Supporting Information for

Regioselective functionalization of the [*closo*-1-CB_9H_{10}]$^-$ anion through iodonium zwitterions

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Preparation of starting materials

Preparation of [*closo*-1-CB_9H_{10}]$^-$[Et_4N]$^+$ (2a[Et_4N]). Salt **2a[Et_4N]** was prepared following literature[1,2] procedures from freshly sublimed $B_{10}H_{14}$ in yields comparable to those reported previously. The total yield for the 3-step process is about 35-40%: ^{1}H NMR (500 MHz, CD_3CN) δ 0.0–1.9 (m, 8H), 1.21 (tt, J = 7.3 Hz, J = 1.9 Hz, 12H), 3.16 (q, J = 7.3 Hz, 8H), 4.75 (s, 1H), 5.28 (q, J = 152 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 7.7, 53.1, 54.3 (br); ^{11}B NMR (160 MHz, CD_3CN) δ –24.4 (d, J = 136 Hz, 4B), –18.9 (d, J = 150 Hz, 4B), 30.1 (d, J = 154 Hz, 1B).

Preparation of [*closo*-1-CB_9H_9-1-C_5H_{11}]$^-$[Et_4N]$^+$ (2c-[Et_4N]). Well-dried [*closo*-1-CB_9H_{10}]$^-$$Cs^+$ **(2a-[Cs]**, 508 mg, 2.00 mmol, P_2O_5, 100 ^{o}C, 0.25 Tr, 12 hr) was dissolved in freshly distilled THF (10 mL) and the solution was cooled to –10 °C. A solution of *n*-BuLi (2.5 M, 1.04 mL, 2.60 mmol) was added slowly over 10 min under Ar atmosphere. The solution was stirred for 1 hr at –10 °C, warmed to room temperature and stirred for additional 30 min, while a milky precipitate was formed signifying the formation of the reactive carboranyllithium intermediate. The suspension was cooled to 0 °C and 1-iodopentane (515 mg, 0.34 mL, 2.6 mmol) was added dropwise. The reaction mixture was warmed to room temperature and stirred overnight. MeOH (5 mL) was added, and the solvents were evaporated to dryness. 6M aqueous HCl (15 mL) and Et_2O (15 mL) were added to the residue and the suspension was stirred for 1 hr. The organic layer was separated and the aqueous layer was extracted with Et_2O (4 × 15 mL). The organic extracts were combined and the solvent was removed in *vacuo*. The ^{11}B NMR spectrum of the crude mixture showed about 80% conversion. Water (10 mL) was added to the residue followed by a slow dropwise addition of a concentrated aqueous solution of [Et_4N]$^+$$Br^-$ (0.85 equiv., 358 mg, 1.7 mmol). The resulting precipitate containing about 90% of **2c** (based on the ^{11}B NMR spectrum) was collected, washed with H_2O and dried. Traces of the unreacted iodopentane were removed under vacuum (Kugel-Rohr, 80 ^{o}C, 0.25 Tr) and the crude product was separated from small amounts of the unreacted **2a** by column chromatography (hexanes/AcOEt, 2:3) to give 454 mg (71% yield) of [*closo*-1-CB_9H_9-1-C_5H_{11}]$^-$[Et_4N]$^+$ **(2c-[Et_4N])** as a yellowish solid. The analytical sample was obtained by recrystallization (EtOH/H_2O): mp 102-103 ^{o}C; ^{1}H NMR (500

MHz, CD_3CN) δ 0.0–1.65 (m, 8H), 0.96 (t, J = 7.2 Hz, 3H), 1.20 (tt, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 12H), 1.41–1.55 (m, 4H), 1.96–2.03 (m, 2H), 3.08 (t, J = 8.2 Hz, 2H), 3.16 (q, J = 7.3 Hz, 8H), 5.02 (q, J = 148 Hz, 1H, BH); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 7.7, 14.6, 23.5, 33.0, 33.2, 35.1, 53.1 (t, J = 2.5 Hz), 74.1; ^{11}B NMR (160 MHz, CD_3CN) δ –24.2 (d, J = 136 Hz, 4B), –16.4 (d, J = 148 Hz, 4B), 25.9 (d, J = 152 Hz, 1B); MALDI MS: *m/z* 181–190 (max at 188 [M-1]); HRMS ESI (-) *m/z*: calcd for $C_6H_{20}B_9$ 191.2403; found 191.2409. Anal. Calcd. for $C_{14}H_{40}B_9N$: C, 52.58; H, 12.61; N, 4.38. Calcd for $C_{14}H_{40}B_9N•H_2O$: C, 49.78; H, 12.53; N, 4.15. Found: C, 49.85; H, 12.73; N, 3.99.

Reaction of 2a with $PhI(OAc)_2$.[3] Following a literature procedure[3] to a cold (0–5 °C) solution of [*closo*-1-$CB_9H_{10}]^-[Et_4N]^+$ (**2a-[Et$_4$N]**, 5.0 mmol) in 75% aqueous CF_3COOH (45 mL), $PhI(OAc)_2$ (3.38 g, 5.51 mmol) was added in five portions at 5 min intervals. The reaction mixture was stirred for 1 hr at the same temperature and the resulting solid material was collected by filtration, washed with water and dried in *vacuo* giving a white solid mixture of isomers **5[6]a** and **5[10]a** in a ratio of 2.7:1 (27% of **5[10]a** by ^1H NMR) and a typical yield of 95%:

Major isomer **5[6]a**: ^1H NMR (500 MHz, CD_3CN) δ 0.4–2.2 (m, 8H), 5.14 (s), 5.11 (q, J = 163 Hz, 1H), 7.43 (t, J = 8.1 Hz, 2H), 7.66 (t, J = 7.7 Hz, 1H), 7.73 (d, J = 8.2 Hz, 2H); ^{11}B NMR (160 MHz, CD_3CN) δ –26.7 (1B), –23.7 (2B), –21.4 (2B), –17.6 (2B), –16.6 (1B), 22.9 (1B).

Minor isomer **5[10]a**: ^1H NMR (500 MHz, CD_3CN) δ 0.6–2.0 (m, 8H), 5.88 (br s, 1H), 7.46 (t, J = 7.9 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 8.09 (d, J = 7.5 Hz, 2H); ^{11}B NMR (160 MHz, CD_3CN) δ –19.4 (d, J = 147 Hz, 4B), –17.6 (d, J = 158 Hz, 4B), 21.3 (s, 1B).

The mixture was used immediately for the next step.

Reaction of 2c with $PhI(OAc)_2$. Reaction with **2c-[Et$_4$N]** (300 mg, 0.94 mol) was conducted as described for **2a-[Et$_4$N]** with modified isolation of the iodonium zwitterions. Thus, the reaction mixture was diluted with H_2O and stirred for additional 5 min giving a semi-crystalline product sticking to the reaction flask walls. The supernatant liquid was decanted, the residue was washed with cold H_2O, and dissolved in CH_2Cl_2. The resulting solution was washed with 5% aqueous $NaHCO_3$ and passed through a thin layer of silica gel using a mixture of hexanes and CH_2Cl_2 (1:9) as the eluent. The solvents were evaporated under reduced pressure (*cold bath*!) giving an

oily mixture of isomers **5[6]c** and **5[10]c** in an approximate ratio of 4:5 (55% of **5[10]c** by ^{1}H NMR) and yield of 95%:

Minor isomer **5[6]c**: ^{1}H NMR (500 MHz, CD_3CN) characteristic signals δ 3.01 (t, *J* = 8.2 Hz, 2H), 5.02 (q, *J* = 148 Hz, 1H, BH), 7.41 (t, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 6.1 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 2H); ^{11}B{^{1}H} NMR (160 MHz, CD_3CN) δ –23.9 (1B), –21.0 (2B), –16.8 (2B), –13.6 (1B), –12.7 (2B), 21.2 (1B).

Major isomer **5[10]c**: ^{1}H NMR (500 MHz, CD_3CN) characteristic signals δ 3.14 (t, *J* = 8.2 Hz, 2H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 6.1 Hz, 1H), 8.06 (d, *J* = 7.6 Hz, 1H); ^{11}B{^{1}H} NMR (160 MHz, CD_3CN) δ –19.3 (4B), –15.3 (4B), 19.3 (1B).

The mixture was used immediately for the next step.

Isomer separation

With MeCN. Preparation of [*closo*-1-CB_9H_9-10-IPh] (5[10]a).[3] The mixture of regioisomers **5[6]a** and **5[10]a** (2.893 g, 8.97 mmol) was dissolved in MeCN (30 mL) and the solution was stirred at 60 °C for 16 hr. The solvent was evaporated under reduced pressure and the residue was separated by column chromatography (CH_2Cl_2/hexane 1:4) to give 0.670 g (22% yield based on **2a**) of **5[10]a** as a colorless solid: mp 129-131 °C dec; ^{1}H NMR (500 MHz, CD_3CN) δ 0.6–2.0 (m, 8H), 5.88 (br s, 1H), 7.46 (t, *J* = 7.9 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 65.6 (br), 106.8, 132.5, 132.8, 137.0; ^{11}B NMR (160 MHz, CD_3CN) δ –19.4 (d, *J* = 147 Hz, 4B), –17.6 (d, *J* = 158 Hz, 4B), 21.3 (s, 1B).

With Pyridine in MeCN. Preparation of [*closo*-1-CB_9H_9-6-NC_5H_5] (9[6]a) and [*closo*-1-CB_9H_9-10-IPh] (5[10]a). To a stirred solution of a mixture of regioisomers **5[6]a** and **5[10]a** (450 mg, 1.39 mmol) in MeCN (4 mL), pyridine (200 mg, 2.53 mmol) was added. Stirring was continued for 20 hr at room temperature. The solvent and the excess pyridine were evaporated under reduced pressure and the residue was purified by column chromatography (CH_2Cl_2/hexane 1:3 gradient to 1:1) to give 149 mg (33% yield) of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**) as the first fraction and 149 mg (54% yield) of 6-pyridinium **9[6]a** as colorless solids.

[*closo*-1-CB_9H_9-6-NC_5H_5] (9[6]a). Mp 118 °C; R_f = 0.17 (CH_2Cl_2/hexane 1:2); ^{1}H NMR (500 MHz, CD_3CN) δ 0.1–2.35 (m, 7H), 5.15 (s, 1H), 5.28 (q, *J* = 157 Hz, 1H), 7.71 (t, *J* = 7.0 Hz, 2H), 8.24 (td, J_1 = 7.7 Hz, J_2 = 0.4 Hz, 1H), 8.46 (d, *J* = 5.4 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz,

CD_3CN) δ 55.3 (br), 127.9, 144.8, 147.4; ^{11}B NMR (160 MHz, CD_3CN) δ –26.7 (d, *J* = 137 Hz, 1B), –21.6 (d, *J* = 150 Hz, 2B), –20.1 (d, *J* = 158 Hz, 2B), –15.2 (d, *J* = 154 Hz, 2B), –6.4 (s, 1B), 26.0 (d, *J* = 155 Hz, 1B); UV (MeCN), λ_{max} (log ε) 264.0 nm (3.87); HRMS ESI (-) *m/z*: calcd for $C_6H_{13}B_9N$ 198.1885; found 198.1893. Anal. calcd. for $C_6H_{14}B_9N$: C, 36.49; H, 7.15; N 7.09. Found: C, 36.68; H, 7.22; N, 6.91.

With acetamidine in MeCN. Preparation of [*closo*-1-CB_9H_9-6-$NHC(NH_2)Me$] (10[6]a) and [*closo*-1-CB_9H_9-10-IPh] (5[10]a). To a stirred solution of a mixture of regioisomers **5[6]a** and **5[10]a** (2.49 g, 7.72 mmol) in MeCN (23 mL) acetamidine[4] (0.54 g, 9.30 mmol) was added. After stirring for 1.5 hr at room temperature, acetic acid (180 mg, 3.00 mmol) was added. The solvent was evaporated under reduced pressure and the residue was subjected to column chromatography (CH_2Cl_2/hexane 1:2 gradient to CH_2Cl_2) to afford 753 mg (30% yield) of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**) as the first fraction and 760 mg (56% yield) of [*closo*-1-CB_9H_9-6-$NHC(NH_2)Me$] (**10[6]a**) as colorless solids.

[*closo*-1-CB_9H_9-6-$NHC(NH_2)Me$] (10[6]a). Mp 150-151 °C; R_f = 0.2 (CH_2Cl_2); ^1H NMR (500 MHz, CD_3CN) δ 0.1–2.1 (m, 7H), 2.04 (s, 3H), 5.02 (br s, 1H), 5.21 (q, *J* = 150 Hz, 1H), 6.58 (br s, 1H), 7.15 (br s, 1H), 7.52 (br s, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 21.1, 55.8 (br), 170.2; ^{11}B NMR (160 MHz, CD_3CN) δ –27.7 (d, *J* = 141 Hz, 1B), –20.5 (d, *J* = 157 Hz, 2B), –19.5 (d, *J* = 161 Hz, 2B), –15.7 (d, *J* = 154 Hz, 2B), –13.7 (s, 1B), 23.0 (d, *J* = 144 Hz, 1B); IR (KBr) ν 2551, 2516 and 2479 (BH), 1648 (C=N), 1606, 464 cm^{-1}; HRMS ESI (-) *m/z*: calcd for $C_3H_{14}B_9N_2$ 177.1994; found 177.2002. Anal. Calcd. for $C_3H_{15}B_9N_2$: C, 20.42; H, 8.57; N 15.88. Found: C, 20.57; H, 8.60; N, 15.76.

With $[Et_4N]^+[CN]^-$ in MeCN. Preparation of [*closo*-1-CB_9H_8-1-C_5H_{11}-6-$CN]^-[Et_4N]^+$ (11[6]c-[Et_4N]) and [*closo*-1-CB_9H_8-1-C_5H_{11}-10-IPh] (5[10]c). To a stirred solution of a mixture of regioisomers **5[6]c** and **5[10]c** (280.0 mg, 0.71 mmol) in MeCN (5 mL) $[Et_4N]^+[CN]^-$ (49.0 mg, 0.31 mmol) was added. The progress of the reaction was monitored using ^{11}B NMR spectroscopy. After stirring for 1 hr at 0 °C the reaction was complete. After evaporation of the solvent (cold bath) the products were separated by column chromatography (SiO_2) starting with hexanes (elution of iodobenzene), followed by hexanes/CH_2Cl_2 4:1 (elution of **5[10]c**), and finally CH_2Cl_2/MeCN 10:1 (elution of **11[6]c-[Et_4N]**) giving 150 mg of **5[10]c** (containing

approximately 3% of **5[6]c**) and 121 mg (49% yield) of ~92% pure [*closo*-1-CB_9H_8-1-C_5H_{11}-6-CN]$^-$[Et_4N]$^+$ (**11[6]a-[Et_4N]**) as a yellow oil. Pure [*closo*-1-CB_9H_8-1-C_5H_{11}-10-IPh] (**5[10]c**) was obtained by heating the product in MeCN at 60 ^oC. The progress of the reaction was monitored using ^{11}B NMR spectroscopy and after 2 h it showed that the entire [*closo*-1-CB_9H_8-1-C_5H_{11}-6-IPh] (**5[6]c**) was consumed. The solvent was evaporated, the residue was passed through a silica gel pad using hexanes/CH_2Cl_2 (4:1) as an eluent giving 140 mg (50% yield) of pure **5[10]c** as a white solid, which was recrystallized from *n*-heptane.

[*closo*-1-CB_9H_8-1-C_5H_{11}-10-IPh] (5[10]c): mp 65–66 ^oC; ^1H NMR (500 MHz, CD_3CN) δ 0.65–1.85 (m, 8H), 0.96 (t, J = 7.3 Hz, 3H), 1.38–1.55 (m, 4H), 1.91–1.99 (m, 2H), 3.13 (t, J = 8.3 Hz, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 8.06 (d, J = 7.5 Hz, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 14.5, 23.4, 32.8, 32.9, 34.7, 106.6, 132.5, 132.8, 137.0 (the C(1) signal of the boron cluster was not observed); ^{11}B NMR (160 MHz, CD_3CN) δ –18.9 (d, J = 143 Hz, 4B), –14.9 (d, J = 155 Hz, 4B), 19.6 (s, 1B); EI MS: *m/z* 388-394 (max at 391 [M-1]). Anal. Calcd. for $C_{12}H_{24}B_9I$: C, 36.72; H, 6.16. Found: C, 36.71; H, 6.22.

[*closo*-1-CB_9H_8-1-C_5H_{11}-6-CN]$^-$[Et_4N]$^+$ (11[6]a-[Et_4N]). Crude product was purified by column chromatography (CH_2Cl_2/MeCN 30:1) to give 97 mg of **11[6]a-[Et_4N]** as a colourless oil: ^1H NMR (500 MHz, CD_3CN) δ 0.20–1.65 (m, 8H), 0.96 (t, J = 7.2 Hz, 3H), 1.20 (tt, J_1 = 7.2 Hz, J_2 = 1.9 Hz, 12H), 1.41-1.54 (m, 4H), 1.95-2.00 (m, 2H), 3.08 (t, J = 8.3 Hz, 2H), 3.16 (q, J = 7.3 Hz, 8H), 5.02 (q, J = 157 Hz, 1H, BH); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 7.7, 14.5, 23.5, 32.8, 33.0, 34.6, 53.1; $^{13}C\{^1H\}$ NMR (151 MHz, acetone-d_6) δ 7.6, 14.4, 23.3, 32.6, 32.9, 34.6, 52.9 (t, J = 2.9 Hz), 74.8 (brs), 131.3 (q, J = 93 Hz); ^{11}B NMR (160 MHz, CD_3CN) δ –27.9 (s, 1B), –23.8 (d, 1B), –22.9 (d, J = 134 Hz, 2B), –16.2 (d, J = 143 Hz, 2B), –15.4 (d, J = 143 Hz, 2B), 25.6 (d, J = 158 Hz, 1B); ^{11}B NMR (193 MHz, acetone-d_6) δ –27.7 (s, 1B), –23.3 (d, J = 154 Hz, 1B), –22.8 (d, J = 131 Hz, 2B), –16.1 (d, J = 154 Hz, 2B), –15.3 (d, J = 154 Hz, 2B), 26.0 (d, J = 156 Hz, 1B); IR (KBr) ν 2553 (B–H), 2203 (CN) cm^{-1}; MALDI MS: *m/z* 212–217 (max at 214 [M]); HRMS ESI(-), *m/z*: calcd for $C_7H_{19}B_9N$ 216.2355, found 216.2358. Anal. Calcd. for $C_{15}H_{39}B_9N_2$: C, 52.25; H, 11.40; N, 8.13. Found: C, 52.17; H, 11.23; N, 8.05.

