93179
H	3.64420	-2.59744	3.21737
H	3.22273	-4.04636	2.28593
H	2.44337	-3.74185	3.83813
C	-2.51725	-0.54822	2.83906
H	-1.65278	-1.13485	3.12356
C	0.54626	-3.40942	1.82685
H	0.07081	-3.81755	2.72435

H	0.89184	-4.24773	1.21431
H	-0.22562	-2.87433	1.25975
Cl	4.02555	0.97118	1.72500
Cl	3.90432	1.19434	-1.80885

Calculated XYZ coordinates for complex **10** at T₁ state

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diCl-IPr_L1_modify_triplet.out Energy: -1774183.2904177

Cu	-0.56753	1.00061	-0.61304
N	0.44037	2.67220	-0.51727
N	-2.19620	1.89456	-1.00678
N	1.58475	-1.13429	0.16251
N	-0.48322	-1.65736	0.49131
N	-1.52685	3.86381	0.15234
H	-1.85601	4.70254	0.61023
C	-1.92598	-1.56124	0.50889
C	0.31925	-0.67107	0.00709
C	-2.52727	-0.83636	1.55316
C	-2.64345	-2.20141	-0.52290
C	0.26775	-2.72901	0.95418
C	-3.92329	-0.71583	1.51383
H	-4.43289	-0.15420	2.28998
C	1.57637	-2.40514	0.73368
C	-4.66422	-1.31561	0.49967
H	-5.74463	-1.20891	0.48823
C	-4.03388	-2.05973	-0.50063
H	-4.63537	-2.52947	-1.27069
C	-1.73009	-0.23750	2.70659
H	-0.66906	-0.44947	2.54303
C	2.78437	-0.43255	-0.22948
C	3.50472	0.25151	0.76822
C	3.16224	-0.48217	-1.58162
C	5.05236	0.92528	-0.98409
H	5.94671	1.46472	-1.28187

C	4.31721	0.22718	-1.94044
H	4.64352	0.23178	-2.97520
C	3.02520	0.28707	2.21700
H	2.52576	-0.66524	2.42795
C	2.34016	-1.21273	-2.63648
H	1.59176	-1.82777	-2.12629
C	-0.15961	3.79423	0.02158
C	1.77984	2.72750	-0.80317
H	2.18528	1.85801	-1.29975
C	0.62786	4.88993	0.43705
H	0.13857	5.73574	0.91311
C	1.98693	4.90308	0.20007
H	2.58884	5.75243	0.50327
C	-2.53084	3.08056	-0.37823
C	-4.87215	2.76048	-0.89601
H	-5.90465	3.08476	-0.83921
C	-3.86877	3.49022	-0.27753
H	-4.09983	4.40769	0.25783
C	2.57224	3.79595	-0.48203
H	3.62354	3.77442	-0.74059
C	-4.50692	1.59676	-1.64091
H	-5.24846	1.01196	-2.17284
C	1.98543	1.40972	2.42408
H	1.63142	1.40870	3.46041
H	1.12015	1.28809	1.76788
H	2.42366	2.38924	2.20917
C	4.65374	0.93378	0.35393
H	5.24381	1.48205	1.07896
C	3.19659	-2.16614	-3.48945

H	3.74659	-2.87303	-2.86060
H	3.92248	-1.62271	-4.10275
H	2.55630	-2.73746	-4.16929
C	-2.12469	-0.90027	4.04152
H	-1.49734	-0.51766	4.85321
H	-2.00238	-1.98691	3.99512
H	-3.16831	-0.68957	4.29697
C	-1.87844	1.29325	2.77652
H	-1.52303	1.77470	1.86115
H	-1.29480	1.69099	3.61263
H	-2.92241	1.59001	2.91845
C	-1.92900	-2.97913	-1.62503
H	-0.99296	-3.36738	-1.21051
C	4.17165	0.41652	3.23283
H	4.94756	-0.33624	3.06255
H	3.78281	0.28250	4.24691
H	4.63879	1.40619	3.19484
C	1.58352	-0.20090	-3.52076
H	2.28153	0.45154	-4.05538
H	0.92428	0.44123	-2.92401
H	0.96780	-0.72022	-4.26165
C	-2.72639	-4.19483	-2.12504
H	-3.03134	-4.84018	-1.29582
H	-2.11013	-4.78586	-2.80956
H	-3.62498	-3.89630	-2.67468
C	-3.19851	1.20930	-1.66837
H	-2.88098	0.31339	-2.18670
C	-1.55563	-2.05128	-2.79949
H	-2.45542	-1.66866	-3.29348

H	-0.96957	-2.59558	-3.54722
H	-0.95698	-1.19699	-2.46546
Cl	-0.42346	-4.12720	1.63750
Cl	2.99209	-3.29630	1.04989

Calculated XYZ coordinates for complex **11** at S₀ state

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Cu	0.049080	0.483550	0.055400
N	1.512650	1.749991	-0.369500
N	-1.502480	1.606560	-0.573950
N	0.997251	-2.322700	0.300010
N	-1.015299	-2.080340	1.010670
N	-0.131700	3.360250	0.285650
H	-0.201720	4.298440	0.654830
C	-2.302449	-1.495180	1.291060
C	0.009911	-1.391210	0.429650
C	-2.426029	-0.620380	2.385750
C	-3.372669	-1.818991	0.429870
C	-0.664889	-3.399510	1.266390
H	-1.345639	-4.092410	1.734840
C	-3.676249	-0.015681	2.581440
H	-3.813480	0.670529	3.411600
C	0.606481	-3.553880	0.814270
H	1.261652	-4.410379	0.802590
C	-4.746089	-0.292671	1.735360
H	-5.702469	0.196689	1.886260
C	-4.599389	-1.195031	0.680260
H	-5.450629	-1.402191	0.043070
C	-1.284039	-0.343610	3.358750
H	-0.397359	-0.883790	3.016230
C	2.288941	-2.075759	-0.292030
C	3.372591	-1.830339	0.575360
C	2.419631	-2.140599	-1.692970
C	4.795841	-1.711259	-1.395630

H	5.782521	-1.576208	-1.829230
C	3.702291	-1.942119	-2.225270
H	3.847491	-1.985889	-3.299920
C	3.162281	-1.701929	2.082340
H	2.328471	-2.354549	2.362560
C	1.246941	-2.430839	-2.623090
H	0.373531	-2.671520	-2.011470
C	1.190110	2.981691	0.068750
C	2.817210	1.472061	-0.586750
H	3.032210	0.470361	-0.942110
C	2.172200	3.954611	0.349390
H	1.882139	4.935381	0.713270
C	3.502850	3.651771	0.139420
H	4.276210	4.384371	0.341500
C	-1.359320	2.874960	-0.155250
C	-3.685240	3.358899	-0.553910
H	-4.531530	4.038209	-0.546950
C	-2.445880	3.775970	-0.112210
H	-2.300651	4.791370	0.243240
C	3.836480	2.383641	-0.352720
C	-3.828210	2.045579	-1.022980
C	2.744851	-0.259399	2.441940
H	2.542941	-0.177229	3.515670
H	1.841971	0.040981	1.900610
H	3.545860	0.444031	2.190620
C	4.631461	-1.651279	-0.010760
H	5.494831	-1.459348	0.614280
C	1.513831	-3.649909	-3.525910
H	1.773212	-4.533149	-2.933570

H	2.332411	-3.463739	-4.228520
H	0.620821	-3.882740	-4.115590
C	-1.623919	-0.866040	4.768630
H	-0.772589	-0.720920	5.442370
H	-1.866099	-1.933400	4.747660
H	-2.482529	-0.336610	5.195300
C	-0.915510	1.151010	3.400340
H	-0.618880	1.510440	2.410290
H	-0.078450	1.316930	4.086690
H	-1.758340	1.762070	3.741700
C	-3.184869	-2.787070	-0.739050
H	-2.448249	-3.536540	-0.431380
C	4.377401	-2.141639	2.915310
H	4.719481	-3.142059	2.631600
H	4.111411	-2.159999	3.977020
H	5.219221	-1.450099	2.805560
C	0.900071	-1.190010	-3.469100
H	1.743871	-0.899709	-4.104450
H	0.650011	-0.332390	-2.832930
H	0.040731	-1.393390	-4.116570
C	-4.464759	-3.549511	-1.117700
H	-4.919799	-4.032121	-0.246890
H	-4.228358	-4.325491	-1.852630
H	-5.211929	-2.891341	-1.573280
C	-2.721800	1.213060	-1.001300
H	-2.794929	0.184620	-1.320080
C	-2.603099	-2.069030	-1.975590
H	-3.334579	-1.369601	-2.393820
H	-2.356539	-2.796540	-2.756510

H	-1.689289	-1.518430	-1.731410
C	5.273360	1.992881	-0.566270
C	-5.169040	1.571399	-1.512320
F	-6.073380	1.498419	-0.501750
F	-5.682890	2.425369	-2.427980
F	-5.103560	0.347389	-2.084580
F	6.073930	3.074112	-0.692160
F	5.425490	1.234981	-1.674230
F	5.748080	1.268632	0.482960

Calculated XYZ coordinates for complex **11** at S₁ state

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IPr_3-diCF3-L2_optS1.out Energy: -1619947.0903797

Cu	0.32903	-0.39351	0.24746
N	1.54084	-1.83782	0.43655
N	-1.25493	-1.57048	0.35784
N	0.89931	2.35991	-0.23327
N	-1.12075	2.08780	-0.88468
N	0.00986	-3.35229	-0.57129
H	-0.07233	-4.24194	-1.04216
C	-2.38391	1.47043	-1.19035
C	-0.09597	1.45310	-0.28377
C	-2.41919	0.55277	-2.24732
C	-3.50361	1.82736	-0.41767
C	-0.76634	3.38142	-1.21703
H	-1.44937	4.04531	-1.72226
C	-3.63997	-0.08329	-2.48855
H	-3.71909	-0.80627	-3.29427
C	0.51109	3.55816	-0.79813
H	1.17592	4.40511	-0.85528
C	-4.76064	0.21830	-1.72830
H	-5.70095	-0.28466	-1.92768
C	-4.69817	1.17555	-0.71910
H	-5.59589	1.40318	-0.15758
C	-1.23423	0.32251	-3.17635
H	-0.34753	0.79478	-2.74270
C	2.21103	2.05263	0.27546
C	3.18715	1.62311	-0.63855
C	2.44010	2.19767	1.65333

C	4.72257	1.49877	1.23292
H	5.71519	1.27995	1.61040
C	3.72600	1.90790	2.11259
H	3.95510	2.00554	3.16842
C	2.89328	1.43108	-2.12022
H	1.94812	1.93221	-2.35393
C	1.33366	2.60519	2.61452
H	0.52294	3.05654	2.03281
C	1.31345	-2.97304	-0.31540
C	2.81152	-1.62112	0.90395
H	2.94195	-0.75711	1.54869
C	2.37788	-3.77624	-0.75409
H	2.17468	-4.62743	-1.39764
C	3.65653	-3.51130	-0.33719
H	4.48591	-4.13314	-0.64942
C	-1.17465	-2.83288	-0.15218
C	-3.52199	-3.17756	0.26391
H	-4.41821	-3.78597	0.20945
C	-2.35130	-3.62401	-0.26873
H	-2.29150	-4.59817	-0.74341
C	3.85915	-2.42271	0.57436
C	-3.55000	-1.91548	0.92249
C	2.71792	-0.05896	-2.45398
H	2.54974	-0.18968	-3.52737
H	1.86161	-0.49803	-1.93047
H	3.60483	-0.63578	-2.17265
C	4.45364	1.34579	-0.12161
H	5.24050	1.00039	-0.78281
C	1.79127	3.65435	3.63508

H	2.24460	4.51887	3.14228
H	2.51928	3.24714	4.34342
H	0.93372	4.00390	4.21715
C	-1.49494	1.00971	-4.52626
H	-0.62761	0.90127	-5.18476
H	-1.69436	2.07755	-4.39500
H	-2.36031	0.56692	-5.02984
C	-0.89790	-1.15952	-3.36968
H	-0.67528	-1.64685	-2.41723
H	-0.02063	-1.26190	-4.01546
H	-1.72100	-1.70543	-3.84134
C	-3.41461	2.89448	0.67363
H	-2.83591	3.72898	0.26109
C	3.96831	2.06717	-3.01101
H	4.12336	3.12055	-2.76089
H	3.66613	2.00595	-4.06046
H	4.92950	1.55285	-2.91839
C	0.76280	1.36757	3.32498
H	1.53651	0.85967	3.90969
H	0.35491	0.63946	2.61150
H	-0.04768	1.65061	4.00314
C	-4.77878	3.46481	1.07258
H	-5.34013	3.82177	0.20451
H	-4.63683	4.30946	1.75241
H	-5.38849	2.72429	1.59998
C	-2.41422	-1.15378	0.91662
H	-2.39826	-0.16689	1.36110
C	-2.66967	2.41029	1.93018
H	-3.24155	1.63176	2.44259

H	-2.54400	3.24099	2.63136
H	-1.67365	2.01844	1.70389
C	5.22662	-2.16332	1.12267
C	-4.79605	-1.48684	1.62876
F	-5.86581	-1.47471	0.80553
F	-5.10317	-2.33057	2.63346
F	-4.69046	-0.25511	2.16431
F	5.84444	-3.30426	1.47354
F	5.20509	-1.36720	2.20898
F	6.03014	-1.55955	0.21208

Calculated XYZ coordinates for complex **11** at T₁ state

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IPr_3-diCF3-L2_B3LYP-D3_TD.out Energy: -1620413.9406764

Cu	0.31100	-0.37717	0.16604
N	1.64493	-1.72201	0.38229
N	-1.15834	-1.65513	0.46764
N	0.66446	2.40302	-0.43539
N	-1.34647	1.93899	-1.04218
N	0.18935	-3.44706	-0.37173
H	0.14747	-4.37730	-0.76640
C	-2.57335	1.21466	-1.28034
C	-0.25780	1.40922	-0.43067
C	-2.56758	0.23517	-2.28834
C	-3.70149	1.52720	-0.48965
C	-1.09994	3.24636	-1.43580
H	-1.84110	3.83121	-1.95658
C	-3.73822	-0.52081	-2.44399
H	-3.77723	-1.29598	-3.20289
C	0.17071	3.54345	-1.04708
H	0.76371	4.43783	-1.15449
C	-4.85610	-0.27484	-1.65283
H	-5.75214	-0.87429	-1.77872
C	-4.84475	0.75115	-0.70528
H	-5.73732	0.93149	-0.12013
C	-1.39503	0.03876	-3.24667
H	-0.59041	0.72192	-2.95888
C	2.00850	2.22552	0.06616
C	3.00984	1.83756	-0.84790
C	2.24700	2.45520	1.43715

C	4.58314	1.93128	1.00418
H	5.59559	1.80907	1.37348
C	3.56364	2.29261	1.88584
H	3.79717	2.45208	2.93306
C	2.71598	1.54572	-2.31550
H	1.67916	1.82720	-2.52463
C	1.12425	2.81588	2.40298
H	0.26190	3.14585	1.81531
C	1.46875	-2.95883	-0.22193
C	2.91489	-1.36429	0.75807
H	3.00371	-0.42372	1.29113
C	2.57254	-3.72610	-0.63284
H	2.40477	-4.65980	-1.16278
C	3.85259	-3.32387	-0.31265
H	4.71435	-3.91585	-0.59464
C	-1.01987	-2.96869	0.06431
C	-3.33070	-3.42273	0.61053
H	-4.18485	-4.08893	0.65092
C	-2.13675	-3.83864	0.07885
H	-2.02257	-4.85049	-0.29978
C	4.01243	-2.12416	0.45982
C	-3.41918	-2.09732	1.13981
C	2.84807	0.03747	-2.60950
H	2.62119	-0.16557	-3.66109
H	2.16060	-0.55208	-1.99442
H	3.86173	-0.31995	-2.40334
C	4.30759	1.69623	-0.34191
H	5.10967	1.38436	-1.00152
C	1.49871	3.97378	3.34562

H	1.84143	4.84881	2.78484
H	2.29033	3.68964	4.04608
H	0.62751	4.26694	3.93978
C	-1.81042	0.41318	-4.68432
H	-0.94924	0.34826	-5.35772
H	-2.20605	1.43275	-4.73025
H	-2.58401	-0.26267	-5.06325
C	-0.81732	-1.38581	-3.19567
H	-0.44322	-1.62940	-2.19884
H	0.01429	-1.48350	-3.90072
H	-1.57147	-2.13539	-3.45702
C	-3.67947	2.67434	0.52796
H	-3.18529	3.52337	0.04104
C	3.60958	2.37609	-3.25595
H	3.51883	3.44733	-3.04943
H	3.32214	2.20253	-4.29787
H	4.66449	2.10274	-3.15438
C	0.68983	1.57363	3.20799
H	1.52255	1.18072	3.80053
H	0.34038	0.76702	2.55047
H	-0.13020	1.82129	3.88936
C	-5.08171	3.15877	0.92957
H	-5.69376	3.40193	0.05562
H	-4.99539	4.06040	1.54346
H	-5.61248	2.40934	1.52575
C	-2.33506	-1.26354	1.02322
H	-2.37372	-0.23960	1.36530
C	-2.86028	2.34896	1.79674
H	-3.35822	1.57973	2.39199

H	-2.77148	3.24452	2.42053
H	-1.84793	2.00781	1.56572
C	5.38289	-1.69137	0.87601
C	-4.67626	-1.67684	1.83096
F	-5.77115	-1.84982	1.04066
F	-4.90108	-2.41246	2.95021
F	-4.65944	-0.37317	2.20950
F	6.15253	-2.74395	1.23846
F	5.36259	-0.82269	1.91744
F	6.05106	-1.06395	-0.14023