Conversions of [closo-CB_9H_8-1-R-10-IPh] (5[10]).

Preparation of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-I]$^-$[Et_4N]$^+$ (3[10]c-[Et_4N]). **Method A:** To a stirred solution of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-IPh] (**5[10]c**, 50.0 mg, 0.127 mmol) in dry MeCN (1 mL)

$[Et_4N]^+I^-$ (49 mg, 0.191 mmol) was added. The mixture was heated overnight at 60 ºC. The solvent was evaporated under reduced pressure and the resulting crude product was purified by column chromatography (hexanes/CH_2Cl_2 2/1 gradient to CH_2Cl_2) giving 55 mg (97% yield) of pure **3[10]c-[Et4N]**.

Method B: To a solution of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-IPh] **(5[10]c**, 71 mg, 0.181 mmol) in dry THF (3 mL) 2.5 M *n*-BuLi in hexanes (0.18 mL, 0.45 mmol) was added dropwise at –10 ºC under argon. The reaction mixture was stirred at –5 ºC and progress of the reaction was monitored by TLC. After 1 hr H_2O (3 mL) was added, THF was removed under reduced pressure, and the clear solution was extracted with hexanes (3x). The aqueous layer was treated with concentrated solution of $[Et_4N]^+Br^-$ (46 mg, 0.22 mmol). The resulting milky suspension was extracted with CH_2Cl_2 (3x) and dried ($MgSO_4$). The solvent was evaporated to give 70 mg of crude product, which contained 7% of the [*closo*-1-CB_9H_8-1-C_5H_{11}-10-Ph]$^-$ derivative. Pure **3[10]c-[Et_4N]** was isolated as a white solid by extraction of the 10-phenyl derivative from the crude solid with Et_2O followed by recrystallization (MeOH): mp 102-103 ºC; ^{1}H NMR (500 MHz, CD_3CN) δ 0.30–1.80 (m, 8H), 0.96 (t, J = 7.2 Hz, 3H), 1.20 (tt, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 12H), 1.41–1.53 (m, 4H), 1.95–1.99 (m, 2H), 3.01 (t, J = 8.3 Hz, 2H), 3.15 (t, J = 7.2 Hz, 8H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 7.7, 14.5, 23.5, 32.8, 33.1, 35.1, 53.1 (C-1 signal of the boron cluster was not observed); ^{11}B NMR (160 MHz, CD_3CN) δ –20.2 (d, J = 139 Hz, 4B), –16.1 (d, J = 151 Hz, 4B), 13.2 (s, 1B); MALDI MS: *m/z* 313-318 (max at 316 [M]); HRMS ESI(-), *m/z* calcd for $C_6H_{19}B_9I$: 317.1369, found: 317.1371. Anal. Calcd. for $C_{14}H_{39}B_9IN$: C, 37.73; H, 8.82; N, 3.14. Found: C, 37.89; H, 8.96; N, 3.19.

[*closo*-1-CB_9H_8-1-C_5H_{11}-10-Ph]$^-$ [Et_4N]$^+$: H NMR (500 MHz, CD_3CN) characteristic signals in the mixture δ 7.17 (t, J = 7.2 Hz, 1H), 7.26 (t, J = 7.3 Hz, 2H), 7.88 (d, J = 7.9 Hz, 2H); ^{11}B NMR {^{1}H}(160 MHz, CD_3CN) δ –23.2 (4B), –17.3 (4B), 36.3 (1B); EI MS: *m/z* 264-268 (max at 266 [M]); HRMS ESI (-) *m/z*: calcd for $C_{12}H_{24}B_9$ 267.2716; found 267.2724.

Preparation of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-($NC_5H_4OC_7H_{15}$)] (6[10]c). A solution of [*closo*-1-CB_9H_9-1-C_5H_{11}-10-IPh] (**5[10]c**, 35.0 mg, 0.089 mmol) in 4-heptyloxypyridine (0.4 mL) was stirred at 85 ºC for 6 hr. After completion of the reaction (confirmed by TLC) all volatiles were removed via Kugelrohr distillation (80 ºC, 0.25 Tr). The crude product was purified by passing through a silica gel pad using CH_2Cl_2 as an eluent giving 33.0 mg (95% yield) of [*closo*-1-

CB_9H_8-1-C_5H_{11}-10-($NC_5H_4OC_7H_{15}$)] (**6[10]c**) as white crystals. The analytical sample was obtained by crystallization from *n*-heptane: mp 94-95 °C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.65-2.05 (m, 8H), 0.91 (t, *J* = 7.0 Hz, 3H), 0.97 (t, *J* = 7.2 Hz, 3H), 1.28-1.58 (m, 12H), 1.87 (quint, *J* = 7.0 Hz, 2H), 1.95-2.03 (m, 2H), 3.16 (t, *J* = 8.3 Hz, 2H), 4.32 (t, *J* = 6.6 Hz, 2H), 7.36 (d, *J* = 7.4 Hz, 2H), 9.03 (d, *J* = 7.4 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 14.4, 14.5, 23.4, 23.5, 26.4, 29.3, 29.7, 32.5, 32.97, 33.02, 33.9, 71.7, 113.9, 149.5, 171.3 (the C-1 signal of the boron cluster was not observed); ^{11}B NMR (160 MHz, CD_3CN) δ –21.6 (d, *J* = 139 Hz, 4B), –17.1 (d, *J* = 154 Hz, 4B), 36.4 (s, 1B); EI MS: *m/z* 379–384 (382 max, [M]); HRMS ESI(+), *m/z*: calcd for $C_{18}H_{38}B_9NONa$ 406.3689, found 406.3688. Anal. Calcd. for $C_{18}H_{38}B_9ON$: C, 56.62; H, 10.03; N, 3.67. Found: C, 56.65; H, 10.07; N, 3.62.

Preparation of [*closo*-1-CB_9H_9-10-NC_5H_5] (9[10]a). A solution of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 150 mg, 0.465 mmol) in pyridine (0.50 g, 6.3 mmol) was stirred at 45 °C for 6 hr. Pyridine was removed under reduced pressure and the crude product was purified by column chromatography (CH_2Cl_2/hexane 1:2, R_f = 0.17) to give 86 mg (93% yield) of 10-pyridinium derivative **9[10]a** as a colorless solid: mp 134-135 °C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.7–2.1 (m, 8H), 5.28 (s, 1H), 8.01 (td, J_1 = 6.7 Hz, J_2 = 0.9 Hz, 2H), 8.49 (tt, J_1 = 7.8 Hz, J_2 = 1.4 Hz, 1H), 9.34 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 55.6 (br), 128.2, 145.3, 148.1; ^{11}B NMR (160 MHz, CD_3CN) δ –21.7 (d, *J* = 136 Hz, 4B), –19.7 (d, *J* = 154 Hz, 4B), 38.6 (s, 1B); UV (MeCN), λ_{max} (log ε) 265.5 nm (4.01); HRMS ESI (-) *m/z*: calcd for $C_6H_{13}B_9N$ 198.1885; found 198.1894. Anal. Calcd. for $C_6H_{14}B_9N$: C, 36.49; H, 7.15; N 7.09. Found: C, 36.59; H, 7.25; N, 6.98.

Preparation of [*closo*-1-CB_9H_9-10-$NHC(NH_2)Me$] (10[10]a). Acetamidine hydrochloride (437 mg, 4.62 mmol) was added in one portion to sodium ethoxide solution, which was prepared from sodium (101 mg, 4.4 mmol) and ethanol (2.7 mL).[4] The mixture was stirred for 10 min at room temperature and ethanol was evaporated at reduced pressure. MeCN (6 mL) was added to the residue, the resulting suspension was filtered through Celite and concentrated to *ca*. 4 mL. [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 354 mg, 1.10 mmol) was added and the resulting solution was stirred for 4 hr at 40 °C. The solvent was evaporated in *vacuo* and the crude product was purified by column chromatography (SiO_2, CH_2Cl_2) to afford 171 mg (89% yield) of 10-acetmidinium

derivative **10[10]a** as a colorless solid: mp 135 °C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.4–2.0 (m, 8H), 2.42 (s, 3H), 4.98 (br s, 1H), 7.29 (br s, 1H) , 7.38 (br s, 1H), 8.42 (br s, 1H); $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) δ 21.0, 51.7 (br), 168.6; ^{11}B NMR (160 MHz, CD_3CN) δ –24.1 (d, J = 137 Hz, 4B), –20.5 (d, J = 154 Hz, 4B), 33.0 (s, 1B); IR (KBr) ν 3458, 3380 and 3354 (N–H), 2557 and 2487 (B–H), 1657 (C=N), 1592 cm^{-1}. Anal. Calcd for $C_3H_{14}B_9N_2$: C, 20.54; H, 8.04; N, 15.97. Found: C, 20.46; H, 8.15; N, 15.94.

Preparation of [*closo*-1-CB_9H_9-10-CN]$^-$[Et_4N]$^+$ (11[10]a-[Et_4N]). A solution of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 45.0 mg, 0.140 mmol) and [Et_4N]$^+$[CN]$^-$ (26 mg, 0.168 mmol) in MeCN (1 mL) was stirred at room temperature for 7 hr. After evaporation of the solvent the crude product was purified by column chromatography (CH_2Cl_2 gradient to CH_2Cl_2/MeCN 10:1, R_f = 0.19 at CH_2Cl_2/MeCN 10:1) to give 37.0 mg (96% yield) of [*closo*-1-CB_9H_9-10-CN]$^-$[Et_4N]$^+$ (**11[10]a-[Et_4N]**) as a colorless solid: mp 237-239 °C dec.; ^{1}H NMR 500 MHz, CD_3CN) δ 0.3–1.9 (br m, 8H), 1.21 (tt, J = 7.3 Hz, J = 1.8 Hz, 12H), 3.16 (q, J = 7.3 Hz, 8H), 5.16 (br s, 1H); (500 MHz, acetone-d_6) δ 0.5–2.0 (m, 8H), 1.40 (tt, J_1 = 7.2 Hz, J_2 =1.8 Hz, 12H), 3.49 (q, J = 7.3 Hz, 8H), 5.03 (br s, 1H); $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) δ 7.7, 53.1, 61.6 (br), 131.8 (q, J = 105 Hz); (126 MHz, acetone-d_6) δ 7.7, 53.0 (t, J = 3.1 Hz), 60.5 (br), 131.5 (q, J = 106 Hz); ^{11}B NMR (160 MHz, CD_3CN) δ –21.0 (d, J = 140 Hz, 4B), –18.3 (d, J = 154 Hz, 4B), 20.1 (s, 1B); (160 MHz, acetone-d_6) δ –21.9 (d, J = 141 Hz, 4B), –19.1 (d, J = 152 Hz, 4B), 19.8 (s, 1B); IR (KBr) ν 2562, 2553 and 2513 (B-H), 2201 (C≡N), 1460 cm^{-1}; HRMS ESI (-) *m/z*: calcd for $C_2H_9B_9N$ 146.1572; found 146.1576. Anal. Calcd. for $C_{10}H_{29}B_9N_2$: C, 43.73; H, 10.64; N 10.20. Found: C, 43.51; H, 10.89; N, 9.96.

Preparation of [*closo*-1-CB_9H_9-10-$SCHNMe_2$] (12[10]a). A solution of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 70 mg, 0.217 mmol) in *N,N*-dimethylthioformamide (0.30 g, 3.36 mmol) was stirred at 80 °C for 1.5 hr. Excess *N,N*-dimethylthioformamide was removed under reduced pressure and the resulting crude product was purified by column chromatography (CH_2Cl_2/hexane 1:1, R_f = 0.28) to afford 39.0 mg (87% yield) of zwitterion **12[10]a** as a white solid: mp 249–250 °C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.4–2.0 (m, 8H), 3.50 (s, 3H), 3.57 (s, 3H), 5.25 (br s, 1H), 9.54 (s, 1H); $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) δ 42.5, 49.5, 58.9 (br), 185.4; ^{11}B NMR (160 MHz, CD_3CN) δ –21.1 (d, J = 142 Hz, 4B), –18.8 (d, J = 154 Hz, 4B),

30.9 (s, 1B); HRMS ESI (-) *m/z*: calcd for $C_4H_{15}B_9NS$ 208.1763; found 208.1767. Anal. Calcd. for $C_4H_{16}B_9NS$: C, 23.15; H, 7.77; N 6.75. Found: C, 23.32; H, 7.91; N, 6.76.

Preparation of [*closo*-1-CB_9H_9-10-OCOPh]$^-$[Me_4N]$^+$ (13[10]a-[Me_4N]). To a stirred solution of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 35.0 mg, 0.109 mmol) in MeCN (0.4 mL) $[Me_4N]^+PhCOO^-$ (36 mg, 0.185 mmol) was added. The mixture was heated at 40 ^oC for 9 hr. The solvent was evaporated under reduced pressure and the resulting crude product was purified by column chromatography (CH_2Cl_2 gradient to CH_2Cl_2/MeCN 5:1, R_f = 0.17 at CH_2Cl_2/MeCN 5:1) to give 31.0 mg (91% yield) of benzoyloxy derivative **13[10]a-[Me_4N]** as a colorless solid: mp 236-238 ^oC; ^1H NMR (500 MHz, CD_3CN) δ 0.3–1.8 (m, 8H), 3.06 (s, 12H), 4.46 (br s, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 1H), 8.24 (dd, J_1 = 7.1 Hz, J_2 = 1.5 Hz, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 40.1 (br), 56.3 (t, *J* = 3.9 Hz), 129.5, 130.7, 133.1, 134.6, 167.1; ^{11}B NMR (160 MHz, CD_3CN) δ –26.5 (d, *J* = 141 Hz, 4B), –22.9 (d, *J* = 151 Hz, 4B), 42.7 (s, 1B); IR (KBr) ν 2552 and 2550 (B–H), 1695 (C=O), 1479, 1290, 1205, 710 cm^{-1}; HRMS ESI (-) *m/z*: calcd for $C_8H_{14}B_9O_2$ 241.1831; found 241.1841. Anal. Calcd. for $C_{12}H_{26}B_9NO_2$: C, 45.96; H, 8.36; N 4.47. Found: C, 46.11; H, 8.57; N, 4.32.

Preparation of [*closo*-1-CB_9H_9-10-N_3]$^-$[Bu_4N]$^+$ (14[10]a-[Bu_4N]). To a stirred solution of [*closo*-1-CB_9H_9-10-IPh] (**5[10]a**, 28.0 mg, 0.087 mmol) in THF (1.2 mL), $[Bu_4N]^+N_3^-$ (29 mg, 0.102 mmol) was added. After stirring for 2 hr at room temperature the solvent was evaporated under reduced pressure and the crude product was purified by column chromatography (CH_2Cl_2, R_f = 0.45) to yield 34.0 mg (95% yield) of azide **14[10]a-[Bu_4N]** as a colorless oil: ^1H NMR (500 MHz, CD_3CN) δ 0.3–1.8 (m, 8H), 0.97 (t, *J* = 7.4 Hz, 12H), 1.35 (sex, *J* = 7.4 Hz, 8H), 1.59 (quint, *J* = 8.0 Hz, 8H), 3.07 (pseudo t, *J* = 8.6 Hz, 8H), 4.52 (br s, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 13.9, 20.4, 24.4, 43.8 (br), 59.4 (t, *J* = 2.7 Hz); ^{11}B NMR (160 MHz, CD_3CN) δ –25.3 (d, *J* = 139 Hz, 4B), –21.6 (d, *J* = 152 Hz, 4B), 39.2 (s, 1B); IR (film) ν 2548 and 2515 (B–H), 2117 (N_3) cm^{-1}; HRMS ESI (-) *m/z*: calcd for $CH_9B_9N_3$ 162.1634; found 162.1637.

Functional group transformations

Preparation of [*closo*-1-CB_9H_9-10-N_2] (4[10]a). To a cooled (–15 ^oC) stirred solution of amine **8[10]a** (66 mg, 0.49 mmol) and pyridine (193 mg, 2.44 mmol) in MeCN (2 mL) $[NO]^+[BF_4]^-$

(171 mg, 1.46 mmol) was added in four portions at 5 min intervals. The reaction mixture was stirred for 2 hr at the same temperature and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography (CH_2Cl_2/petroleum ether 1:2, R_f = 0.62) to give 46 mg (65% yield) of **4[10]a** as a colorless solid: mp 125-139 °C dec.; ^{1}H NMR (500 MHz, CD_3CN) δ 1.1–2.4 (br m, 8H), 6.18 (br s, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 77.0 (br); ^{11}B NMR (160 MHz, CD_3CN) δ –16.1 (d, *J* = 148 Hz, 4B), –15.4 (d, *J* = 120 Hz, 4B), 17.1 (s, 1B); IR (KBr) ν 2589 and 2550 (B–H), 2283 (N≡N) cm^{-1}; UV (MeCN), λ_{max} (log ε) 215.0 nm (4.30). Anal. Calcd for $CH_9B_9N_2$: C, 8.20; H, 6.20; N, 19.14. Found: C, 8.45; H, 6.40; N, 18.88.

Preparation of [*closo*-1-CB_9H_9-6-NH_3] (8[6]a). Acetamidinium **10[6]a** (100 mg, 0.567 mmol) was added to a solution of KOH (318 mg, 5.67 mmol) in MeOH (3.8 mL) and the reaction mixture was stirred at 60 °C for 16 hr. After evaporation of MeOH under reduced pressure the residue was acidified with ca.18 % HCl and extracted with Et_2O (3 x 10 mL). The organic layers were combined and dried (Na_2SO_4). After evaporation of the solvent in *vacuo*, the crude material was purified by column chromatography (SiO_2, CH_2Cl_2/MeCN 10:1, R_f = 0.26) to afford 41 mg (76% yield) of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**) as a colorless solid: mp >300 °C dec.; ^{1}H NMR (500 MHz, CD_3CN) δ 0.0–2.1 (m, 7H), 4.76 (t, *J* = 44.8 Hz, 3H), 4.95 (s, 1H), 5.13 (q, *J* = 161 Hz, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, CD_3CN) δ 53.9 (br); ^{11}B NMR (160 MHz, CD_3CN) δ –27.3 (d, *J* = 146 Hz, 1B), –21.6 (d, *J* = 153 Hz, 2B), –20.3 (d, *J* = 160 Hz, 2B), –15.2 (d, *J* = 154 Hz, 2B), –12.7 (s, 1B), 25.9 (d, *J* = 150 Hz, 1B); HRMS ESI (-) *m/z*: calcd for $CH_{11}B_9N$ 136.1729; found 136.1734. Anal. Calcd for $CH_{12}B_9N$: C, 8.87; H, 8.93; N, 10.34. Found: C, 9.20; H, 9.10; N, 10.00.

Preparation of [*closo*-1-CB_9H_9-10-NH_3] (8[10]a). A solution of potassium hydroxide (0.44 g, 7.84 mmol) and acetamidinium **10[10]a** (137 mg, 0.78 mmol) in methanol (7 mL) was stirred at 60 °C for 9 hr. Solvents were removed under reduced pressure, and the residue was acidified with *ca*.18 % hydrochloric acid and extracted with diethyl ether (3 x 10 mL). The organic layers were combined and dried (Na_2SO_4). After evaporation of the solvent in *vacuo*, the crude material was purified by column chromatography (SiO_2, CH_2Cl_2/MeCN, 10:1) to afford 83 mg (78% yield) of amine **8[10]a** as a colorless crystalline solid: mp >250 °C; ^{1}H NMR (500 MHz, CD_3CN)

δ 0.4–1.9 (m, 8H), 5.01 (br s, 1H), 6.54 (br t, J = 47.9 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) δ 52.2 (br); ^{11}B NMR (160 MHz, CD_3CN) δ –23.1 (d, J = 140 Hz, 4B), –20.0 (d, J = 154 Hz, 4B), 33.4 (s, 1B); HRMS ESI (-) *m/z*: calcd for $CH_{11}B_9N$ 136.1729; found 136.1732. Anal. Calcd for $CH_{12}B_9N$: C, 8.87; H, 8.93; N, 10.34. Found: C, 9.11; H, 8.84; N, 9.96.

Preparation of [*closo*-1-CB_9H_9-6-(NHCONHPh)]$^-$[Et_4N]$^+$ (15[6]a-[Et_4N]). To a stirred solution of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**, 25 mg, 0.185 mmol) and *N,N*-diisopropylethylamine (48 mg, 0.369 mmol) in THF (0.4 mL), PhNCO (31.0 mg, 0.259 mmol) was added. Stirring was continued for 4 hr at ambient temperature and the mixture was concentrated at the reduced pressure. The residue was acidified with 5% aqueous solution of HCl and extracted with Et_2O (3x15 mL). The organic layers were combined and concentrated under reduced pressure. A solution of $[Et_4N]^+$ OH^- (1 mL, 35 wt. % in water) was added and the mixture was extracted with CH_2Cl_2 (3x15 mL). The organic layers were combined and dried (Na_2SO_4). Evaporation of the solvent in *vacuo*, followed by column chromatography of the resulting crude product (SiO_2, CH_2Cl_2/MeCN 10:3, R_f = 0.15) gave 65 mg (92% yield) of urea **15[6]a-[Et_4N]** as a white solid: mp 68-69 °C; ^1H NMR (500 MHz, CD_3CN) δ 0.0–2.0 (m, 7H), 1.19 (tt, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 12H), 3.14 (q, J = 7.3 Hz, 8H), 4.30 (br s, 1H), 4.87 (s, 1H), 5.15 (q, J = 146 Hz, 1H), 6.95 (t, J = 7.4 Hz, 1H), 7.25 (t, J = 7.9 Hz, 2H), 7.50 (d, J = 7.9 Hz, 2H), 8.50 (br s, 1H); (500 MHz, acetone-d_6) δ 0.0–2.2 (br m, 7H), 1.33 (tt, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 12H), 3.40 (q, J = 7.3 Hz, 8H), 4.33 (br s, 1H), 4.79 (s, 1H), 5.27 (q, J = 146 Hz, 1H), 6.91 (t, J = 7.3 Hz, 1H), 7.24 (t, J = 7.9 Hz, 2H), 7.58 (d, J = 7.9 Hz, 2H), 8.79 (br s, 1H); $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_3CN) δ 7.7, 53.1, 54.7 (br), 119.2, 122.6, 129.8, 141.6, 159.0; (126 MHz, acetone-d_6) δ 7.6, 52.9, 54.2 (br), 118.7, 122.0, 129.4, 141.9, 158.7; ^{11}B NMR (160 MHz, CD_3CN) δ –28.2 (d, J = 135 Hz, 1B), –18.5 (d, J = 148 Hz, 4B), –15.0 (d, J = 149 Hz, 2B), –11.7 (s, 1B), 22.0 (d, J = 139 Hz, 1B); (160 MHz, acetone-d_6) δ –27.8 (d, J = 136 Hz, 1B), –18.2 (d, J = 146 Hz, 4B), –14.6 (d, J = 151 Hz, 2B), –11.4 (s, 1B), 22.3 (d, J = 142 Hz, 1B); HRMS ESI (-) *m/z*: calcd for $C_8H_{16}B_9N_2O$ 255.2100; found 255.2111. Anal. Calcd. for $C_{16}H_{36}B_9N_3O$: C, 50.08; H, 9.46; N, 10.95. Found: C, 49.82; H, 9.20; N, 10.71.

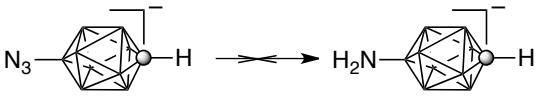
Preparation of [*closo*-1-CB_9H_9-6-(NHCSNHC$_6$H$_3$(CF$_3$)$_2$-3,5)]$^-$[Et_4N]$^+$ (16[6]a-[Et_4N]). A mixture of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**, 17 mg, 0.126 mmol), *N,N*-diisopropylethylamine (32

mg, 0.251 mmol) and 3,5-bis(trifluoromethyl)phenyl isothiocyanate (102 mg, 0.378 mmol) in THF (0.35 mL) was stirred at 40 ^{o}C for 15 hr. The solvent was evaporated under reduced pressure and the residue was acidified with 5% aqueous solution of HCl and extracted with Et_2O (3x15 mL). The organic layers were combined and concentrated under reduced pressure. A solution of $[Et_4N]^+$ OH^- (1 mL, 35 wt. % in water) was added and a mixture was extracted with CH_2Cl_2 (3x15 mL). The organic layers were combined and dried (Na_2SO_4). After evaporation of the solvent the crude product was purified by a column chromatography (SiO_2, CH_2Cl_2/MeCN 10:1, R_f = 0.22) to yield 46.0 mg (69% yield) of thiourea derivative **16[6]a-[Et4N]** as a colorless solid: mp 123-124 ^{o}C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.0–2.1 (br m, 7H), 1.19 (tt, J_1 = 7.3 Hz, J_2 = 1.8 Hz, 12H), 3.14 (q, J = 7.3 Hz, 8H), 5.01 (s, 1H), 5.28 (q, J = 146 Hz, 1H), 6.18 (s, 1H), 7.73 (s, 1H), 8.46 (s, 2H), 9.93 (br s, 1H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 7.7, 53.0 (t, J = 3.0 Hz), 56.3 (br s), 123.4, 123.5, 124.9 (q, J = 272 Hz), 131.8 (q, J = 33 Hz), 143.1, 184.4; ^{19}F NMR (188 MHz, CD_3CN) δ –62.77; ^{11}B NMR (160 MHz, CD_3CN) δ –26.9 (d, J = 145 Hz, 1B), –18.6 (d, J = 152 Hz, 4B), –15.1 (d, J = 152 Hz, 2B), –12.9 (s, 1B), 22.1 (d, J = 145 Hz, 1B); HRMS ESI (-) *m/z*: calcd for $C_{10}H_{14}B_9F_6N_2S$ 407.1619; found 407.1634. Anal. Calcd. for $C_{18}H_{34}B_9F_6N_3S$: C, 40.35; H, 6.40; N, 7.84. Found: C, 40.34; H, 6.40; N, 7.99.

Preparation of [*closo*-1-CB_9H_9-6-(NHAlaBoc)]$^-$ $[Et_4N]^+$ (17[10]a-[Et_4N]). To a solution of *L*-Boc-Ala-OH (19 mg, 0.1 mmol) in THF (0.6 mL) at 0 ^{o}C DCC (23 mg, 0.11 mmol) was added. After 25 min at 0 ^{o}C [*closo*-1-CB_9H_9-6-NH_2]$^-$ $[Et_4N]^+$ (**8[6]a-[Et_4N]**, 26 mg, 0.1 mmola) was added and stirring was continued at ambient temperature for 18 hr. The solvent was evaporated and the residue was purified by column chromatography (CH_2Cl_2/MeCN, 10:6) to give 18.0 mg of about 90% pure amide **17[10]a-[Et_4N]**: ^{1}H NMR (500 MHz, CD_3CN) δ major signals 0.1–2.0 (br m, 7H), 1.08 (d, J = 7.1 Hz, 3H), 1.20 (tt, J_1 = 7.2 Hz, J_2 = 1.9 Hz, 12H), 1.39 (s, 9H), 3.16 (q, J = 7.3 Hz, 8H), 3.76 (br s, 1H), 4.70 (br s, 1H), 4.51–5.52 (br m, 1H), 5.47 (br s, 1H), 5.79 (s, 1H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 7.7, 19.2, 28.6, 52.2 (br), 53.1 (t, J = 3.0 Hz), 79.7, 156.2, 175.9; ^{11}B NMR (160 MHz, CD_3CN) δ –28.6 (d, J = 135 Hz, 1B), –19.9 (d, J = 129 Hz, 2B), –19.0 (d, J = 151 Hz, 2B), –15.9 (d, J = 146 Hz, 2B), –12.6 (s, 1B), 25.2 (d, J = 151 Hz, 1B); HRMS ESI(-), *m/z*: calcd for $C_9H_{24}B_9N_2O_3$ 307.2624; found: 307.2632. Further attempts at purification gave no improvement.

Preparation of [*closo*-1-CB_9H_9-10-(SC_5H_9)] (18[10]a). A mixture of [*closo*-1-CB_9H_9-10-$SCHNMe_2$] (**12[10]a**, 33 mg, 0.159 mmol), 1,5-dibromopentane (40 mg, 0.175 mmol), $[Me_4N]^+OH^-•5H_2O$ (86 mg, 0.477 mmol) in MeCN (2.5 mL) was stirred at 70 °C overnight. The solvent was removed *in vacuo* and the residue was purified by column chromatography (CH_2Cl_2/hexane 1:3, R_f = 0.45) to give 25.0 mg (71% yield) of sulfonium **18[10]a** as a white solid: mp 150–151 °C; ^{1}H NMR (500 MHz, CD_3CN) δ 0.6–2.0 (br m, 8H), 1.64-1.73 (m, 1H), 1.98–2.05 (m, 3H), 2.27–2.37 (m, 2H), 3.36 (td, J_1 = 12.3 Hz, J_2 = 2.3 Hz, 2H), 3.65 (dt, J_1 = 12.6 Hz, J_2 = 2.4 Hz, 2H), 5.59 (br s, 1H); (500 MHz, acetone-d_6) δ 0.6–1.9 (br m, 8H), 1.75–1.85 (m, 1H), 1.95–2.15 (m, 3H), 2.39–2.48 (m, 2H), 3.45 (td, J_1 = 6.7 Hz, J_2 = 2.2 Hz, 2H), 3.79 (d, J = 12.9 Hz, 2H), 5.57 (s, 1H); ^{13}C{^{1}H} NMR (126 MHz, CD_3CN) δ 24.5, 24.6, 40.8, 65.3 (br); (126 MHz, acetone-d_6) δ 24.5, 40.5, 65.3 (br); ^{11}B NMR (160 MHz, CD_3CN) δ –20.6 (d, J = 142 Hz, 4B), –17.7 (d, J = 156 Hz, 4B), 28.5 (s, 1B); (160 MHz, acetone-d_6) δ –21.4 (d, J = 143 Hz, 4B), –18.5 (d, J = 155 Hz, 4B), 27.3 (s, 1B); HRMS ESI (-) *m/z*: calcd for $C_6H_{18}B_9S$ 221.1967; found 221.1977. Anal. Calcd. for $C_6H_{19}B_9S$: C, 32.67; H, 8.68. Found: C, 32.71; H, 8.61.

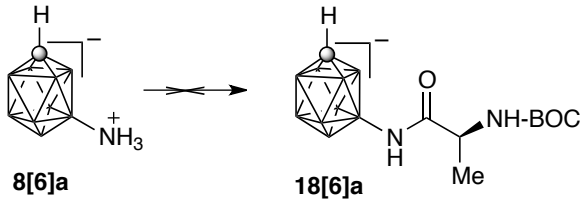
Attempted Reduction of [*closo*-1-CB_9H_9-10-N_3]$^-$ (14[10]a).



14[10]a **8[10]a**

1. To a solution of [*closo*-1-CB_9H_9-10-N_3]$^-$ (**14[10]a**, 34 mg, 0.084 mmol) in THF (1 mL) Pd/C (10%,7 mg) was added and the stirred suspension was saturated with H_2 gas supplied from a balloon. After 24 h at ambient temperature unreacted substrate was fully recovered and conformed by ^{11}B NMR and TLC.
2. To a solution of [*closo*-1-CB_9H_9-10-N_3]$^-$ (**14[10]a**, 12 mg, 0.031 mmol) in CD_3CN (0.45 mL) Ph_3P (24 mg, 0.093 mmol) was added and the solution was stirred for 6 h at 45 °C. No reaction was detected by ^{31}P, ^{11}B and ^{1}H NMR spectroscopy. Also no reaction was detected after 24 h at 60 °C.

Attempted bioconjugation of [*closo*-1-CB_9H_9-6-NH_2]$^-$ (8[6]a).



A solution of [*closo*-1-CB_9H_9-6-NH_2]$^-$ [NEt_4]$^+$ (**8[6]a-[NEt$_4$]**, 20 mg, 0.076 mmol, 1 eq.) and methyl ester Boc-Ala-OMe (140 mg, 0.688 mmol, 9 eq.) in THF (0.2 mL) was stirred at ambient temperature for 4 days. No reaction was detected by NMR or TLC.

2. Details of ESI(-) MS data acquisition

All experiments were performed on a Waters Synapt HDMS fitted with an atmospheric pressure ionization electrospray source (Waters Corporation, Milford, MA, USA). The instrument was operated in negative-ion mode.
Capillary voltage: 2.5 kV;
Cone: 40.0 V;
Source Offset: 50 V;
Source temp.: 80 °C;
Desolvation temp.: 150 °C;
Cone gas flow: 50 L/h;
Desolvation gas flow: 800 L/h;

For accurate mass acquisition, a lock-mass of leucine enkephalin ([M − H]− = 554.2615) was used. Data collection and processing were controlled by MassLynx 4.1 software (Waters Corp.).