Calculated XYZ coordinates for complex **12** at S₀ state

94

IPr_4-diCF3-L3_modify.out Energy: -1620472.7322958

Cu	-0.00012	-0.16534	0.41443
N	-1.45563	1.30819	0.72899
N	1.45630	1.30781	0.72824
N	-1.07281	-2.72701	-0.60137
N	1.07211	-2.72727	-0.60165
N	0.00041	3.09711	0.15099
H	0.00049	4.06862	-0.12662
C	2.44761	-2.32408	-0.44995
C	-0.00020	-1.95795	-0.25433
C	3.04211	-1.57675	-1.48312
C	3.12676	-2.69966	0.72570
C	0.67881	-3.93875	-1.15605
H	1.39451	-4.67275	-1.49083
C	4.37987	-1.19604	-1.30764
H	4.87494	-0.61167	-2.07667
C	-0.67995	-3.93858	-1.15587
H	-1.39591	-4.67248	-1.49030
C	5.08526	-1.55907	-0.16150
H	6.12524	-1.26484	-0.05187
C	4.46530	-2.30104	0.84545
H	5.02854	-2.56974	1.73274
C	2.27917	-1.16477	-2.73719
H	1.30916	-1.67067	-2.72866
C	-2.44816	-2.32357	-0.44908
C	-3.04293	-1.57605	-1.48197
C	-3.12694	-2.69908	0.72680

C	-5.08559	-1.55813	-0.15959
H	-6.12548	-1.26373	-0.04958
C	-4.46538	-2.30027	0.84706
H	-5.02833	-2.56895	1.73454
C	-2.28039	-1.16414	-2.73631
H	-1.31041	-1.67009	-2.72809
C	-2.41666	-3.43007	1.86079
H	-1.53197	-3.92326	1.44542
C	-1.27280	2.59891	0.40571
C	-2.71610	0.88897	0.98622
H	-2.81409	-0.15595	1.24636
C	-2.35171	3.50064	0.28346
H	-2.18264	4.53661	0.01043
C	-3.63162	3.03851	0.52853
C	1.27358	2.59870	0.40560
C	3.63244	3.03808	0.52865
C	2.35255	3.50043	0.28387
H	2.18354	4.53656	0.01145
C	-3.82984	1.70379	0.90413
H	-4.81676	1.30806	1.10782
C	3.83055	1.70312	0.90349
H	4.81743	1.30717	1.10692
C	-2.00107	0.35208	-2.73473
H	-1.44734	0.63871	-3.63485
H	-1.40666	0.63758	-1.86183
H	-2.93459	0.92509	-2.71299
C	-4.38054	-1.19512	-1.30596
H	-4.87580	-0.61058	-2.07475
C	-3.28056	-4.52028	2.51659

H	-3.67232	-5.22187	1.77337
H	-4.12959	-4.09648	3.06296
H	-2.68222	-5.08560	3.23814
C	3.00810	-1.59632	-4.02337
H	2.39520	-1.36141	-4.89975
H	3.20896	-2.67241	-4.02483
H	3.96436	-1.07636	-4.14139
C	1.99996	0.35148	-2.73543
H	1.40594	0.63702	-1.86229
H	1.44589	0.63819	-3.63533
H	2.93356	0.92438	-2.71406
C	2.41674	-3.43047	1.85996
H	1.53192	-3.92366	1.44488
C	-3.00983	-1.59575	-4.02219
H	-3.21067	-2.67184	-4.02351
H	-2.39731	-1.36086	-4.89884
H	-3.96616	-1.07582	-4.13980
C	-1.92191	-2.40966	2.90813
H	-2.76677	-1.87616	3.35824
H	-1.25141	-1.67186	2.45371
H	-1.37370	-2.91426	3.71032
C	3.28075	-4.52066	2.51566
H	3.67233	-5.22229	1.77240
H	2.68254	-5.08592	3.23737
H	4.12990	-4.09684	3.06184
C	2.71674	0.88836	0.98520
H	2.81464	-0.15669	1.24482
C	1.92227	-2.40989	2.90727
H	2.76723	-1.87627	3.35706

H	1.37428	-2.91435	3.70970
H	1.25163	-1.67221	2.45288
C	-4.83043	3.94787	0.36331
C	4.83132	3.94748	0.36428
F	-5.55494	3.57707	-0.72052
F	-4.47468	5.23876	0.19466
F	-5.64693	3.87803	1.43664
F	4.47563	5.23826	0.19465
F	5.64662	3.87822	1.43857
F	5.55708	3.57626	-0.71856

Calculated XYZ coordinates for complex **12** at S₁ state

94

IPr_4-diCF3-L3_optS1.out Energy: -1619943.4072819

Cu	0.03732	-0.28584	-0.42955
N	1.21894	-0.47991	1.16973
N	1.48849	0.08944	-1.54402
N	-2.66635	-0.10469	1.07181
N	-2.73536	-0.29266	-1.05954
N	2.77702	1.02574	0.22938
H	3.56094	1.62335	0.44556
C	-2.29338	-0.40280	-2.42710
C	-1.88616	-0.29376	-0.01192
C	-2.04219	0.78116	-3.13859
C	-2.13818	-1.68820	-2.97247
C	-4.03833	-0.09975	-0.64686
H	-4.85905	-0.06287	-1.34519
C	-1.63418	0.64369	-4.46696
H	-1.41824	1.53070	-5.05361
C	-3.99296	0.02570	0.70222
H	-4.76929	0.19931	1.43018
C	-1.49062	-0.61075	-5.04599
H	-1.17907	-0.69346	-6.08233
C	-1.72980	-1.76454	-4.30494
H	-1.59814	-2.73467	-4.77240
C	-2.17284	2.16168	-2.51259
H	-2.61436	2.05070	-1.51667
C	-2.16781	0.02671	2.41555
C	-1.53789	1.22813	2.76409
C	-2.34190	-1.05169	3.30166

C	-1.09990	0.24419	4.93513
H	-0.66528	0.32432	5.92618
C	-1.79097	-0.91059	4.57483
H	-1.89996	-1.70770	5.30166
C	-1.51712	2.44732	1.85049
H	-2.03358	2.19700	0.91857
C	-3.09379	-2.31468	2.88673
H	-3.92422	-2.00815	2.24191
C	2.33011	0.27845	1.27135
C	0.85511	-1.27762	2.19692
H	-0.02330	-1.88453	2.02818
C	3.02906	0.34171	2.50506
H	3.89211	0.99033	2.60319
C	2.61369	-0.44146	3.54778
C	2.49457	0.93868	-1.14305
C	2.97560	1.56617	-3.40913
C	3.21493	1.69808	-2.03534
H	3.97986	2.37885	-1.67598
C	1.51731	-1.31198	3.39429
H	1.18204	-1.95965	4.19319
C	2.03795	0.59290	-3.83628
H	1.87425	0.40119	-4.89054
C	-0.09590	2.88364	1.47596
H	-0.12739	3.79217	0.86761
H	0.42317	2.11649	0.89593
H	0.50722	3.09546	2.36508
C	-0.98376	1.30269	4.04554
H	-0.47532	2.20940	4.35868
C	-3.71155	-3.06499	4.07091

H	-4.30699	-2.40181	4.70471
H	-2.94910	-3.54310	4.69444
H	-4.36775	-3.85774	3.70133
C	-3.11287	3.06351	-3.32416
H	-3.25561	4.01773	-2.80890
H	-4.09328	2.59779	-3.46157
H	-2.70222	3.28360	-4.31418
C	-0.79343	2.81552	-2.33441
H	-0.13314	2.20792	-1.70680
H	-0.90125	3.79774	-1.86433
H	-0.28848	2.95271	-3.29549
C	-2.35052	-2.94549	-2.14299
H	-2.93027	-2.67546	-1.25354
C	-2.29480	3.60568	2.49484
H	-3.31170	3.30258	2.76083
H	-2.35949	4.44737	1.79884
H	-1.80163	3.96229	3.40444
C	-2.21262	-3.26480	2.05891
H	-1.36489	-3.62504	2.65304
H	-1.82716	-2.78774	1.15164
H	-2.79087	-4.14037	1.74828
C	-3.14588	-4.02335	-2.88989
H	-4.08425	-3.62386	-3.28460
H	-3.38332	-4.84737	-2.21107
H	-2.57857	-4.44414	-3.72553
C	1.33947	-0.11983	-2.91341
H	0.61253	-0.86877	-3.20421
C	-0.99849	-3.49973	-1.66545
H	-0.36246	-3.76775	-2.51514

H	-1.14287	-4.39437	-1.05233
H	-0.44867	-2.76848	-1.05890
C	3.31651	-0.38282	4.88540
C	3.65521	2.43765	-4.40392
F	2.47047	0.05918	5.83575
F	4.37445	0.43759	4.87004
F	3.73951	-1.59909	5.25888
F	4.70141	3.10089	-3.87396
F	4.11161	1.74274	-5.46745
F	2.81834	3.38167	-4.91344