3. Details of XRD analysis

X-Ray data collection. Single-crystal X-ray diffraction measurement for 4[10]a, 9[6]a and 9[10]a and 10[10]a was performed with a Supernova Dual Source diffractometer equipped with an Atlas detector at 100 K whereas for 10[10]b it was performed with a SuperNova Single Source diffractometer equipped with an Eos detector at 90 K. The measurements for 4[10]a and 10[10]a were conducted u using the Mo*K*α radiation (λ = 0.71073 Å), whereas the measurements for 9[6]a and 9[10]a were performed using the Cu-*K*α radiation (λ = 0.71073 Å). The crystals were positioned at ~50 mm from the CCD detectors. A total number of 1862 frames were collected at 1° intervals with a counting time of 15 and 70 s for 4[10]a, 5433 frames at 1° intervals with a counting time of 2.5, 4 and 5 s for 9[6]a, 4858 frames at 1° intervals with a counting time of 1.5, 2.5 and 3 s for 9[10]a and 887 frames at 1° intervals with a counting time of 15 and 50 s for 10[10]a. The data were corrected for Lorentzian and polarization effects. Data

reduction and analysis were carried out with the CrysAlis program.[5] All structures were solved by direct methods using SHELXS-97 and refined using SHELXL-97[6] within the Olex2 program.[7] The refinement was based on F^2 for all reflections except those with very negative F^2. Weighted R factors (wR) and all goodness-of-fit (GooF) values are based on F^2. Conventional R factors are based on F with F set to zero for negative F^2. The $F_o^2 > 2\sigma(Fo^2)$ criterion was used only for calculating the R factors and it is not relevant to the choice of reflections for the refinement. The R factors based on F^2 are about twice as large as those based on F. Scattering factors were taken from the International Tables for Crystallography.[8] The positions of all hydrogen atoms in compounds 4[10]a and 10[10]a were located in difference Fourier map and refined *freely, whereas* in case of derivatives 9[6]a and 9[10]a the treatment of hydrogen atoms during refinement was mixed. In the 9[6]a most of the H-atoms were positioned geometrically, with C–H and B–H equal to 0.95 and 1.21 Å, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C,B)$. The exception was made for the H-atoms bonded to the C(6) and the B(2) atoms. The positions of the aforementioned hydrogens were located in difference map and refined *freely*. In case of derivative 9[10]a H-atom linked to the C(6) atom was found from the difference Fourier map and then refined as freely. The positions of remaining H-atoms in this derivative were positioned geometrically, with C–H and B–H equal to 0.95 and 1.21 Å, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C,B)$. The figures for this publication were prepared using Olex2 and Mercury programs.[7,9]

The structures are deposited at CCDC (1585235–1585238).

Table S1. Crystal data and refinement details for selected compounds.[a]

	4[10]a	**9[6]a**	**9[10]a**	**10[10]a**
Empirical formula	$CH_9B_9N_2$	$C_6H_{14}B_9N$	$C_6H_{14}B_9N$	$C_3H_{15}B_9N_2$
Formula weight	146.39	197.47	197.47	176.46
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	*Pbcm*	*Pbca*	$P2_1/n$	$P2_1/n$
a/Å	10.05044(13)	10.26745(13)	10.27824(14)	11.9956(2)
b/Å	9.06474(12)	11.60263(12)	8.91573(11)	7.28546(18)
c/Å	18.4188(2)	19.0717(2)	12.86546(18)	12.7122(3)
β/°	90	90	101.8937(14)	105.760(2)
Volume/Å^3	1678.04(4)	2272.00(4)	1153.65(3)	1069.20(4)
Z	8	8	4	4
Goodness-of-fit on F^2	1.069	1.052	1.055	1.049
Final *R* indexes [$I>=2\sigma$ (I)]	$R_1 = 0.0322$, w$R_2 = 0.0962$	$R_1 = 0.0397$, w$R_2 = 0.1056$	$R_1 = 0.0399$, w$R_2 = 0.1024$	$R_1 = 0.0404$, w$R_2 = 0.1060$
Final *R* indexes [all data]	$R_1 = 0.0374$, w$R_2 = 0.0995$	$R_1 = 0.0431$, w$R_2 = 0.1096$	$R_1 = 0.0422$, w$R_2 = 0.1052$	$R_1 = 0.0531$, w$R_2 = 0.1149$

[a] Temperature 100 K (except for **9[10]a**, where $T = 90$ K) and $\lambda = 1.54184$ Å (except for **4[10]a**, where $\lambda = 0.71073$ Å).

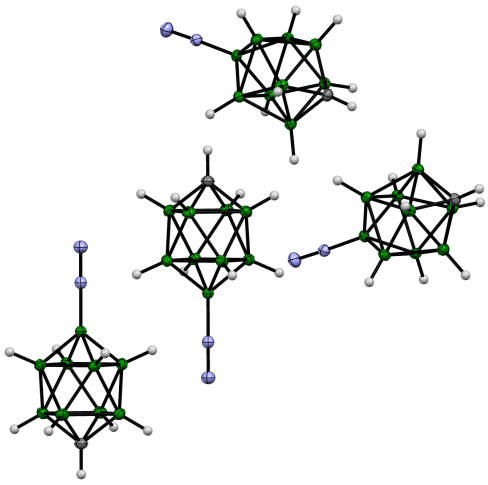


Figure S1. Partial packing diagram for **4[10]a** showing two pairs of unique molecules. Thermal ellipsoid diagram drawn at 50% probability and the numbering system according to the chemical structure.

4. Comparison of molecular structures parameters of [*closo*-1-CB_9H_8-1-COOH-10-X]$^-$ derivatives

Table S2. Selected interatomic distances and angles for derivatives of carboxylic acids [*closo*-1-CB_9H_8-1-COOH-10-X]$^-$.[a]

	2b-[Et_4N] [b] X = H	**9[10]b** [c,d] X = Pyridine	**4[10]b** [c] X = N_2
C(1)–COOH	1.484(4)	1.482(5)	1.486(2)
C(1)–B(2) avrg	1.613(5)	1.601(4)	1.606(1)
C(1)···B(2-5) [e]	0.934	0.927(3)	0.922
B(2)–B(3) avrg	1.858(11)	1.847(9)	1.859(8)
B(2)–B(6) avrg	1.811(9)	1.800(4)	1.805(2)
B(6)–B(7) avrg	1.845(9)	1.850(7)	1.879(6)
B(6)–B(10) avrg	1.707(17)	1.676(4)	1.670(2)
B(10)···B(6-9) [e]	1.101	1.048(3)	1.013
B(10)–N –		1.527(3)	1.498(2)
C(1)···B(10)	3.543	3.471(1)	3.429
B–C(1)–C	125.3(39)	125.3(12)	125.0(10)
B–B(10)–X	130.2(4) [f]	128.7(14) [g]	127.3(18) [g]

[a] Except for unique in each molecule distances C(1)–C, B(10)–N and the cage size C(1)···B(10), all parameters are average values and the esd refers to the distribution of the measured values. [b] Ref.[10] . [c] Ref.[11]. [d] Four molecules. [e] The height of the square pyramid. [f] X = H. [g] X = N.

5. Comparison of NMR chemical shifts and Hammett constants

Table S3. NMR chemical shifts for selected atoms in [*closo*-1-CB_9H_9-10-R]$^-$ (in (CD_3CN) and in analogous Ph–R derivatives (in DMSO-d_6).

		[*closo*-1-CB_9H_9-10-R]$^-$			Ph–R
Substituent B(10)–R	σ_p [a]	C(1)–H ^{1}H NMR /ppm	C(1) ^{13}C NMR /ppm	B(10) ^{11}B NMR /ppm	C(4)–H ^{1}H NMR /ppm
H	0.0	4.75	54.3	30.1	7.36 [b]
$^+$IPh	[c]	5.88	65.6	21.3	7.69 [d]
$^+NC_5H_5$	–	5.28	55.6	38.6	7.75 [e]
$[NHCNH_2Me]^+$	–	4.98	51.7	33.0	–
$^+SCHNMe_2$	–	5.25	58.9	30.9	–
OCOPh	0.13	4.46	40.1	42.7	7.33 [f]
N_3	0.08	4.52	43.8	39.2	7.19 [g]
CN	0.66	5.16	61.6	20.1	7.62 [h]
$^+S(CH_2)_5$	0.90 [i]	5.59	65.3	28.5	7.77 [i,j]
$^+NH_3$	0.60	5.01	52.2	33.4	–
$^+N_2$	1.91	6.18	77.0	17.1	8.25 [k]

[a] Substituent Hammett constant from ref [12]. [b] Ref [13]. [c] Ref [14]. [d] $CF_3SO_3^-$ salt; ref [15]. [e] Cl- salt; ref[16]. [f] Ref[17]. [g] Ref[18]. [h] Ref[19]. [i] Value for the $^+SMe_2$ group. [j] $CF_3SO_3^-$ salt; ref[20]. [k] $[BF_4]^-$ salt; ref. [21]

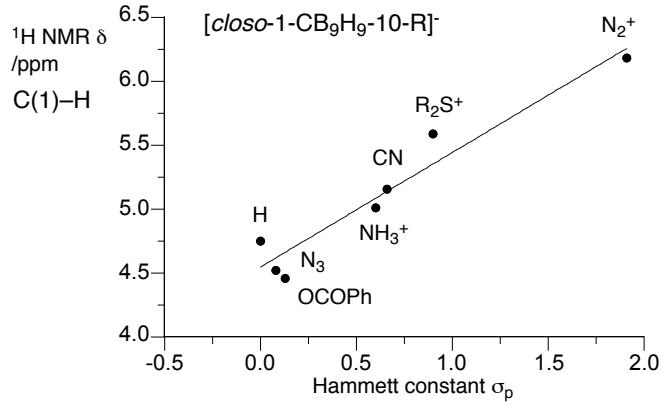


Figure S2. Correlation of the C(1)–H ^{1}H NMR chemical shifts (δ) in [*closo*-1-CB_9H_9-10-R]$^-$ obtained in CD_3CN with Hammett substituent constants σ_p. Best fit line: $\delta = 4.55+0.89\bullet\sigma_p$, r_2 = 0.93.

The established in Figure S2 relationship between ^{1}H NMR chemical shift for the C(1)–H in [*closo*-1-CB_9H_9-10-R]$^-$ derivatives and substituent constants σ_p allows for an estimate of

parameters for substituents for which the σ_p values are not known. Thus, for substituents PhI^+, $C_5H_5N^+$, Me_2CHS^+, and $MeC(NH_2)NH^+$ the σ_p value can be estimated as 1.5, 0.8, 0.8, 0.5, respectively, with an uncertainty of ±0.1. The estimated value $\sigma_p = 1.5\pm0.1$ for the PhI^+ group is consistent with a significant acidity of 4-PhI^+PhCOOH (apparent $pK_a^{'}$ = 4.6, lower limit, in $MeCN/H_2O$, 15:1).[14] A correlation of apparent $pK_a^{'}$ values obtained in ref [14] for a series of six 4-substituted benzoic acids in $MeCN/H_2O$ (15:1) with their σ_p values[12] ($r^2 = 0.970$) gave $\sigma_p = 1.4\pm0.1$ for the PhI^+ group in position 4.

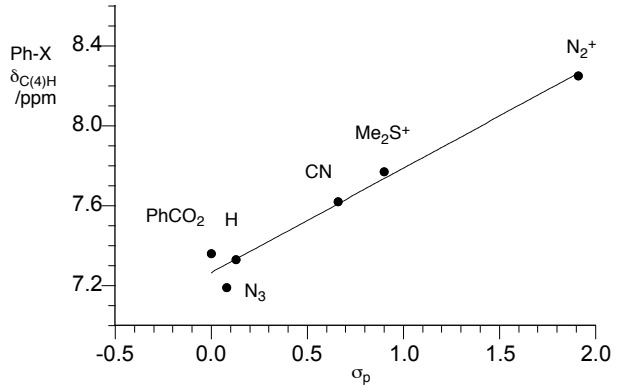


Figure S3. Correlation of the C(4)–H ^{1}H NMR chemical shifts (δ) in Ph-X obtained in DMSO-d_6 with Hammett substituent constants σ_p. Best fit line: $\delta = 7.27(4)+0.52(5)\bullet\sigma_p$, $r^2 = 0.970$.

Using the correlation in Figure S3, the σ_p value for the PhI^+ group can estimated as 0.77(5). This is in stark contrast to the estimates from the correlation for [*closo*-1-CB_9H_9-10-R]$^-$ in Figure S2.

6. Details of TD-DFT calculation and partial output data

Excitation energies calculated with the CAM-B3LYP/6-31++G(2d,p)//M062x/6-31G(2d,p) method are systematically overestimated give slightly better correlation with experiment than with CAM-B3LYP/6-31++G(2d,p)//B3LYP/6-31G(2d,p) method (E_{exp} = -1.3±0.40 + 1.19±0.07• E_{theor} eV, $r^2 = 0.988$). Both methods perform significantly better than that without long-range correlation and diffuse functions (the B3LYP/6-31G(2d,p)// B3LYP/6-31G(2d,p)) method; E_{exp} = -1.26±0.56 + 0.81±0.12• E_{theor} eV, $r^2 = 0.935$); these values are systematically underestimated relatively to the experiment.

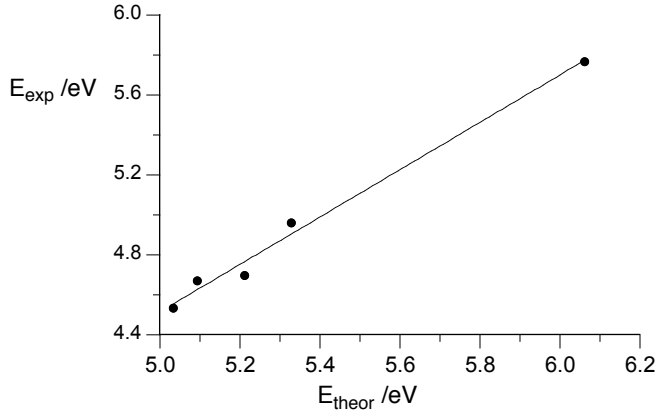


Figure S4. Correlation between theoretical (TD CAM-B3LYP/6-31++G(2d,p) // M06-2x/6-31G(2d,p) method) and experimental excitation energies in MeCN. Best fit function E_{exp} = -1.4±0.37 + 1.18±0.07• E_{theor} eV, r^2 = 0.990.

4[1]a

```
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-E      4.5199 eV  274.31 nm f=0.0000 <S**2>=0.000
      32 -> 38         0.10430
      33 -> 39        -0.10430
      36 -> 39        -0.47409
      37 -> 38         0.47409
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -376.333470417
 Copying the excited state density for this state as the 1-particle RhoCI
density.
 Excited State   2: Singlet-E     4.6083 eV  269.05 nm  f=0.0000 <S**2>=0.000
      36 -> 38         0.47979
      37 -> 39        -0.47979
 Excited State   3: Singlet-E     4.6439 eV  266.98 nm  f=0.0000 <S**2>=0.000
      32 -> 38         0.10860
      33 -> 39         0.10860
      36 -> 39         0.47806
      37 -> 38         0.47806
 Excited State   4: Singlet-E     5.0724 eV  244.43 nm  f=0.0028 <S**2>=0.000
      35 -> 38         0.69316
 Excited State   5: Singlet-E     5.0724 eV  244.43 nm  f=0.0028 <S**2>=0.000
      35 -> 39         0.69316
 Excited State   6: Singlet-E    5.3292 eV  232.65 nm  f=0.3095 <S**2>=0.000
      36 -> 38         0.48683
      37 -> 39         0.48683
 Excited State   7: Singlet-E    5.3782 eV  230.53 nm  f=0.0143 <S**2>=0.000
      34 -> 38         0.68787
 Excited State   8: Singlet-E    5.3782 eV  230.53 nm  f=0.0143 <S**2>=0.000
      34 -> 39         0.68787
```

4[10]a

```
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-E    4.8145 eV  257.52 nm  f=0.0000 <S**2>=0.000
      35 -> 38         0.49413
      36 -> 39         0.49413
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -376.402608080
 Copying the excited state density for this state as the 1-particle RhoCI
density.
 Excited State   2: Singlet-E    4.8760 eV  254.28 nm  f=0.0000 <S**2>=0.000
      35 -> 38         0.49490
      36 -> 39        -0.49490
 Excited State   3: Singlet-E    4.8852 eV  253.80 nm  f=0.0000 <S**2>=0.000
      35 -> 39         0.49444
      36 -> 38         0.49444
 Excited State   4: Singlet-E    5.4362 eV  228.07 nm  f=0.0041 <S**2>=0.000
      34 -> 38         0.17098
      37 -> 39         0.67371
 Excited State   5: Singlet-E    5.4363 eV  228.07 nm  f=0.0041 <S**2>=0.000
      34 -> 39        -0.17098
      37 -> 38         0.67371
 Excited State   6: Singlet-E    5.6510 eV  219.40 nm  f=0.0243 <S**2>=0.000
      34 -> 39         0.67043
      37 -> 38         0.17750
 Excited State   7: Singlet-E    5.6510 eV  219.40 nm  f=0.0243 <S**2>=0.000
      34 -> 38         0.67043
      37 -> 39        -0.17750
 Excited State   8: Singlet-E    6.0625 eV  204.51 nm  f=0.7784 <S**2>=0.000
      32 -> 38        -0.10399
      33 -> 39        -0.10399
      35 -> 39        -0.48194
      36 -> 38         0.48194
 Excited State   9: Singlet-E    6.5096 eV  190.46 nm  f=0.0000 <S**2>=0.000
      30 -> 38         0.11799
      31 -> 39         0.11799
      32 -> 39        -0.46359
      33 -> 38         0.46359
```

9[1]a

```
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-A1   5.0332 eV  246.33 nm  f=0.2433 <S**2>=0.000
      47 -> 52         0.14319
      51 -> 52         0.67457
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -515.093339806
 Copying the excited state density for this state as the 1-particle RhoCI
density.
 Excited State   2: Singlet-A2   5.1269 eV  241.83 nm  f=0.0000 <S**2>=0.000
      50 -> 52         0.66411
      50 -> 58         0.16554
```

```
 Excited State   3: Singlet-B2   5.2770 eV  234.95 nm  f=0.0460 <S**2>=0.000
      41 -> 53         0.10052
      43 -> 53         0.11166
      46 -> 52         0.52778
      47 -> 53        -0.15302
      48 -> 52         0.36961
      51 -> 53        -0.18104
 Excited State   4: Singlet-B1   5.5673 eV  222.70 nm  f=0.0032 <S**2>=0.000
      49 -> 52         0.69505
 Excited State   5: Singlet-B2   5.8182 eV  213.10 nm  f=0.0177 <S**2>=0.000
      46 -> 52        -0.31465
      48 -> 52         0.58059
      48 -> 58         0.11332
      51 -> 53         0.15406
 Excited State   6: Singlet-A2    5.8527 eV  211.84 nm  f=0.0000 <S**2>=0.000
      51 -> 55         0.54467
      51 -> 57        -0.37362
      51 -> 61        -0.17811

 Excited State   7: Singlet-A1   6.1340 eV  202.13 nm  f=0.0848 <S**2>=0.000
      43 -> 52        -0.15532
      46 -> 53         0.15752
      47 -> 52         0.41377
      50 -> 55         0.31130
      50 -> 57        -0.20555
      50 -> 61        -0.10208
      51 -> 58        -0.26697
      51 -> 59         0.13870
```

9[6]a

```
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-A    5.2112 eV  237.92 nm  f=0.2548 <S**2>=0.000
      51 -> 52         0.69286
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -515.135839825
 Copying the excited state density for this state as the 1-particle RhoCI
density.
 Excited State   2: Singlet-A    5.3449 eV  231.97 nm  f=0.0426 <S**2>=0.000
      43 -> 53         0.14901
      47 -> 52         0.54944
      48 -> 52        -0.14548
      50 -> 52         0.19975
      51 -> 53         0.30227

 Excited State   3: Singlet-A    5.5775 eV  222.29 nm  f=0.0027 <S**2>=0.000
      47 -> 52        -0.17460
      50 -> 52         0.66920
      51 -> 53        -0.10484
 Excited State   4: Singlet-A    6.0260 eV  205.75 nm  f=0.0176 <S**2>=0.000
      47 -> 52         0.14800
      48 -> 52        -0.15155
```

```
      50 -> 57        -0.26365
      51 -> 53        -0.31642
      51 -> 56         0.15344
      51 -> 59         0.42067
      51 -> 64        -0.18579
 Excited State   5: Singlet-A    6.0743 eV  204.11 nm  f=0.0003 <S**2>=0.000
      48 -> 52         0.59315
      50 -> 57        -0.27944
 Excited State   6: Singlet-A    6.1375 eV  202.01 nm  f=0.0112 <S**2>=0.000
      47 -> 52         0.16628
      48 -> 52         0.27415
      50 -> 57         0.46350
      50 -> 62         0.10722
      50 -> 63        -0.11194
      51 -> 53        -0.20647
      51 -> 59         0.19565
 Excited State   7: Singlet-A    6.2229 eV  199.24 nm  f=0.0075 <S**2>=0.000
      49 -> 52         0.16645
      50 -> 53         0.23452
      50 -> 56        -0.12594
      50 -> 59        -0.31734
      50 -> 64         0.14080
      51 -> 54        -0.10438
      51 -> 57         0.43816
      51 -> 63        -0.10173
Excited State   8: Singlet-A     6.2872 eV  197.20 nm  f=0.0012 <S**2>=0.000
      49 -> 52         0.65401
      50 -> 59         0.10942
```

9[10]a

```
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-A1   5.0930 eV  243.44 nm  f=0.3146 <S**2>=0.000
      51 -> 52         0.69155
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -515.144230385
 Copying the excited state density for this state as the 1-particle RhoCI
density.
 Excited State   2:  Singlet-A2   5.2798 eV  234.83 nm  f=0.0000 <S**2>=0.000
      50 -> 52         0.68786
      50 -> 59        -0.10768
 Excited State   3:  Singlet-B2   5.3319 eV  232.53 nm  f=0.0503 <S**2>=0.000
      44 -> 53         0.17866
      47 -> 52         0.57093
      48 -> 52         0.23903
      51 -> 53         0.27336
 Excited State   4: Singlet-B1   5.8956 eV  210.30 nm  f=0.0063 <S**2>=0.000
      49 -> 52         0.68521
      49 -> 59        -0.12585
 Excited State   5: Singlet-B2   6.0607 eV  204.57 nm  f=0.0051 <S**2>=0.000
      47 -> 52        -0.16449
      48 -> 52         0.63358
```

```
      48 -> 59        -0.13276
      51 -> 53        -0.18472
 Excited State   6: Singlet-A2   6.1138 eV  202.79 nm  f=0.0000 <S**2>=0.000
      50 -> 59         0.10047
      51 -> 56         0.46168
      51 -> 57        -0.39964
      51 -> 61         0.25622
      51 -> 66         0.14711
 Excited State   7: Singlet-B2  6.3143 eV  196.36 nm  f=0.1189 <S**2>=0.000
      47 -> 52        -0.32437
      51 -> 53         0.61560
```

20[1]a

```
Excitation energies and oscillator strengths:
Excited State   1: Singlet-A"   5.3040 eV  233.76 nm  f=0.0678 <S**2>=0.000
      47 -> 59         0.12927
      49 -> 59        -0.11731
      50 -> 59         0.11867
      51 -> 58         0.47661
      53 -> 58        -0.40411
      57 -> 58        -0.21008
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -566.023342654
 Copying the excited state density for this state as the 1-particle RhoCI
density.
Excited State   2: Singlet-A'   5.8489 eV  211.98 nm  f=0.0297 <S**2>=0.000
      49 -> 58        -0.10303
      50 -> 58         0.11600
      52 -> 58        -0.15711
      55 -> 58        -0.18742
      56 -> 58         0.63103

 Excited State   3: Singlet-A"   5.8646 eV  211.41 nm  f=0.0053 <S**2>=0.000
      53 -> 58        -0.27433
      57 -> 58         0.64325

 Excited State   4: Singlet-A'   5.8868 eV  210.61 nm  f=0.1528 <S**2>=0.000
      47 -> 58        -0.11031
      49 -> 58         0.21891
      50 -> 58        -0.23210
      51 -> 59         0.11745
      53 -> 59        -0.11226
      55 -> 58         0.52999
      56 -> 58         0.25697
 Excited State   5: Singlet-A"   6.1097 eV  202.93 nm  f=0.0004 <S**2>=0.000
      54 -> 58         0.68547

 Excited State   6: Singlet-A'   6.3647 eV  194.80 nm  f=0.0091 <S**2>=0.000
      46 -> 58        -0.11999
      52 -> 58         0.67001
```

```
      56 -> 58         0.15593

20[12]a
Excitation energies and oscillator strengths:
 Excited State   1: Singlet-A"   5.3840 eV  230.28 nm  f=0.0674 <S**2>=0.000
      47 -> 59         0.15153
      51 -> 58         0.19499
      54 -> 58         0.57840
      55 -> 59        -0.20399
      57 -> 58        -0.21788
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -566.082227180
 Copying the excited state density for this state as the 1-particle RhoCI
density.
Excited State   2: Singlet-A'   5.8739 eV  211.08 nm  f=0.2356 <S**2>=0.000
      47 -> 58        -0.10023
      54 -> 59         0.15432
      55 -> 58         0.66152
 Excited State   3: Singlet-A'   6.3073 eV  196.57 nm  f=0.0047 <S**2>=0.000
      52 -> 58         0.13247
      56 -> 58         0.68258
 Excited State   4: Singlet-A"   6.3119 eV  196.43 nm  f=0.0024 <S**2>=0.000
      53 -> 58         0.34901
      54 -> 58         0.22765
      57 -> 58         0.55957
```

7. NMR spectra

Copies of ^{1}H, $^{13}C\{^{1}H\}$ and $^{11}B\{^{1}H\}$ NMR spectra organized according to the compound number are shown in Figures S5–S69. Partial analytical data including EI MS for a crude mixture of **3[10]c[Et$_4$N]** and [*closo*-1-CB_9H_9-1-C_5H_{11}-10-Ph]$^-$ $[Et_4N]^+$ is shown in Figures S66–S68.

A stack plot of $^{11}B\{^{1}H\}$ NMR spectra taken for a reaction mixture of **4[10]a** with $[Et_4N]^+$ CN^- at three time intervals is shown in Figures S69.

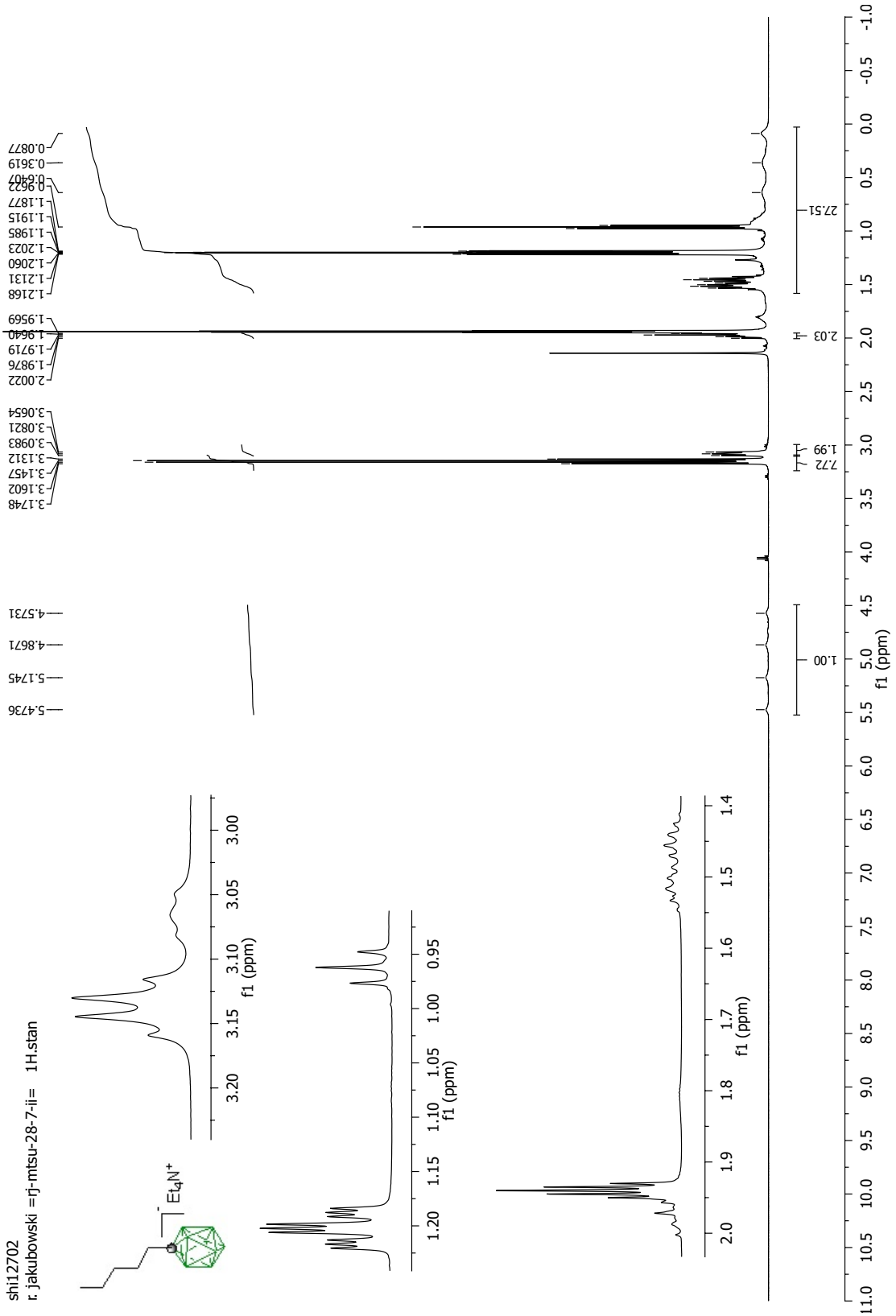


Figure S5. ^{1}H NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}]$^{-}$[Et_4N]$^{+}$ (**2c[Et$_4$N]**; CD_3CN, 500 MHz).

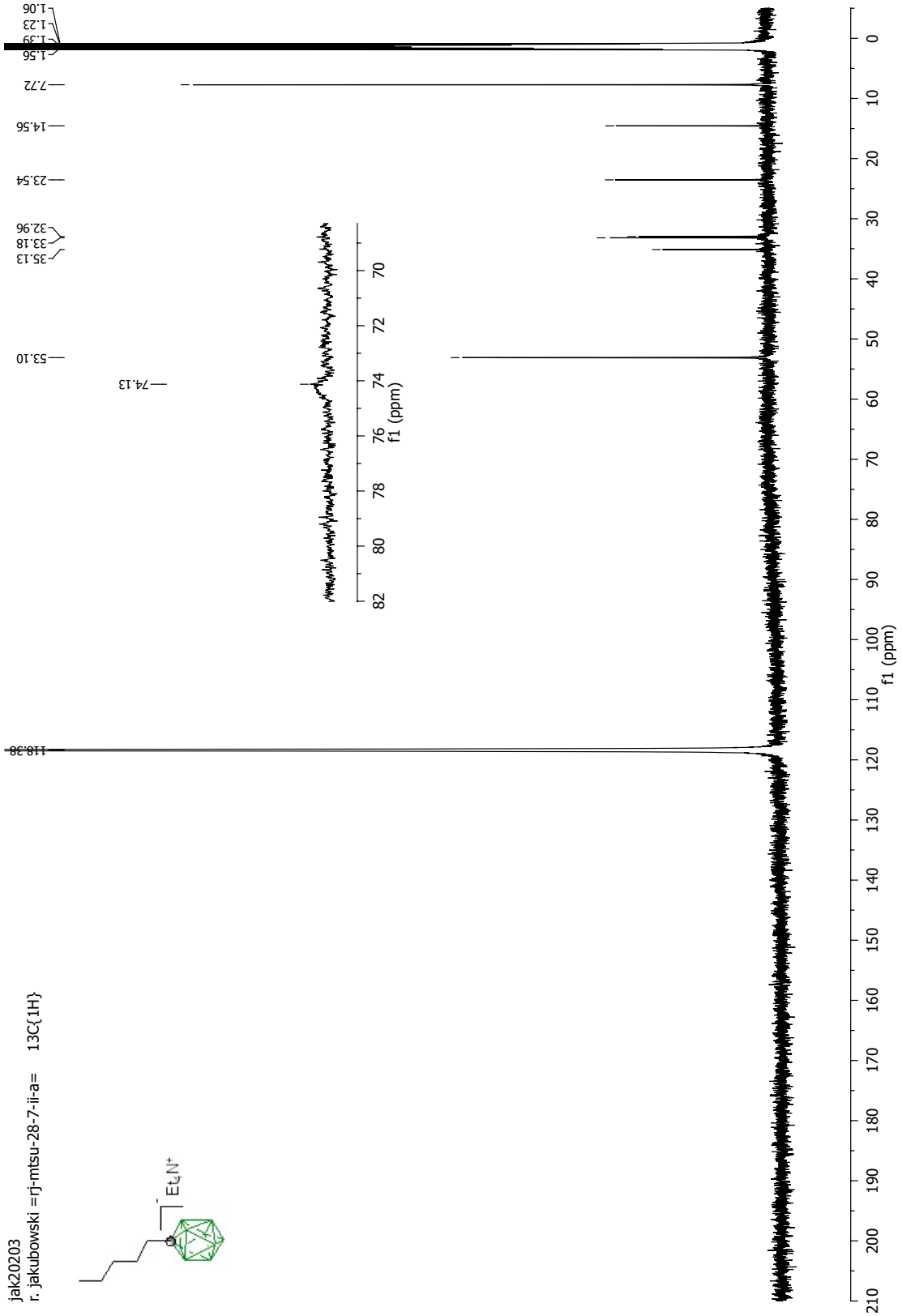


Figure S6. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}]$^-$[Et_4N]$^+$ (**2c[Et$_4$N]**; CD_3CN, 126 MHz).

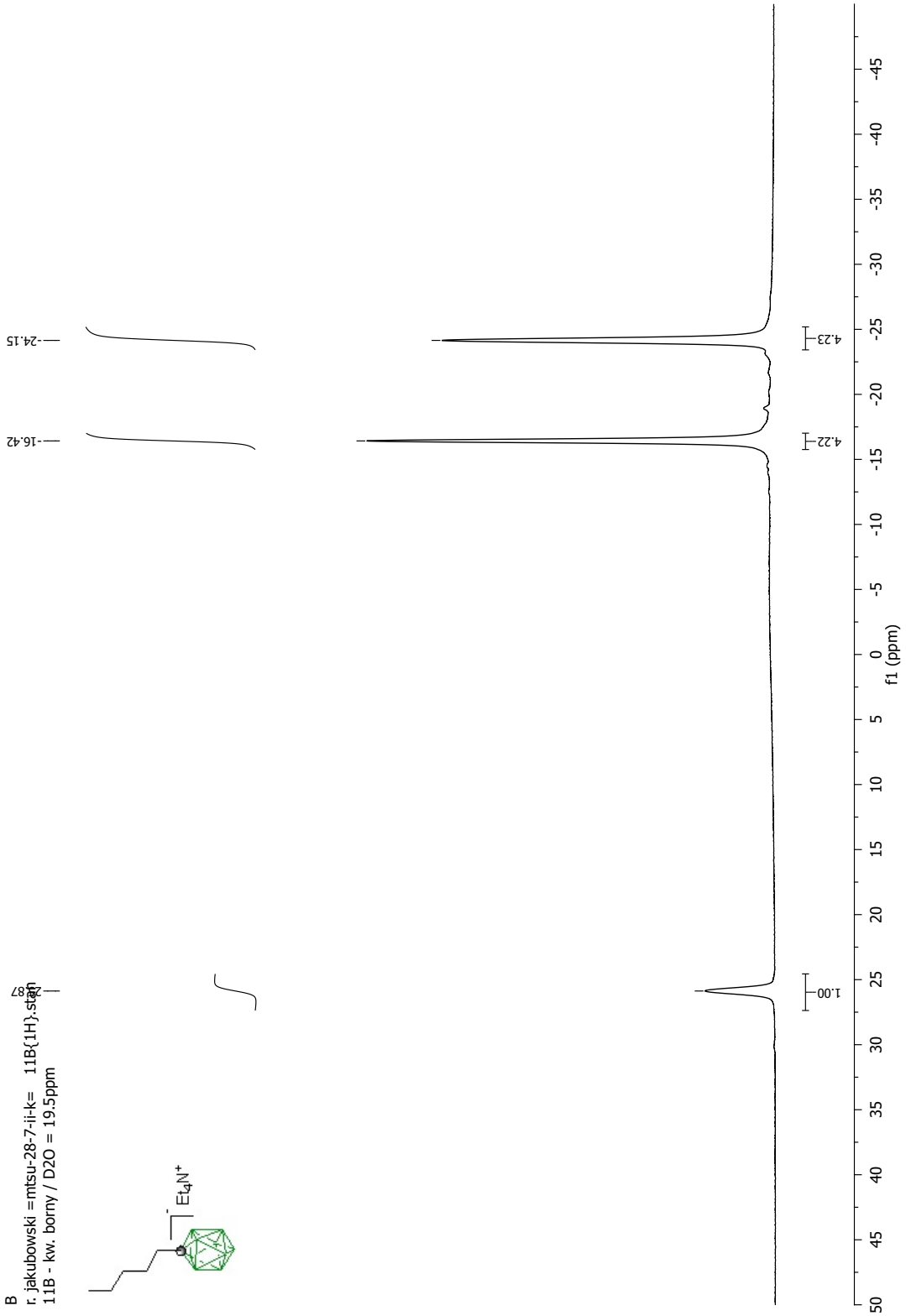


Figure S7. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}]$^-$[Et_4N]$^+$ (**2c[Et$_4$N]**; CD_3CN, 160 MHz).