Calculated XYZ coordinates for complex **12** at T₁ state

94

IPr_4-diCF3-L3_modify_triplet.out Energy: -1620411.3865497

Cu	0.33305	-0.10486	0.44139
N	-1.09849	1.17811	0.83824
N	1.68365	1.16557	0.81346
N	-1.37672	-2.29775	-0.93569
N	0.64292	-2.82303	-0.41129
N	0.30011	3.02854	0.27472
H	0.29512	4.00197	0.00149
C	1.99613	-2.70160	0.08357
C	-0.27386	-1.82894	-0.29788
C	2.98693	-2.23185	-0.80259
C	2.25122	-3.05767	1.42411
C	0.13273	-3.90070	-1.11639
H	0.71835	-4.78445	-1.31416
C	4.29206	-2.14029	-0.30204
H	5.08549	-1.77555	-0.94581
C	-1.14233	-3.56465	-1.45374
H	-1.89559	-4.09621	-2.01312
C	4.58453	-2.49884	1.01324
H	5.60442	-2.42316	1.37844
C	3.57438	-2.94115	1.86974
H	3.81908	-3.19994	2.89438
C	2.67413	-1.79926	-2.23088
H	1.62748	-2.03894	-2.44309
C	-2.60130	-1.55012	-1.11187
C	-2.59601	-0.49233	-2.03845
C	-3.73224	-1.92342	-0.35226

C	-4.88988	-0.03896	-1.37437
H	-5.78580	0.56805	-1.46138
C	-4.87797	-1.13542	-0.50858
H	-5.77579	-1.37261	0.05011
C	-1.41838	-0.21362	-2.96947
H	-0.60884	-0.90734	-2.72415
C	-3.70543	-3.12416	0.59842
H	-3.12123	-3.91481	0.11500
C	-0.93465	2.51511	0.57672
C	-2.32078	0.72933	1.24247
H	-2.36876	-0.32228	1.47866
C	-2.05281	3.37914	0.57922
H	-1.92627	4.42379	0.31446
C	-3.28952	2.89268	0.93969
C	1.56627	2.48001	0.40266
C	3.96171	2.74004	0.36238
C	2.69091	3.25895	0.13046
H	2.57218	4.27567	-0.23058
C	-3.42671	1.52952	1.32461
H	-4.37669	1.12346	1.64519
C	4.08037	1.42566	0.91573
H	5.04840	1.01105	1.16958
C	-0.85568	1.20948	-2.81009
H	-0.01997	1.36454	-3.49958
H	-0.49109	1.38330	-1.79506
H	-1.61423	1.96919	-3.02456
C	-3.76891	0.26976	-2.13873
H	-3.80744	1.10414	-2.83193
C	-5.09794	-3.71533	0.87250

H	-5.63940	-3.92388	-0.05530
H	-5.71199	-3.04578	1.48406
H	-4.99687	-4.65427	1.42509
C	3.53114	-2.55896	-3.26109
H	3.23251	-2.28026	-4.27666
H	3.41607	-3.64253	-3.15553
H	4.59426	-2.32189	-3.15340
C	2.83378	-0.27328	-2.39003
H	2.18531	0.27394	-1.69802
H	2.57565	0.02869	-3.41015
H	3.86251	0.04354	-2.19254
C	1.13916	-3.49594	2.37053
H	0.25693	-3.74179	1.77063
C	-1.81875	-0.48663	-4.43401
H	-2.19803	-1.50583	-4.55924
H	-0.95394	-0.35855	-5.09345
H	-2.59987	0.20420	-4.76759
C	-2.99797	-2.79816	1.93122
H	-3.54792	-2.02898	2.48516
H	-1.97131	-2.45063	1.77973
H	-2.95400	-3.69139	2.56303
C	1.50616	-4.75631	3.17494
H	1.80945	-5.57549	2.51571
H	0.64355	-5.08923	3.76063
H	2.32393	-4.56741	3.87743
C	2.94946	0.69615	1.12443
H	2.98654	-0.31073	1.52230
C	0.75112	-2.33689	3.31187
H	1.60146	-2.03378	3.93147

H	-0.06634	-2.63547	3.97585
H	0.41865	-1.45343	2.75200
C	-4.51223	3.76738	0.91113
C	5.19441	3.50934	0.01907
F	-5.38267	3.34767	-0.04928
F	-4.22093	5.06025	0.65158
F	-5.18172	3.72124	2.08707
F	4.93232	4.80360	-0.28022
F	6.10014	3.49585	1.03108
F	5.83458	2.97401	-1.06455

Calculated XYZ coordinates for complex **13** at S₀ state

96

IPr_4-diOMe-L4_modify.outEnergy: -1341211.8615362

Cu	0.00422	0.26660	0.31901
N	-1.44062	1.74537	0.57781
N	1.48008	1.71145	0.58762
N	-1.08755	-2.36948	-0.47246
N	1.05303	-2.34847	-0.58106
N	0.04314	3.49492	-0.05542
H	0.05627	4.46563	-0.33432
C	2.42897	-1.92525	-0.52340
C	-0.01048	-1.56610	-0.22925
C	2.94766	-1.19030	-1.60441
C	3.18666	-2.27259	0.61290
C	0.64880	-3.59656	-1.03877
H	1.35643	-4.34245	-1.36411
C	4.28799	-0.78835	-1.51940
H	4.72447	-0.21267	-2.32958
C	-0.70755	-3.61077	-0.96787
H	-1.42973	-4.37155	-1.21815
C	5.06878	-1.12285	-0.41494
H	6.10972	-0.81429	-0.37606
C	4.52488	-1.85789	0.64009
H	5.14795	-2.10723	1.49218
C	2.10849	-0.82592	-2.82382
H	1.13567	-1.31669	-2.72722
C	-2.45928	-1.97690	-0.27617
C	-3.12917	-1.33861	-1.33583
C	-3.06193	-2.25492	0.96592

C	-5.09777	-1.24928	0.09146
H	-6.13850	-0.97136	0.23286
C	-4.40274	-1.87845	1.12536
H	-4.90706	-2.07374	2.06590
C	-2.43955	-1.01016	-2.65530
H	-1.46383	-1.50490	-2.66190
C	-2.27110	-2.85571	2.12236
H	-1.37236	-3.32577	1.71094
C	-1.23925	3.03923	0.24935
C	-2.70708	1.37444	0.86474
H	-2.83509	0.33376	1.12944
C	-2.28548	3.96611	0.16814
H	-2.10631	5.00371	-0.09287
C	-3.58954	3.55370	0.44744
C	1.30532	3.01850	0.29902
C	3.64963	3.49945	0.61679
C	2.36185	3.93691	0.30077
H	2.20287	4.98626	0.07629
C	-3.80623	2.21292	0.81894
H	-4.78548	1.81742	1.05030
C	3.83894	2.14173	0.93737
H	4.80509	1.72580	1.18742
C	-2.18155	0.50570	-2.77277
H	-1.67343	0.73296	-3.71596
H	-1.55560	0.86304	-1.95013
H	-3.12235	1.06676	-2.74980
C	-4.46573	-0.97606	-1.12068
H	-5.01661	-0.47457	-1.90992
C	-3.04701	-3.94327	2.88464

H	-3.41198	-4.72321	2.20874
H	-3.90791	-3.53098	3.42130
H	-2.39597	-4.41255	3.62917
C	2.74843	-1.33639	-4.12871
H	2.08537	-1.13533	-4.97673
H	2.93282	-2.41477	-4.08654
H	3.70350	-0.84055	-4.33209
C	1.84689	0.69173	-2.88523
H	1.32458	1.03600	-1.98817
H	1.23083	0.93556	-3.75715
H	2.78480	1.25219	-2.96575
C	2.55431	-2.99175	1.80024
H	1.69106	-3.55590	1.43321
C	-3.22698	-1.53855	-3.86849
H	-3.41383	-2.61409	-3.78532
H	-2.66236	-1.35965	-4.78944
H	-4.19466	-1.03693	-3.97387
C	-1.80650	-1.73323	3.07412
H	-2.66727	-1.21695	3.51390
H	-1.19827	-0.99286	2.54315
H	-1.20395	-2.14549	3.89014
C	3.49763	-3.99788	2.47948
H	3.91980	-4.70369	1.75704
H	2.94930	-4.56938	3.23518
H	4.32747	-3.50004	2.99201
C	2.73059	1.31453	0.90542
H	2.83805	0.26179	1.12756
C	2.02412	-1.95716	2.81622
H	2.84792	-1.36134	3.22567

H	1.52201	-2.45897	3.65007
H	1.30624	-1.27527	2.34862
O	-4.54659	4.49285	0.34443
O	4.61833	4.43202	0.59510
C	5.95918	4.05440	0.93629
H	6.54762	4.96771	0.85584
H	6.00897	3.67269	1.96213
H	6.34476	3.30510	0.23581
C	-5.90479	4.14230	0.64289
H	-6.00342	3.80843	1.68178
H	-6.47968	5.05587	0.49525
H	-6.26713	3.36505	-0.03930