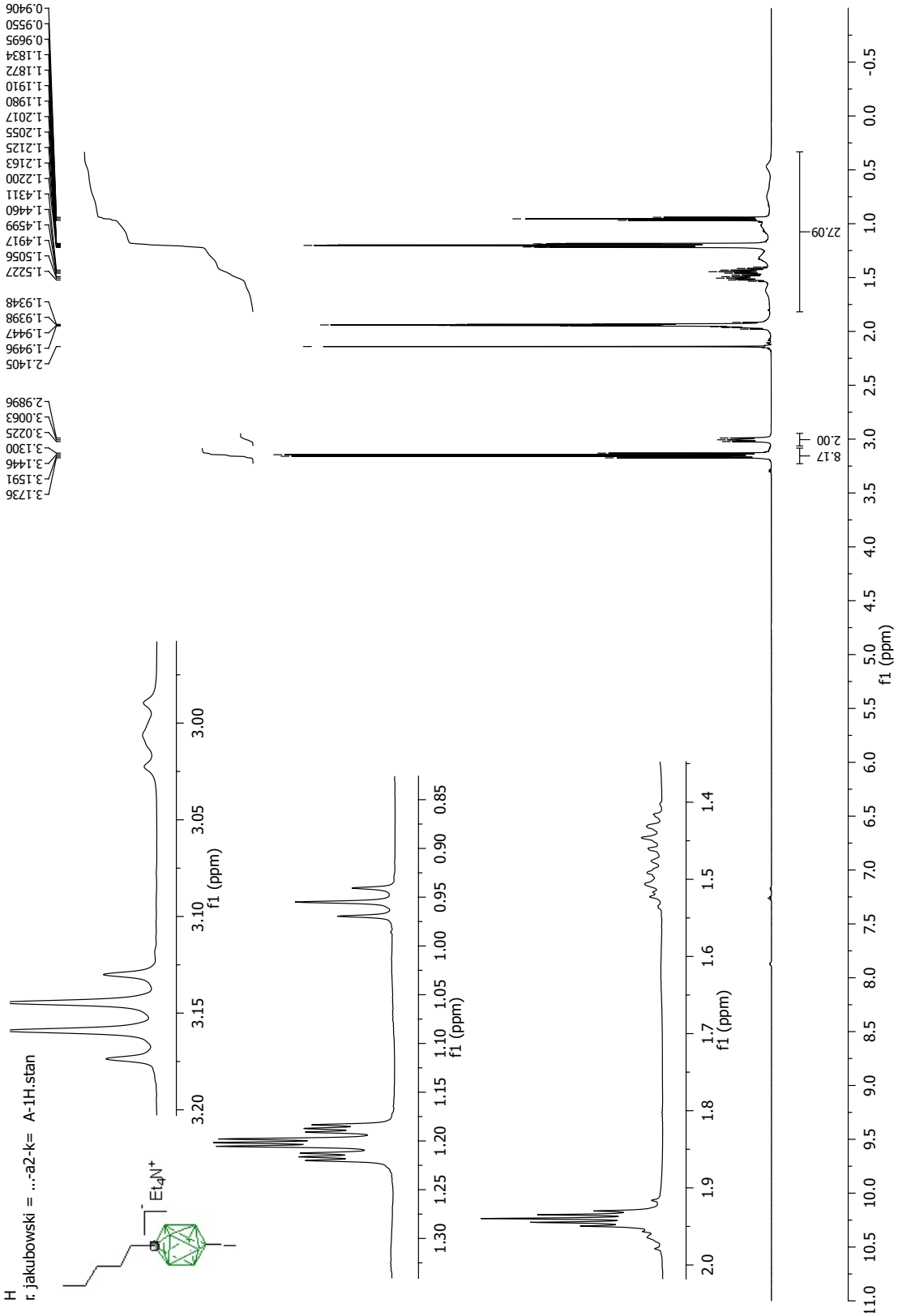


Figure S8. ^{1}H NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-I]$^{-}$[Et_4N]$^{+}$ (**3[10]c[Et_4N]**; CD_3CN, 500 MHz).

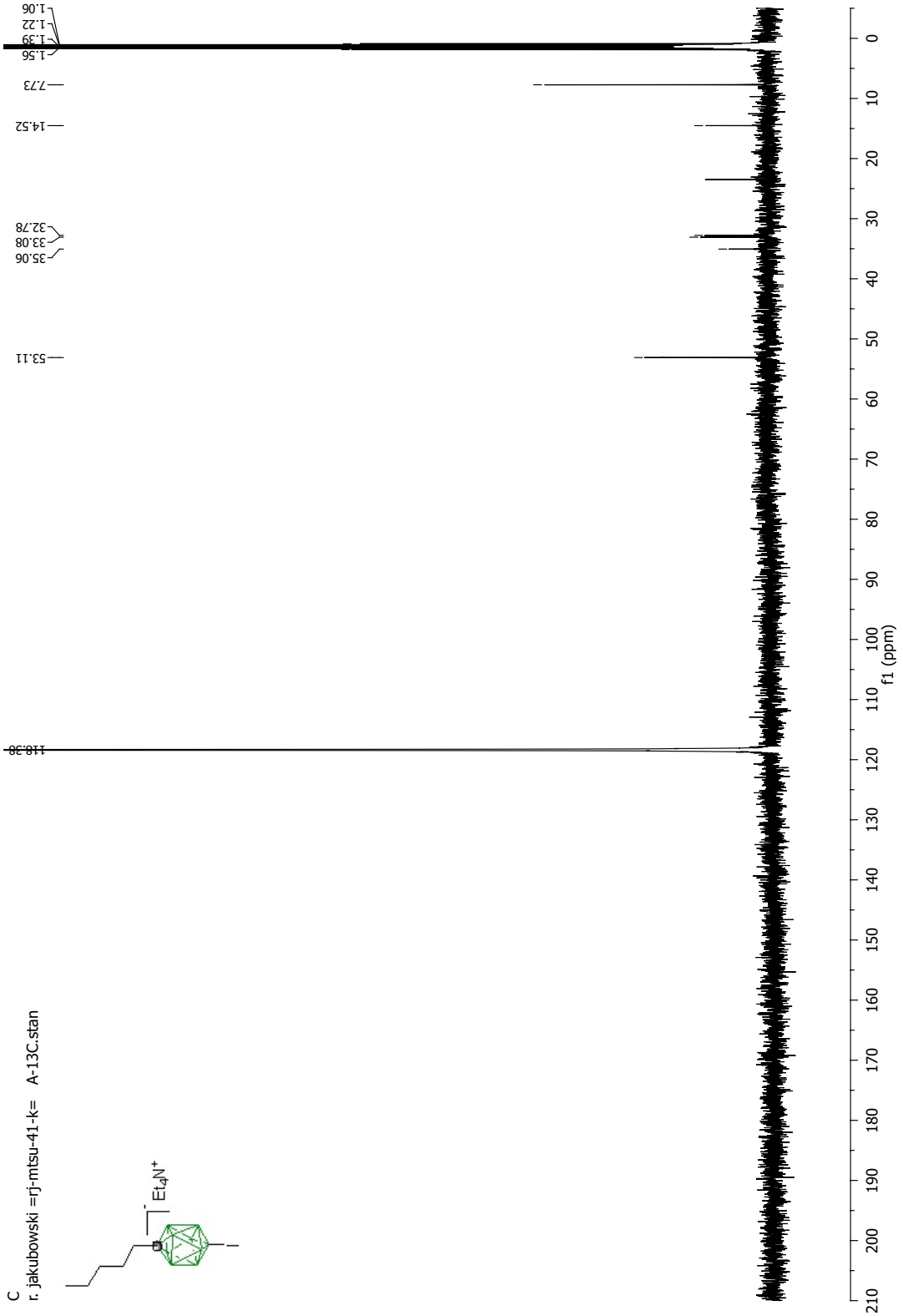


Figure S9. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-I]$^-$[Et_4N]$^+$ (**3[10]c[Et_4N]**; CD_3CN, 126 MHz)

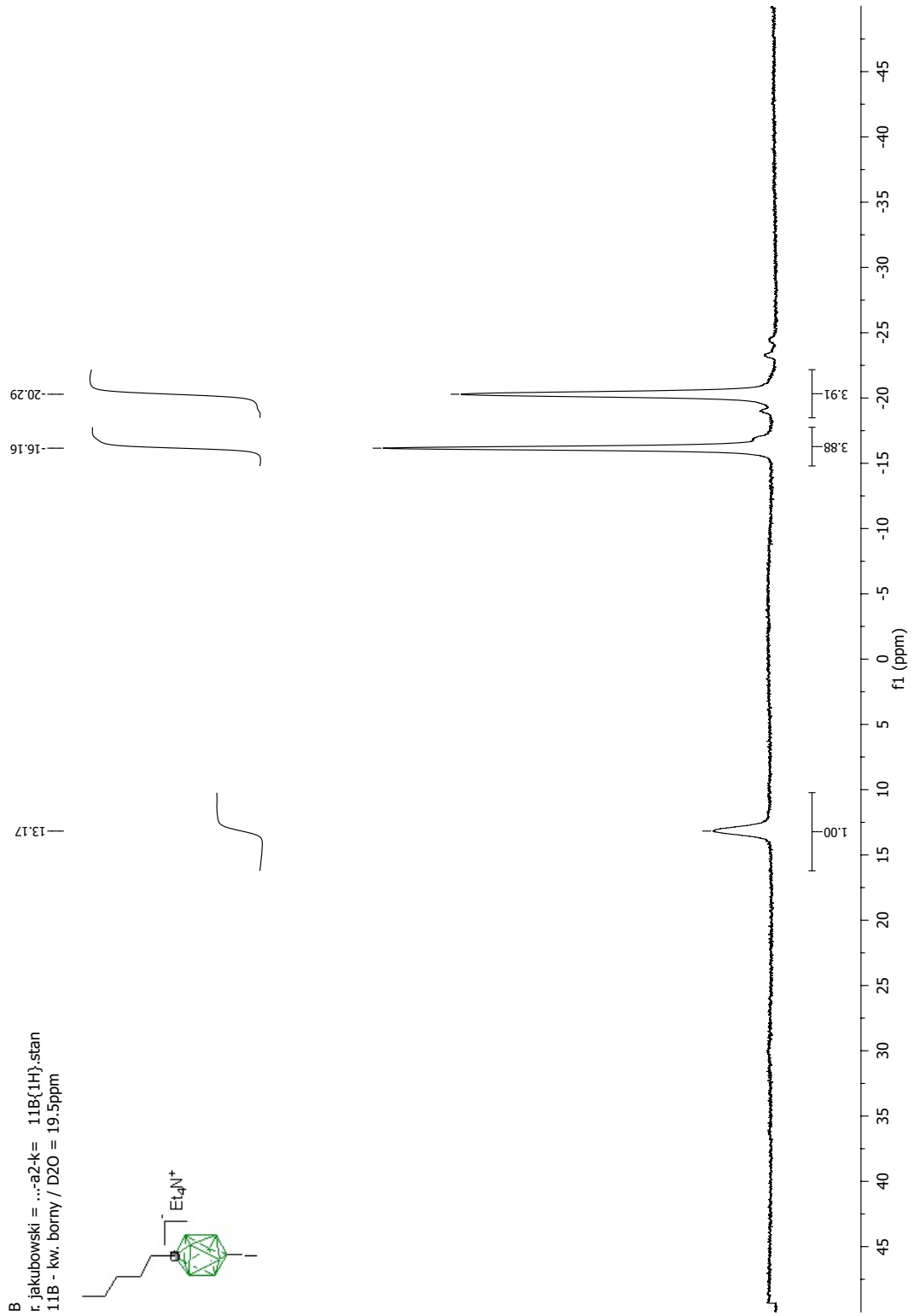


Figure S10. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-I]$^-$[Et_4N]$^+$ (**3[10]c[Et_4N]**; CD_3CN, 160 MHz).

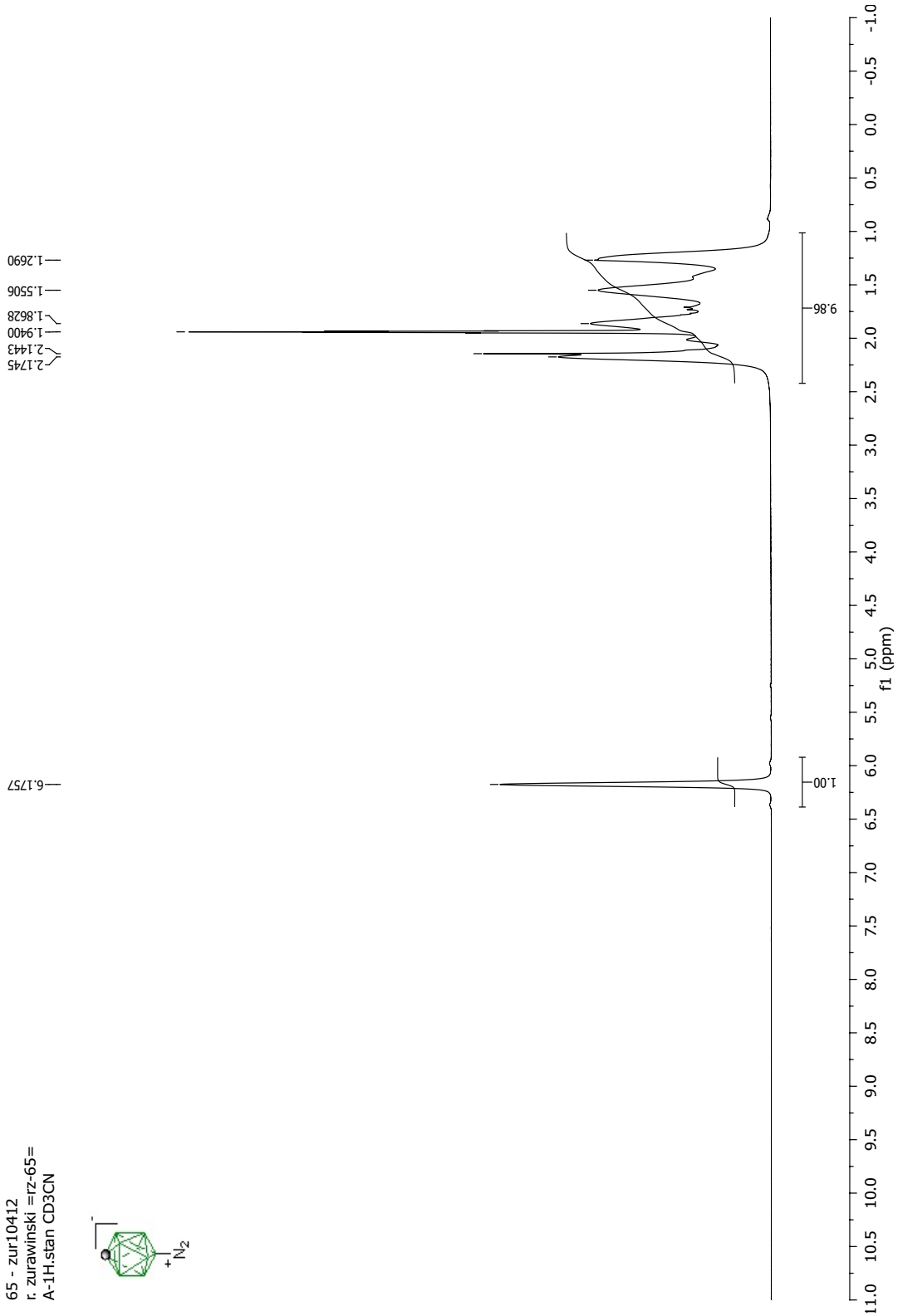


Figure S11. ^{1}H NMR of [*closo*-1-CB_9H_9-10-N_2] (**4[10]a**; CD_3CN, 500 MHz).