Calculated XYZ coordinates for complex **13** at S₁ state

96

IPr_4-diOMe-L4_optS1.out Energy: -1340751.7368546

Cu	0.29802	-0.35334	0.50517
N	1.82631	-0.45959	1.68232
N	1.41958	-0.76742	-1.06765
N	-2.35118	0.35218	0.96704
N	-2.13094	0.49382	-1.19200
N	3.15751	0.44429	-0.04404
H	4.03266	0.91234	-0.22923
C	-1.60628	0.47166	-2.52112
C	-1.46699	0.08354	-0.05456
C	-0.60813	1.39821	-2.87693
C	-2.12317	-0.47744	-3.42389
C	-3.39083	0.98860	-0.85702
H	-4.06759	1.36308	-1.60868
C	-0.11901	1.34367	-4.18390
H	0.64901	2.04085	-4.50011
C	-3.52401	0.90746	0.48451
H	-4.33570	1.19180	1.13510
C	-0.61266	0.41869	-5.09600
H	-0.23175	0.40828	-6.11326
C	-1.60414	-0.48128	-4.72060
H	-1.98153	-1.18748	-5.45185
C	-0.10862	2.44318	-1.88837
H	-0.00968	1.95079	-0.91268
C	-1.93043	0.20639	2.32143
C	-1.27545	1.28955	2.93830
C	-2.14334	-1.02577	2.96532

C	-1.12782	-0.06388	4.94725
H	-0.83692	-0.16180	5.98894
C	-1.73791	-1.13347	4.29933
H	-1.90812	-2.06106	4.83767
C	-1.05090	2.61177	2.22032
H	-1.29838	2.47100	1.16425
C	-2.79031	-2.20126	2.25277
H	-3.08954	-1.86464	1.25592
C	3.01050	0.06726	1.29383
C	1.67460	-0.79592	2.98463
H	0.72353	-1.24516	3.24999
C	4.04027	0.29830	2.18633
H	4.98899	0.70879	1.86010
C	3.85375	-0.00197	3.54315
C	2.65176	-0.23354	-1.15292
C	2.85466	-0.94093	-3.43957
C	3.39580	-0.29645	-2.32151
H	4.38485	0.14212	-2.38649
C	2.63996	-0.57230	3.94605
H	2.43421	-0.84480	4.97245
C	1.60328	-1.56074	-3.32397
H	1.13264	-2.09140	-4.13945
C	0.41551	3.05868	2.27996
H	0.54898	3.97709	1.69963
H	1.07808	2.29299	1.86148
H	0.73925	3.26717	3.30515
C	-0.88420	1.12690	4.27087
H	-0.40040	1.94836	4.79056
C	-4.05198	-2.68483	2.97953

H	-4.77311	-1.87216	3.10784
H	-3.81983	-3.08897	3.97034
H	-4.53498	-3.48113	2.40520
C	-1.12553	3.58453	-1.72660
H	-0.75772	4.31608	-0.99894
H	-2.09421	3.22167	-1.37304
H	-1.28052	4.10196	-2.67938
C	1.27091	3.01059	-2.23334
H	1.99989	2.21782	-2.42972
H	1.63742	3.60780	-1.39284
H	1.23902	3.66931	-3.10809
C	-3.19178	-1.47848	-2.99124
H	-3.90573	-0.94706	-2.35403
C	-1.98880	3.69249	2.77726
H	-3.03712	3.39405	2.68049
H	-1.85191	4.63285	2.23459
H	-1.78937	3.88232	3.83730
C	-1.77864	-3.34132	2.06559
H	-1.43184	-3.73189	3.02887
H	-0.90547	-2.99660	1.49870
H	-2.23415	-4.16954	1.51391
C	-3.99043	-2.06447	-4.15915
H	-4.39562	-1.28253	-4.80823
H	-4.82891	-2.65029	-3.77217
H	-3.38262	-2.73881	-4.77236
C	0.93724	-1.44815	-2.12306
H	-0.03861	-1.89363	-1.98652
C	-2.58950	-2.60884	-2.14000
H	-1.86324	-3.18629	-2.72495

H	-3.37539	-3.29943	-1.81800
H	-2.09569	-2.22253	-1.24159
O	4.88314	0.27208	4.35044
O	3.60249	-0.93105	-4.54410
C	3.10379	-1.56932	-5.71593
H	3.86418	-1.41581	-6.47929
H	2.96536	-2.64171	-5.54575
H	2.16161	-1.11144	-6.03421
C	4.76893	-0.03219	5.73553
H	4.62476	-1.10687	5.88800
H	5.71158	0.27666	6.18331
H	3.94564	0.52768	6.19163

Calculated XYZ coordinates for complex **13** at T₁ state

96

IPr_4-diOMe-L4_modify_triplet.out Energy: -1341138.2475595

Cu	-0.50399	0.19927	0.30153
N	-1.91392	1.44729	0.61398
N	0.85508	1.53228	0.82016
N	-0.49254	-2.49819	-0.45922
N	1.53724	-1.81717	-0.83403
N	-0.51116	3.18517	-0.17090
H	-0.50912	4.12930	-0.53226
C	2.74436	-1.03582	-0.86472
C	0.35158	-1.43436	-0.24535
C	2.79892	0.09489	-1.70880
C	3.82047	-1.43619	-0.04108
C	1.40835	-3.09054	-1.39366
H	2.22650	-3.56320	-1.91297
C	3.97883	0.84898	-1.69264
H	4.06403	1.72864	-2.32013
C	0.13868	-3.51340	-1.16014
H	-0.36924	-4.42505	-1.43239
C	5.05601	0.48190	-0.88805
H	5.96673	1.07440	-0.90313
C	4.97996	-0.65004	-0.07699
H	5.83510	-0.92234	0.53079
C	1.64405	0.45077	-2.64093
H	0.70878	0.26557	-2.09905
C	-1.88499	-2.40474	-0.11428
C	-2.78110	-1.90537	-1.08479
C	-2.28451	-2.78584	1.18454

C	-4.56718	-2.24667	0.53392
H	-5.62343	-2.20040	0.78339
C	-3.65141	-2.69890	1.48555
H	-4.00362	-2.99170	2.46924
C	-2.32336	-1.46272	-2.46930
H	-1.23304	-1.53806	-2.50881
C	-1.27425	-3.22749	2.23575
H	-0.32680	-3.43034	1.72740
C	-1.78794	2.74701	0.21631
C	-3.16014	1.01555	0.99880
H	-3.21384	-0.00558	1.35363
C	-2.86774	3.60254	0.12990
H	-2.74523	4.63675	-0.17224
C	-4.16186	3.12549	0.45077
C	0.70077	2.81498	0.41117
C	2.97183	3.33471	1.04928
C	1.73737	3.73834	0.50793
H	1.60997	4.76405	0.18078
C	-4.29481	1.80583	0.90691
H	-5.24837	1.38501	1.19846
C	3.10236	2.02682	1.54042
H	4.01452	1.65615	1.98574
C	-2.68079	0.01229	-2.73753
H	-2.28608	0.32271	-3.71071
H	-2.25131	0.66424	-1.96922
H	-3.76407	0.17217	-2.74987
C	-4.13592	-1.84076	-0.72893
H	-4.85984	-1.47513	-1.45016
C	-1.69498	-4.51863	2.96014

H	-1.89514	-5.32696	2.24979
H	-2.59479	-4.37167	3.56648
H	-0.89714	-4.84587	3.63453
C	1.64327	-0.46275	-3.88500
H	0.78753	-0.22692	-4.52722
H	1.57884	-1.51976	-3.61323
H	2.55778	-0.31663	-4.47008
C	1.61882	1.92744	-3.06434
H	1.69321	2.59576	-2.20147
H	0.67913	2.14269	-3.58253
H	2.43335	2.16899	-3.75571
C	3.71954	-2.66061	0.87287
H	3.17849	-3.44096	0.32789
C	-2.89295	-2.38492	-3.56491
H	-2.60847	-3.42853	-3.39503
H	-2.51602	-2.08423	-4.54795
H	-3.98664	-2.33651	-3.59553
C	-1.02031	-2.08508	3.24140
H	-1.93807	-1.82246	3.77883
H	-0.65687	-1.18468	2.73087
H	-0.26668	-2.38152	3.97854
C	5.08328	-3.25734	1.25582
H	5.70302	-3.45071	0.37460
H	4.93483	-4.20565	1.78134
H	5.64275	-2.59948	1.93009
C	2.01937	1.17288	1.41199
H	2.06992	0.15054	1.75438
C	2.89760	-2.35331	2.14278
H	3.38888	-1.57798	2.74246

H	2.81262	-3.25039	2.76548
H	1.88434	-2.01923	1.89978
O	-5.16540	4.01853	0.30489
O	3.93794	4.26931	1.06744
C	5.21542	3.93714	1.62833
H	5.82430	4.83371	1.51787
H	5.12047	3.68386	2.69019
H	5.67563	3.10615	1.08213
C	-6.49531	3.62042	0.64891
H	-6.56196	3.34795	1.70902
H	-7.12254	4.49017	0.45506
H	-6.82780	2.78132	0.02566

Calculated XYZ coordinates for complex **14** at S₀ state

95

IPr_4-OMe-4-CF3-L5_modify.out Energy: -1480842.7698542

Cu	0.23674	0.11794	-0.35657
N	1.20277	1.93254	-0.59362
N	-1.59488	1.11181	-0.69052
N	1.92636	-2.11668	0.55290
N	-0.14107	-2.68548	0.55039
N	-0.72081	3.21921	-0.02982
H	-1.00228	4.14838	0.24952
C	-1.57581	-2.65834	0.41668
C	0.68509	-1.64548	0.23505
C	-2.33324	-2.10090	1.46222
C	-2.14715	-3.19897	-0.75276
C	0.56490	-3.76928	1.05803
H	0.07207	-4.67822	1.36452
C	-3.72603	-2.08198	1.30257
H	-4.34765	-1.65091	2.08091
C	1.87490	-3.40980	1.05782
H	2.76295	-3.94028	1.36266
C	-4.32491	-2.61274	0.16187
H	-5.40678	-2.59940	0.06446
C	-3.54443	-3.16666	-0.85477
H	-4.02911	-3.57518	-1.73482
C	-1.69257	-1.52678	2.72104
H	-0.62222	-1.75134	2.69282
C	3.14382	-1.35810	0.41693
C	3.54413	-0.53989	1.48900
C	3.87198	-1.47386	-0.78290

C	5.48989	0.07729	0.16436
H	6.41828	0.63354	0.06963
C	5.06092	-0.73816	-0.88403
H	5.65415	-0.80006	-1.79020
C	2.71694	-0.40173	2.76225
H	1.90622	-1.13504	2.72248
C	3.34986	-2.29052	-1.95946
H	2.59699	-2.98867	-1.58004
C	0.64286	3.13045	-0.32392
C	2.52737	1.92108	-0.85990
H	2.94792	0.94766	-1.07235
C	1.38007	4.31801	-0.29157
H	0.91176	5.27371	-0.08152
C	2.75195	4.27981	-0.55440
C	-1.79286	2.39067	-0.32925
C	-4.17733	2.14166	-0.50634
C	-3.08895	2.94076	-0.21109
H	-3.22870	3.97177	0.09494
C	3.34305	3.03819	-0.85619
H	4.39721	2.92603	-1.06897
C	-3.97900	0.81953	-0.92566
C	2.06388	0.99274	2.84138
H	1.45465	1.07615	3.74756
H	1.41986	1.17376	1.97593
H	2.82315	1.78223	2.86925
C	4.73583	0.18094	1.33237
H	5.07727	0.82741	2.13456
C	4.44136	-3.12721	-2.64827
H	4.97023	-3.76346	-1.93155

H	5.18192	-2.49771	-3.15260
H	3.99147	-3.77123	-3.41059
C	-2.26138	-2.17448	3.99775
H	-1.72202	-1.80836	4.87756
H	-2.16656	-3.26466	3.96754
H	-3.32042	-1.93338	4.13647
C	-1.83331	0.00747	2.76506
H	-1.34231	0.47002	1.90410
H	-1.37291	0.40581	3.67527
H	-2.88691	0.30785	2.75816
C	-1.27937	-3.72173	-1.89327
H	-0.31969	-4.03639	-1.47017
C	3.54520	-0.70343	4.02484
H	4.00976	-1.69319	3.96986
H	2.90317	-0.67573	4.91139
H	4.34168	0.03343	4.17224
C	2.64377	-1.35911	-2.96719
H	3.34836	-0.62933	-3.38192
H	1.82504	-0.81015	-2.48928
H	2.22531	-1.93694	-3.79761
C	-1.88079	-4.94228	-2.60926
H	-2.14506	-5.73366	-1.90079
H	-1.15604	-5.34908	-3.32159
H	-2.77956	-4.68163	-3.17791
C	-2.67692	0.36069	-0.99643
H	-2.46562	-0.65913	-1.28673
C	-0.98719	-2.58420	-2.89540
H	-1.91574	-2.22735	-3.35572
H	-0.32793	-2.93685	-3.69548

H	-0.49856	-1.73659	-2.40361
O	3.39974	5.45472	-0.50287
C	4.80584	5.49356	-0.78871
H	5.00601	5.14665	-1.80838
H	5.09194	6.54033	-0.69398
H	5.36738	4.89098	-0.06626
H	-4.80770	0.16711	-1.16942
C	-5.58824	2.66516	-0.35046
F	-6.19190	2.08481	0.71635
F	-5.62249	4.00130	-0.15947
F	-6.33846	2.38266	-1.43800

Calculated XYZ coordinates for complex **14** at S₁ state

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IPr_4-OMe-4-CF3-L5_optS1.out Energy: -1480345.1626264

Cu	-0.13022	0.00724	-0.43403
N	0.80325	1.70024	-0.96584
N	-1.78361	0.74073	-0.88587
N	2.30396	-1.59332	0.69053
N	0.33281	-2.21200	1.24609
N	-1.05665	2.84210	-0.07817
H	-1.37154	3.74549	0.24415
C	-1.10769	-2.22083	1.32516
C	1.00156	-1.32452	0.47897
C	-1.72637	-1.27666	2.16251
C	-1.81043	-3.15279	0.54365
C	1.20221	-3.02976	1.93760
H	0.85468	-3.80240	2.60469
C	-3.12195	-1.27459	2.18439
H	-3.65148	-0.55615	2.80006
C	2.45154	-2.64435	1.57939
H	3.42415	-3.01124	1.86600
C	-3.84829	-2.18349	1.42596
H	-4.93270	-2.15982	1.45825
C	-3.20217	-3.11708	0.62237
H	-3.79405	-3.81361	0.03876
C	-0.92290	-0.35105	3.06498
H	0.08558	-0.24889	2.64942
C	3.39945	-0.91419	0.05552
C	4.02725	0.12958	0.75250
C	3.77675	-1.33427	-1.22696

C	5.47343	0.39627	-1.17702
H	6.29932	0.90909	-1.66055
C	4.83176	-0.64715	-1.83408
H	5.15858	-0.93397	-2.82867
C	3.56199	0.56734	2.13548
H	3.08132	-0.29083	2.61745
C	3.05474	-2.45039	-1.96766
H	2.38181	-2.95392	-1.26602
C	0.19866	2.86837	-0.64838
C	2.02363	1.73493	-1.52601
H	2.45894	0.77767	-1.78408
C	0.85135	4.08633	-0.82873
H	0.36213	5.02218	-0.58557
C	2.13297	4.10787	-1.37479
C	-2.12467	1.98839	-0.43724
C	-4.46878	1.46657	-0.56024
C	-3.41801	2.38041	-0.25782
H	-3.64146	3.37729	0.10782
C	2.73149	2.89299	-1.75367
H	3.71523	2.83084	-2.19716
C	-4.13196	0.23627	-1.13111
C	2.50750	1.68119	2.02916
H	2.20700	2.01430	3.02732
H	1.61174	1.34085	1.50347
H	2.90697	2.54507	1.48633
C	5.07699	0.77860	0.10086
H	5.59519	1.59275	0.59601
C	4.02609	-3.51084	-2.50172
H	4.65864	-3.90829	-1.70289

H	4.68065	-3.10822	-3.28089
H	3.46817	-4.34247	-2.94178
C	-0.77781	-0.98200	4.45930
H	-0.16672	-0.34405	5.10527
H	-0.30365	-1.96710	4.40604
H	-1.75785	-1.10616	4.93115
C	-1.50908	1.06140	3.15423
H	-1.65747	1.49741	2.16256
H	-0.82716	1.70730	3.71558
H	-2.47029	1.07400	3.67651
C	-1.08658	-4.11988	-0.38333
H	-0.08308	-4.29034	0.02078
C	4.71904	1.00052	3.04324
H	5.51091	0.24684	3.07421
H	4.35086	1.15093	4.06192
H	5.16086	1.94781	2.71814
C	2.19115	-1.87095	-3.09830
H	2.80769	-1.34223	-3.83281
H	1.44645	-1.16333	-2.71562
H	1.65522	-2.66905	-3.62015
C	-1.76776	-5.48918	-0.48027
H	-1.93990	-5.92341	0.50852
H	-1.13581	-6.17639	-1.04999
H	-2.72949	-5.43095	-0.99915
C	-2.81418	-0.09942	-1.31181
H	-2.51778	-1.02772	-1.77987
C	-0.91702	-3.50239	-1.78074
H	-1.89153	-3.32704	-2.24824
H	-0.34759	-4.17448	-2.43039