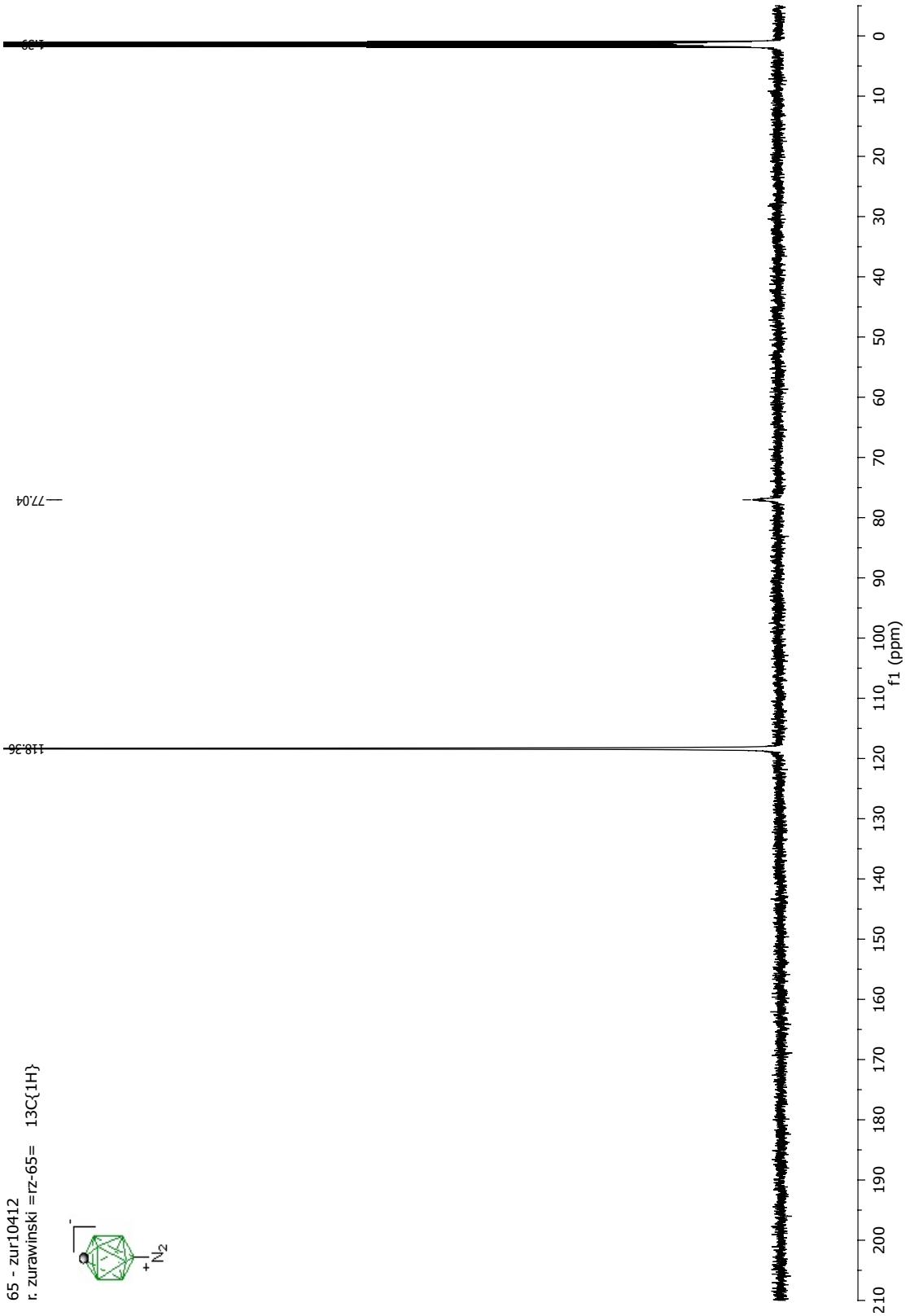


Figure S12. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-N_2] (**4[10]a**; CD_3CN, 126 MHz)

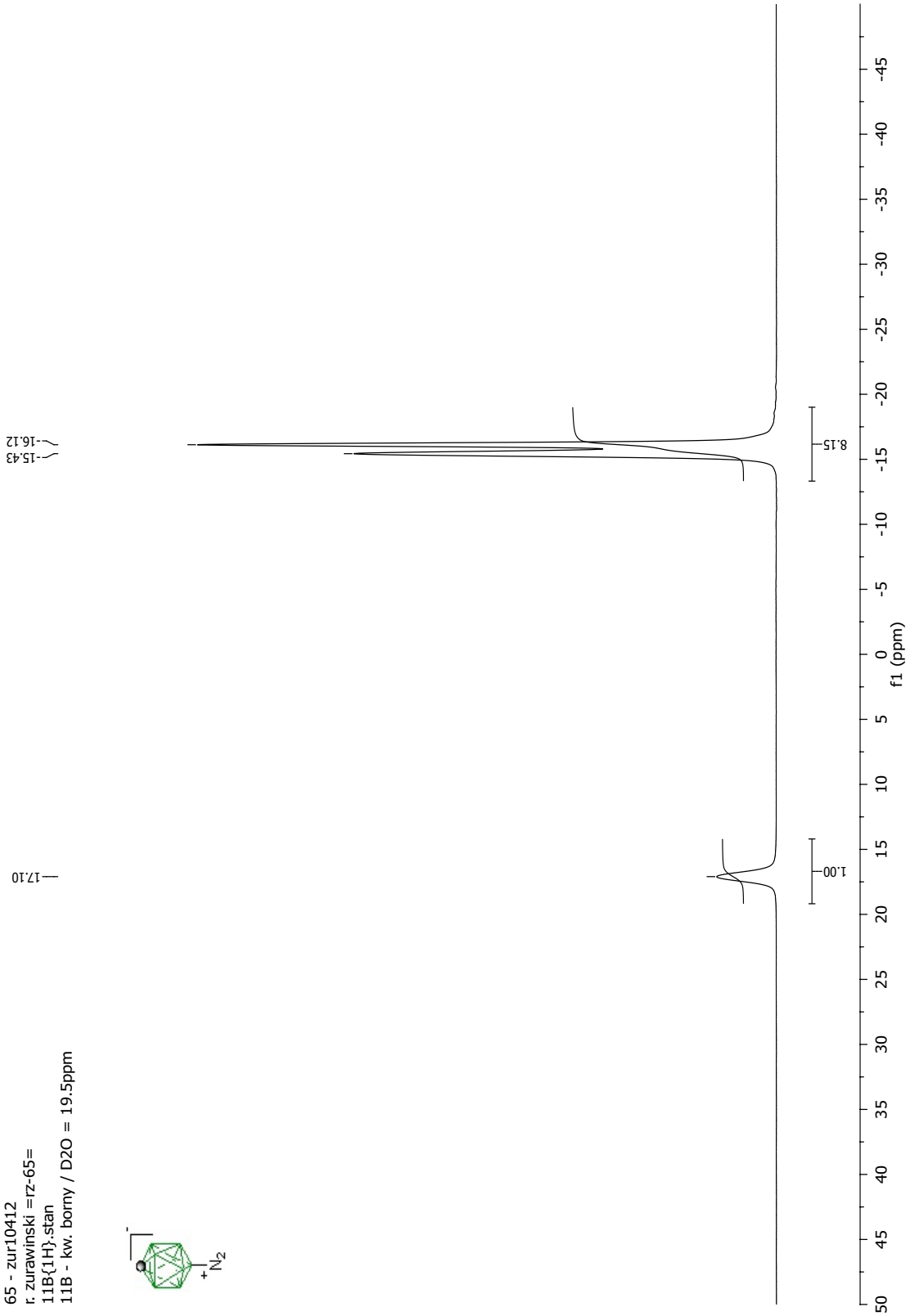


Figure S13. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-N_2] (**4[10]a**; CD_3CN, 160 MHz).

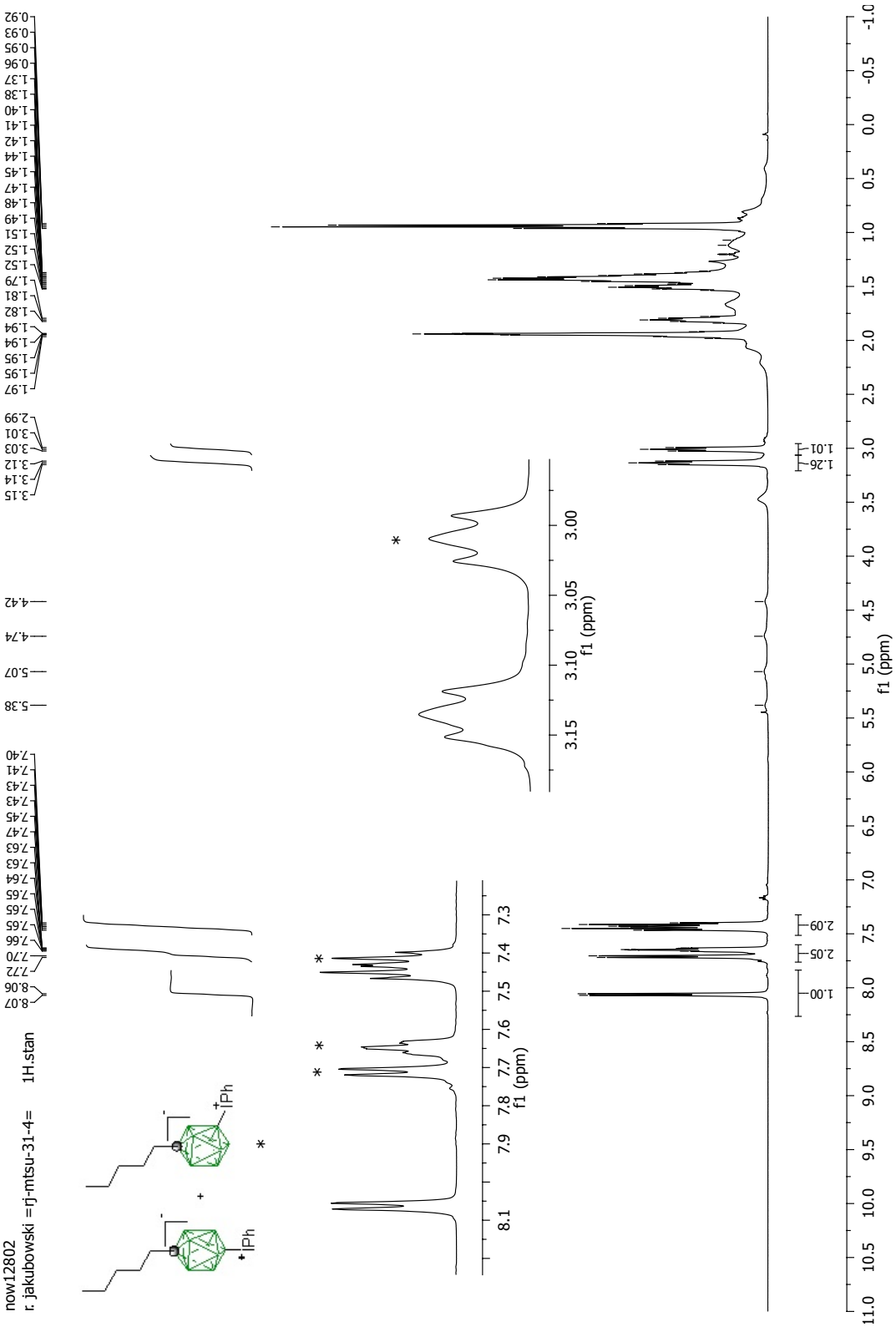


Figure S14. ^{1}H NMR of a crude mixture of [*closo*-1-CB_9H_8-1-C_5H_{11}-IPh] (**5[10]c** and **5[6]c**; CD_3CN, 500 MHz). The asterisk denotes **5[6]c** isomer.

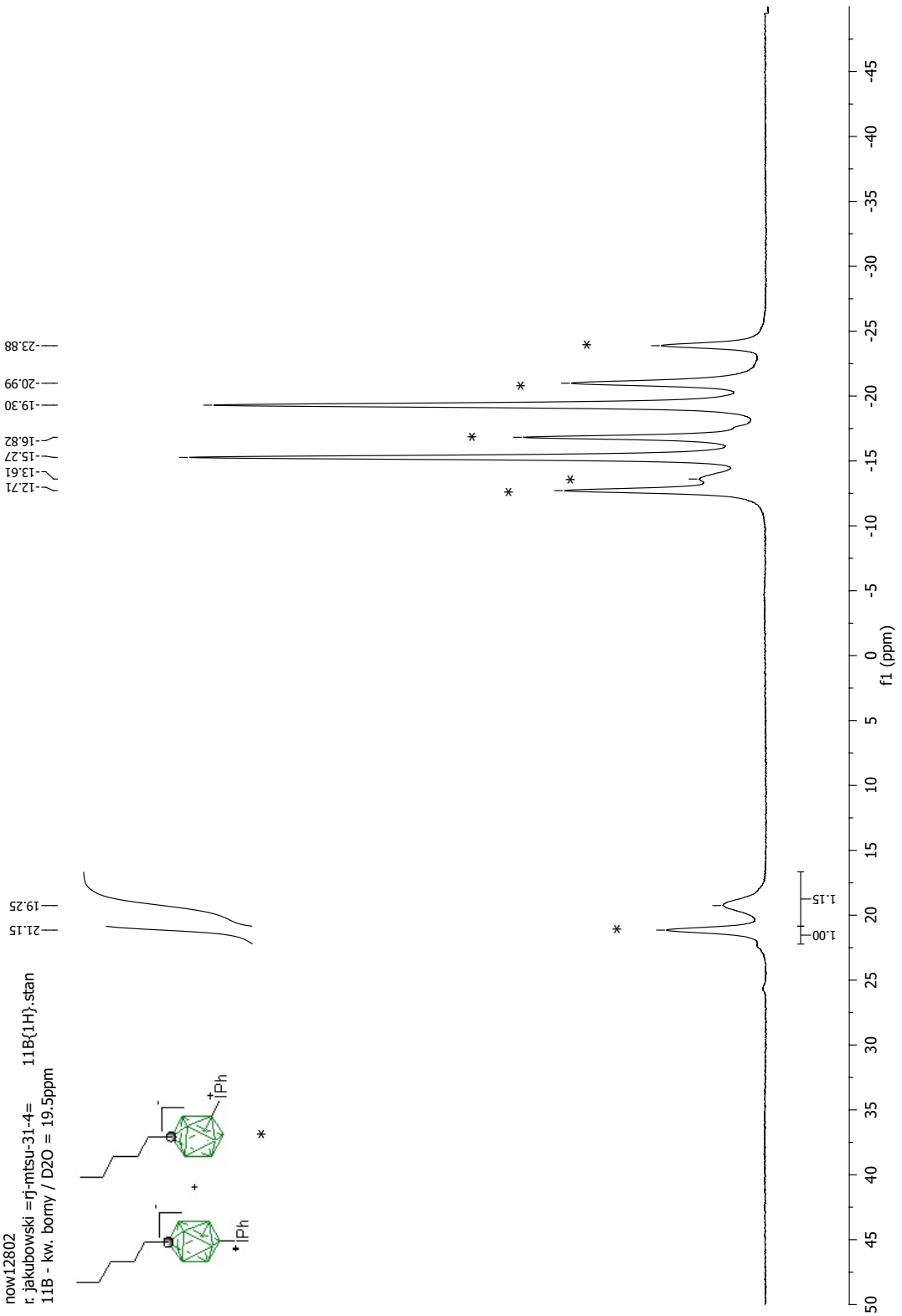


Figure S15. $^{11}B\{^{1}H\}$ NMR of a crude mixture of [*closo*-1-CB_9H_8-1-C_5H_{11}-IPh] (**5[10]c** and **5[6]c**; CD_3CN, 160 MHz). The asterisk denotes **5[6]c** isomer.