H	-0.37940	-2.54851	-1.74095
O	2.69535	5.30650	-1.51790
C	3.98021	5.40403	-2.12656
H	3.95832	5.00450	-3.14521
H	4.20853	6.46762	-2.15591
H	4.73424	4.88197	-1.52874
H	-4.90014	-0.46031	-1.44609
C	-5.87128	1.85000	-0.26665
F	-6.09227	2.00406	1.06901
F	-6.21611	3.03608	-0.82317
F	-6.75778	0.93399	-0.69971

Calculated XYZ coordinates for complex **14** at T₁ state

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IPr_4-OMe-4-CF3-L5_modify_triplet.out Energy: -1480778.8648295

Cu	0.55004	0.24552	-0.31051
N	1.63075	1.84124	-0.47568
N	-1.04534	1.15964	-0.81088
N	1.42542	-2.44334	0.31089
N	-0.68096	-2.37555	0.75621
N	-0.20537	3.25840	-0.02110
H	-0.47181	4.19541	0.24825
C	-2.03865	-1.90289	0.92554
C	0.33052	-1.64244	0.22258
C	-2.26964	-0.90210	1.88667
C	-3.05340	-2.46712	0.12174
C	-0.21651	-3.61150	1.18456
H	-0.86801	-4.32757	1.65904
C	-3.57367	-0.39692	1.97605
H	-3.79694	0.39119	2.68753
C	1.11217	-3.66096	0.89575
H	1.85368	-4.42706	1.05800
C	-4.59168	-0.89620	1.17036
H	-5.59019	-0.47725	1.24421
C	-4.33874	-1.93578	0.27381
H	-5.15617	-2.32431	-0.32174
C	-1.20130	-0.43579	2.87286
H	-0.23703	-0.85523	2.57054
C	2.74708	-2.00813	-0.07373
C	3.58724	-1.47803	0.92804
C	3.12171	-2.11880	-1.42772

C	5.27100	-1.16202	-0.80124
H	6.26748	-0.83741	-1.08655
C	4.40703	-1.67456	-1.76981
H	4.73715	-1.73790	-2.80139
C	3.12609	-1.30627	2.37215
H	2.20773	-1.88372	2.51209
C	2.17245	-2.65895	-2.49050
H	1.31796	-3.11646	-1.98269
C	1.13898	3.08345	-0.20164
C	2.95834	1.69533	-0.70182
H	3.28583	0.69169	-0.94539
C	2.00835	4.18190	-0.07846
H	1.62542	5.17273	0.13864
C	3.37507	4.01061	-0.27813
C	-1.28976	2.46971	-0.44674
C	-3.65474	2.22407	-0.89845
C	-2.55738	3.00470	-0.44805
H	-2.71151	4.03097	-0.12918
C	3.86913	2.72458	-0.61770
H	4.91547	2.52790	-0.80391
C	-3.37698	0.92878	-1.40968
C	2.78207	0.17019	2.65790
H	2.45277	0.29130	3.69480
H	1.97594	0.53012	2.00975
H	3.65149	0.81613	2.49595
C	4.86392	-1.06059	0.52980
H	5.54445	-0.64622	1.26612
C	2.82587	-3.75198	-3.35628
H	3.22788	-4.56172	-2.73926

H	3.64351	-3.35385	-3.96550
H	2.08548	-4.17835	-4.04042
C	-1.51171	-0.98269	4.28163
H	-0.71846	-0.70301	4.98355
H	-1.59620	-2.07434	4.27560
H	-2.45592	-0.57730	4.66007
C	-1.03213	1.09250	2.90108
H	-0.77141	1.48138	1.91441
H	-0.23719	1.36889	3.60161
H	-1.94817	1.59732	3.22201
C	-2.76977	-3.60031	-0.86952
H	-2.06889	-4.29319	-0.39098
C	4.15440	-1.83998	3.38609
H	4.42247	-2.87967	3.17374
H	3.73899	-1.79367	4.39761
H	5.07478	-1.24724	3.38370
C	1.62958	-1.51029	-3.36540
H	2.44237	-1.00318	-3.89629
H	1.10179	-0.75822	-2.76655
H	0.92531	-1.89476	-4.10978
C	-4.01711	-4.42557	-1.22645
H	-4.54256	-4.77385	-0.33189
H	-3.72294	-5.30282	-1.81077
H	-4.72349	-3.85299	-1.83685
C	-2.10295	0.44264	-1.37045
H	-1.84546	-0.52946	-1.75849
C	-2.08679	-3.09741	-2.15930
H	-2.74662	-2.41531	-2.70632
H	-1.85982	-3.94183	-2.81868

H	-1.14738	-2.57561	-1.95227
O	4.13675	5.10617	-0.14935
C	5.55063	5.02241	-0.38745
H	5.75429	4.70659	-1.41625
H	5.92917	6.03180	-0.23194
H	6.02606	4.33753	0.32311
H	-4.16471	0.32000	-1.83649
C	-5.04436	2.70460	-0.73587
F	-5.58342	2.37322	0.49386
F	-5.14366	4.05875	-0.81620
F	-5.89173	2.17150	-1.65438

Calculated XYZ coordinates for complex **15** at S₀ state

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IPr_Me-L6_modify.out Energy: -1222129.4026186

Cu	-0.00322	0.44527	-0.48200
N	1.37843	1.91787	-0.94967
N	-1.48933	1.77517	-1.05943
N	1.12888	-1.96897	0.77592
N	-1.01441	-1.96191	0.87999
N	-0.16961	3.58806	-0.27260
C	-2.38862	-1.55495	0.72350
C	0.03901	-1.24808	0.38714
C	-2.90367	-0.58970	1.60679
C	-3.13878	-2.12634	-0.32402
C	-0.59096	-3.09281	1.56712
H	-1.28598	-3.77526	2.03010
C	-4.22926	-0.18059	1.40429
H	-4.66425	0.56617	2.06131
C	0.76704	-3.09976	1.49764
H	1.49968	-3.78901	1.88648
C	-4.99901	-0.72341	0.37785
H	-6.02663	-0.39813	0.24353
C	-4.46113	-1.68940	-0.47467
H	-5.07798	-2.10398	-1.26454
C	-2.08329	-0.00216	2.75010
H	-1.09989	-0.48100	2.74804
C	2.48628	-1.57661	0.49129
C	3.14297	-0.73243	1.40574
C	3.07897	-2.03784	-0.69915
C	5.07754	-0.80085	-0.06878

H	6.09882	-0.50083	-0.28550
C	4.39651	-1.63381	-0.95699
H	4.89145	-1.96688	-1.86342
C	2.46251	-0.21369	2.66795
H	1.52107	-0.75649	2.79529
C	2.30408	-2.86924	-1.71483
H	1.40398	-3.25332	-1.22522
C	1.11624	3.22172	-0.72707
C	2.61377	1.56049	-1.35486
H	2.76515	0.49884	-1.50273
C	2.11089	4.20246	-0.90009
H	1.88769	5.25070	-0.74978
C	3.38522	3.81586	-1.30108
H	4.15749	4.56626	-1.44049
C	-1.36078	3.10209	-0.85802
C	-3.59414	3.48641	-1.69057
H	-4.40469	4.16457	-1.93955
C	-2.40571	3.99017	-1.17219
H	-2.28448	5.05725	-1.03666
C	3.65030	2.46468	-1.53556
H	4.63001	2.11544	-1.83986
C	-3.72303	2.11127	-1.89745
H	-4.63415	1.67272	-2.28741
C	2.10796	1.28024	2.52390
H	1.61442	1.64266	3.43213
H	1.43414	1.44304	1.67819
H	3.00817	1.88359	2.36133
C	4.45469	-0.35021	1.09454
H	4.99424	0.30646	1.76948

C	3.09831	-4.08377	-2.22645
H	3.44519	-4.71059	-1.39875
H	3.97373	-3.78320	-2.81123
H	2.46655	-4.69617	-2.87806
C	-2.73431	-0.29668	4.11546
H	-2.09721	0.07259	4.92613
H	-2.88443	-1.37126	4.26126
H	-3.70931	0.19306	4.20899
C	-1.84946	1.50874	2.55930
H	-1.32578	1.70793	1.62062
H	-1.24307	1.90436	3.38102
H	-2.79720	2.05818	2.54380
C	-2.51445	-3.12223	-1.29674
H	-1.69657	-3.63248	-0.77768
C	3.30753	-0.46710	3.92992
H	3.56898	-1.52551	4.02884
H	2.74832	-0.16804	4.82257
H	4.23875	0.10892	3.91796
C	1.84299	-1.97144	-2.88191
H	2.70426	-1.54717	-3.41012
H	1.22194	-1.14433	-2.51982
H	1.25340	-2.54754	-3.60233
C	-3.49333	-4.20750	-1.77392
H	-3.97853	-4.70988	-0.93109
H	-2.95575	-4.96124	-2.35790
H	-4.27596	-3.79684	-2.42077
C	-2.64175	1.30345	-1.57545
H	-2.69037	0.22857	-1.69404
C	-1.89448	-2.37504	-2.49663

H	-2.67032	-1.85441	-3.06993
H	-1.39405	-3.07827	-3.17073
H	-1.15503	-1.63808	-2.16703
C	-0.27301	4.82736	0.50729
H	-0.27594	5.73626	-0.10884
H	-1.19353	4.79605	1.09264
H	0.56746	4.87624	1.20192

Calculated XYZ coordinates for complex **15** at S₁ state

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IPr_Me-L6_optS1.out Energy: -1221708.5787170

Cu	0.53340	-0.45969	0.40979
N	1.92539	-1.00110	1.53137
N	1.61122	-1.01206	-1.17552
N	-1.91566	0.78925	1.03060
N	-1.86387	0.79112	-1.11034
N	3.39554	-0.02503	-0.03181
C	-1.43382	0.57944	-2.46499
C	-1.19936	0.34038	-0.02419
C	-0.43899	1.42043	-2.97798
C	-2.03198	-0.46062	-3.19648
C	-2.97788	1.52371	-0.73554
H	-3.63387	1.97039	-1.46560
C	0.01145	1.15051	-4.27319
H	0.78497	1.77327	-4.71204
C	-3.01270	1.51993	0.61964
H	-3.70458	1.95923	1.32030
C	-0.53148	0.10986	-5.01445
H	-0.17197	-0.07842	-6.02128
C	-1.55190	-0.67867	-4.48819
H	-1.98210	-1.46576	-5.09776
C	0.09273	2.62397	-2.21274
H	-0.39639	2.65457	-1.23417
C	-1.50923	0.53025	2.38612
C	-0.61932	1.42933	2.99748
C	-1.99904	-0.62660	3.01428
C	-0.72223	0.02127	4.96911

H	-0.41395	-0.17667	5.99061
C	-1.59475	-0.85333	4.33033
H	-1.95310	-1.73162	4.85781
C	-0.09372	2.67383	2.29699
H	-0.53265	2.71734	1.29479
C	-2.87864	-1.63288	2.28874
H	-3.20386	-1.19006	1.34180
C	3.21684	-0.63285	1.24494
C	1.65827	-1.53525	2.78095
H	0.64189	-1.86398	2.95779
C	4.22891	-0.76467	2.16092
H	5.24117	-0.48398	1.89688
C	3.94612	-1.24823	3.45971
H	4.73374	-1.33146	4.19748
C	2.92693	-0.71397	-1.15497
C	3.18329	-1.66414	-3.35001
H	3.80724	-1.91074	-4.20261
C	3.74029	-1.03415	-2.24368
H	4.79782	-0.80478	-2.21357
C	2.63602	-1.63394	3.74647
H	2.37072	-2.03799	4.71774
C	1.83127	-1.99567	-3.34130
H	1.35641	-2.49210	-4.17833
C	1.43227	2.62500	2.12750
H	1.77972	3.52316	1.60731
H	1.74653	1.75070	1.54740
H	1.94056	2.57830	3.09578
C	-0.23119	1.13950	4.30713
H	0.46159	1.80011	4.81848

C	-4.14318	-1.98393	3.08242
H	-4.71188	-1.08581	3.34043
H	-3.90676	-2.51153	4.01163
H	-4.78777	-2.63873	2.48873
C	-0.27546	3.92352	-2.94488
H	0.03318	4.79097	-2.35356
H	-1.35391	3.99277	-3.11600
H	0.22298	3.98862	-3.91737
C	1.60269	2.53848	-1.95950
H	1.84821	1.68147	-1.32761
H	1.94873	3.44217	-1.44818
H	2.16242	2.44923	-2.89667
C	-3.13883	-1.31989	-2.59531
H	-3.71521	-0.68642	-1.91228
C	-0.52881	3.94620	3.03841
H	-1.61555	3.98672	3.15902
H	-0.21287	4.83415	2.48261
H	-0.07819	4.00068	4.03446
C	-2.06595	-2.89303	1.95195
H	-1.71947	-3.39265	2.86250
H	-1.18313	-2.65167	1.34737
H	-2.67537	-3.60391	1.38597
C	-4.12160	-1.85478	-3.64223
H	-4.49587	-1.05712	-4.29023
H	-4.97766	-2.31686	-3.14258
H	-3.66587	-2.62371	-4.27454
C	1.08504	-1.66287	-2.22646
H	0.02863	-1.88814	-2.16732
C	-2.56322	-2.47686	-1.76249

H	-1.98162	-3.15784	-2.39447
H	-3.37275	-3.05603	-1.30767
H	-1.91904	-2.11618	-0.95419
C	4.57196	0.81239	-0.21146
H	5.51344	0.24821	-0.25953
H	4.45697	1.38641	-1.13349
H	4.62605	1.50903	0.62704

Calculated XYZ coordinates for complex **15** at T₁ state

91

IPr_Me-L6_modify_triplet.out Energy: -1222062.5361885

Cu	0.44982	0.44373	-0.42253
N	1.85594	1.59751	-0.98093
N	-0.88914	1.71805	-1.07027
N	0.64282	-2.06181	0.87301
N	-1.46759	-1.62697	0.87638
N	0.53643	3.36725	-0.17247
C	-2.73503	-0.97694	0.64966
C	-0.27533	-1.16957	0.40673
C	-3.05969	0.13485	1.44546
C	-3.57422	-1.48666	-0.36354
C	-1.28879	-2.77856	1.63532
H	-2.12086	-3.28461	2.09853
C	-4.26064	0.79621	1.15243
H	-4.54718	1.66691	1.73390
C	0.04370	-3.05494	1.63145
H	0.61160	-3.84990	2.08826
C	-5.09880	0.34286	0.13755
H	-6.02647	0.86786	-0.07062
C	-4.76795	-0.79516	-0.60130
H	-5.45083	-1.14499	-1.36726
C	-2.19878	0.58572	2.62159
H	-1.33251	-0.07964	2.68991
C	2.05242	-1.90313	0.60999
C	2.81754	-1.12845	1.50728
C	2.58721	-2.50703	-0.54704
C	4.74903	-1.60160	0.10486

H	5.81134	-1.48811	-0.09005
C	3.96027	-2.34724	-0.77267
H	4.41559	-2.79918	-1.64782
C	2.21412	-0.46501	2.74002
H	1.14135	-0.68055	2.75425
C	1.70904	-3.23624	-1.55673
H	0.72991	-3.40862	-1.09905
C	1.75730	2.94551	-0.75885
C	3.01712	1.10009	-1.52338
H	3.03082	0.03396	-1.71084
C	2.81095	3.80235	-1.03536
H	2.70063	4.86648	-0.86765
C	4.02612	3.28184	-1.52454
H	4.86537	3.94004	-1.71781
C	-0.64747	3.04970	-0.88196
C	-2.75405	3.61205	-1.92796
H	-3.47900	4.35353	-2.24480
C	-1.55510	4.00984	-1.31420
H	-1.33383	5.06011	-1.16999
C	4.11119	1.90302	-1.77506
H	5.01632	1.45531	-2.17117
C	-2.97876	2.24448	-2.13595
H	-3.88223	1.88212	-2.61289
C	2.36613	1.06816	2.68932
H	1.89295	1.52103	3.56682
H	1.89356	1.48440	1.79352
H	3.41946	1.36719	2.68363
C	4.18239	-0.98955	1.22161
H	4.80835	-0.39968	1.88330

C	2.27530	-4.61011	-1.95695
H	2.45105	-5.23960	-1.07895
H	3.22085	-4.51812	-2.50080
H	1.56976	-5.12845	-2.61413
C	-2.97783	0.45169	3.94569
H	-2.32872	0.69743	4.79278
H	-3.35339	-0.56715	4.08591
H	-3.83616	1.13105	3.97528
C	-1.65515	2.01371	2.43659
H	-1.00401	2.07318	1.56181
H	-1.07174	2.31060	3.31475
H	-2.46707	2.73802	2.31129
C	-3.18542	-2.72065	-1.17811
H	-2.60702	-3.38219	-0.52384
C	2.81869	-1.04407	4.03409
H	2.68939	-2.13017	4.08379
H	2.33369	-0.60129	4.91015
H	3.89059	-0.83091	4.10163
C	1.48748	-2.34394	-2.79619
H	2.43571	-2.13554	-3.30313
H	1.03500	-1.38317	-2.52056
H	0.82000	-2.83463	-3.51146
C	-4.39669	-3.53037	-1.66959
H	-5.08618	-3.76242	-0.85187
H	-4.05726	-4.47411	-2.10763
H	-4.95608	-2.99784	-2.44612
C	-2.02528	1.33470	-1.72009
H	-2.15121	0.27204	-1.85712
C	-2.27044	-2.34892	-2.36398

H	-2.79439	-1.69168	-3.06717
H	-1.97097	-3.24994	-2.90978
H	-1.35946	-1.84324	-2.03018
C	0.54972	4.62073	0.57851
H	0.62935	5.51521	-0.05530
H	-0.37225	4.68400	1.16032
H	1.40028	4.60282	1.26330

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