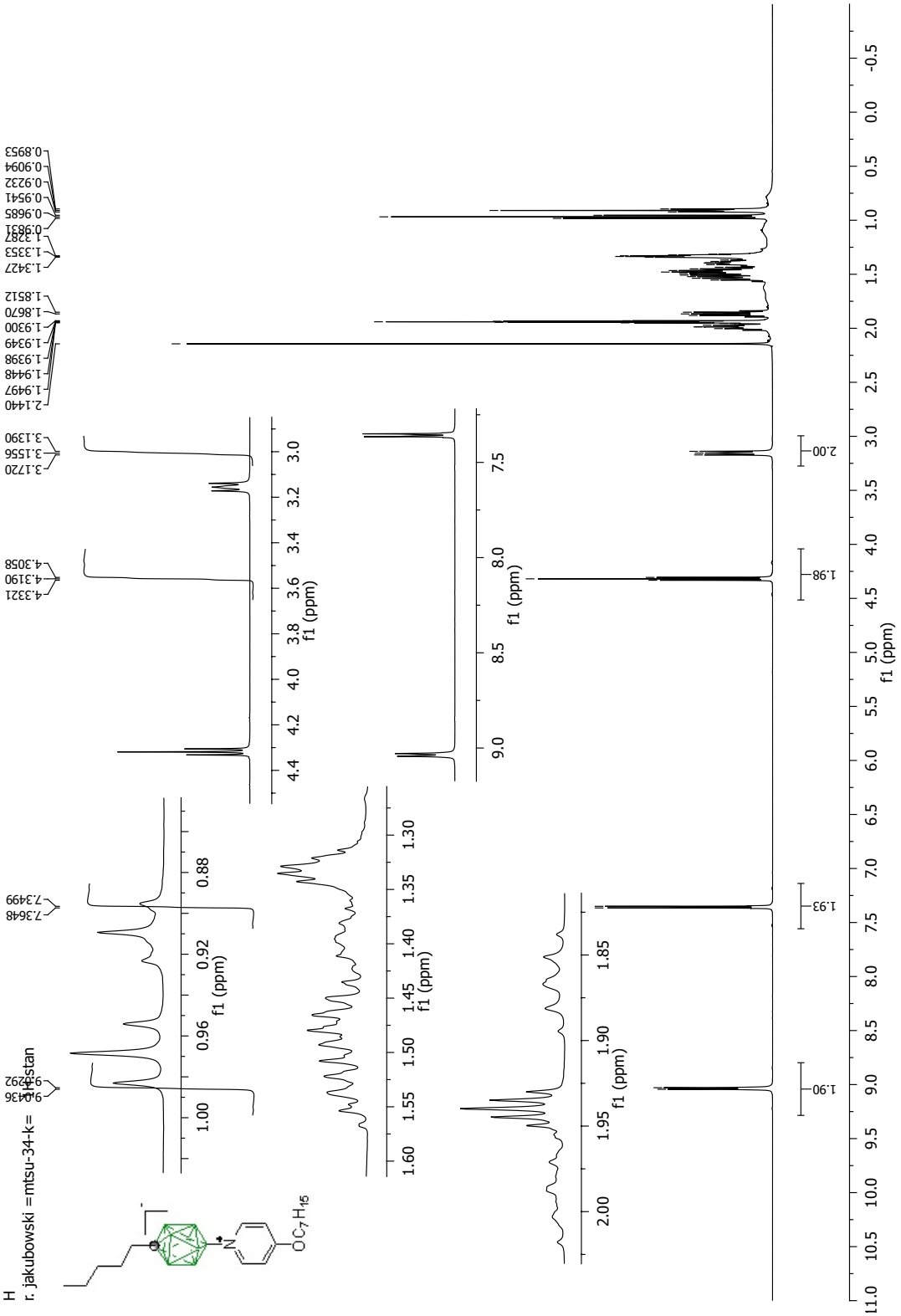


Figure S16. ^{1}H NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}-10-($NC_5H_4OC_7H_{15}$-4)] (**6[10]c**; CD_3CN, 500 MHz).

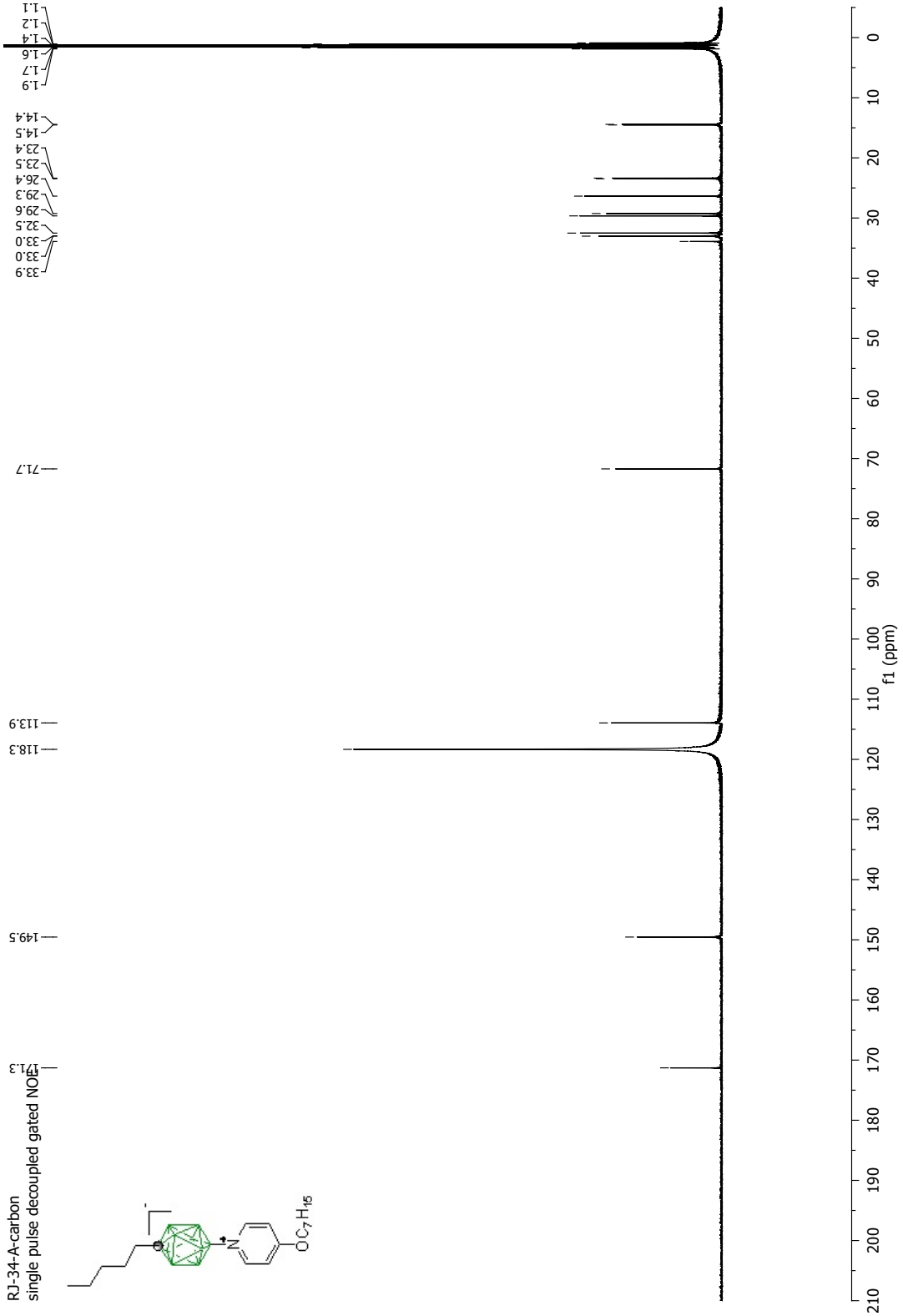


Figure S17. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}-10-($NC_5H_4OC_7H_{15}$-4)] (**6[10]c**; CD_3CN, 126 MHz)

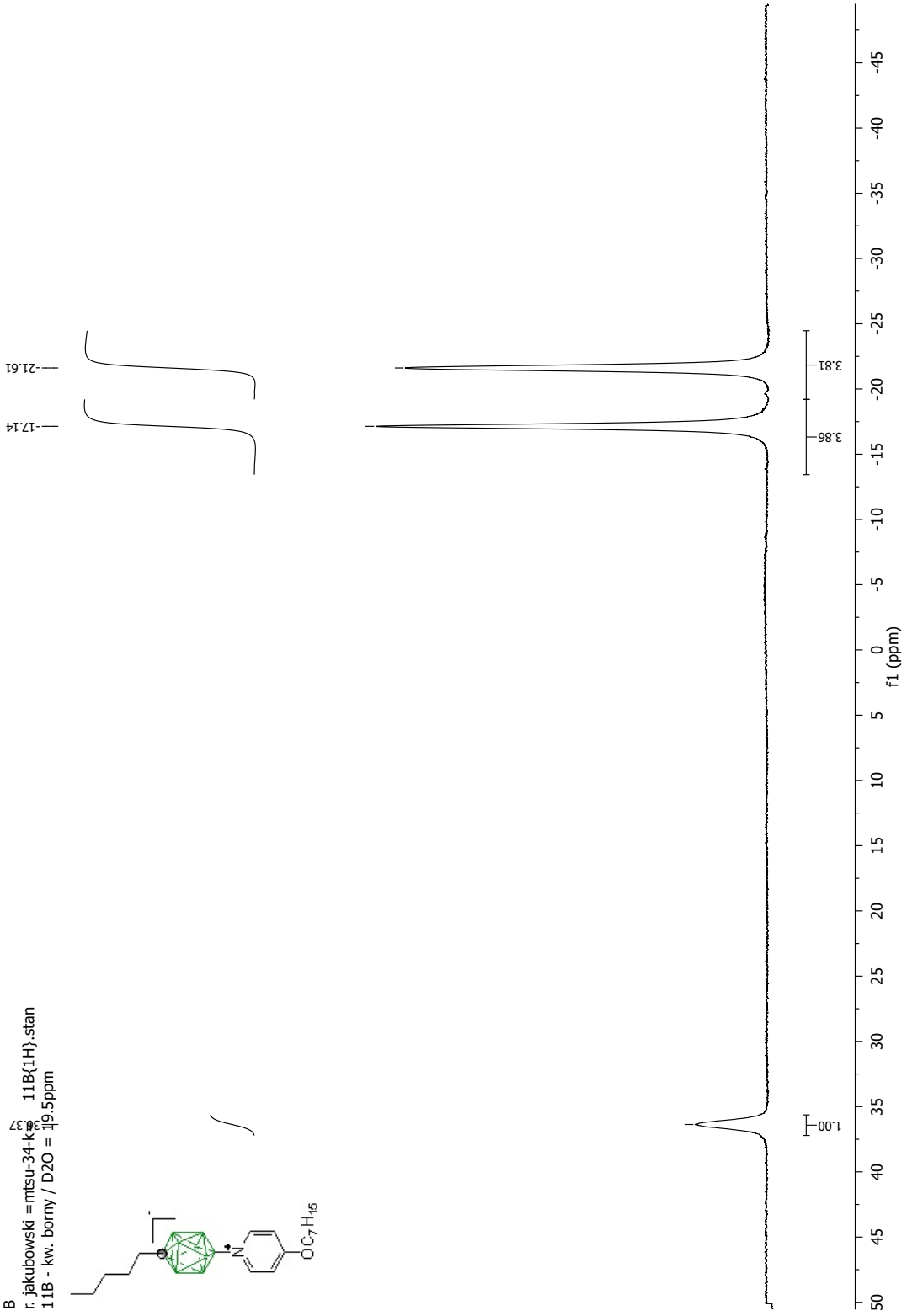


Figure S18. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-1-C_5H_{11}-10-($NC_5H_4OC_7H_{15}$-4)] (**6[10]c**; CD_3CN, 160 MHz).

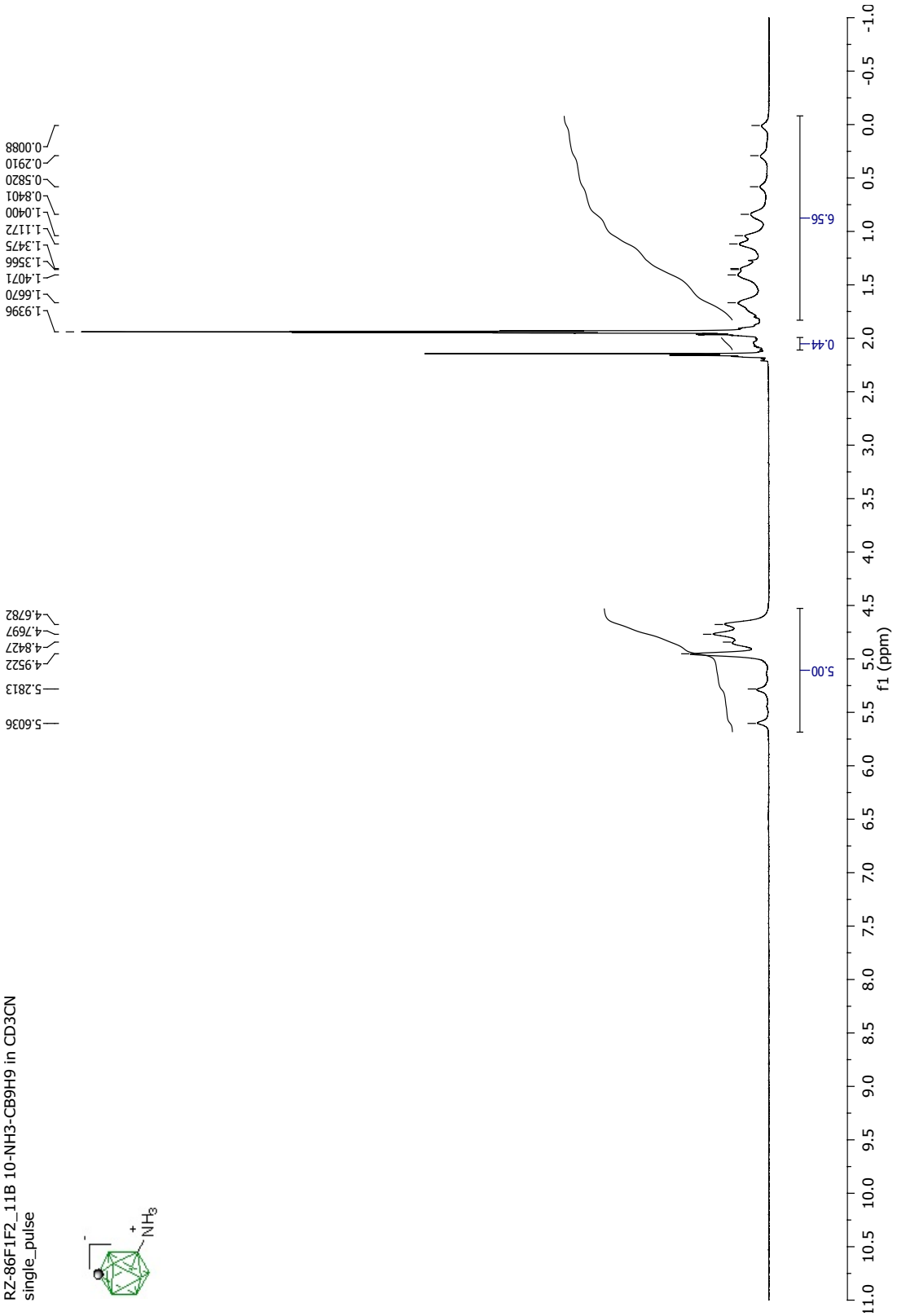


Figure S19. ^{1}H NMR of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**; CD_3CN, 500 MHz).

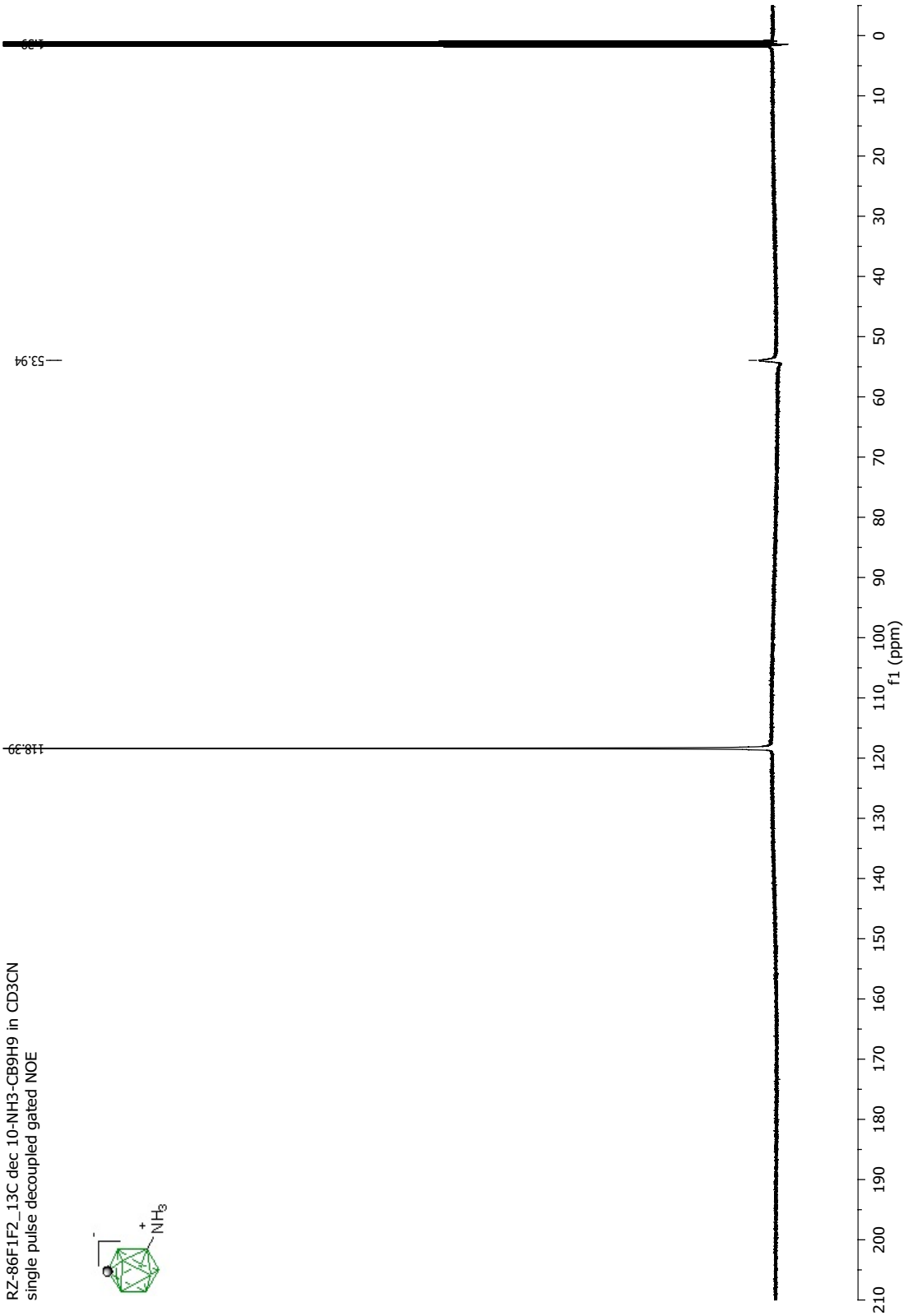


Figure S20. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**; CD_3CN, 126 MHz)

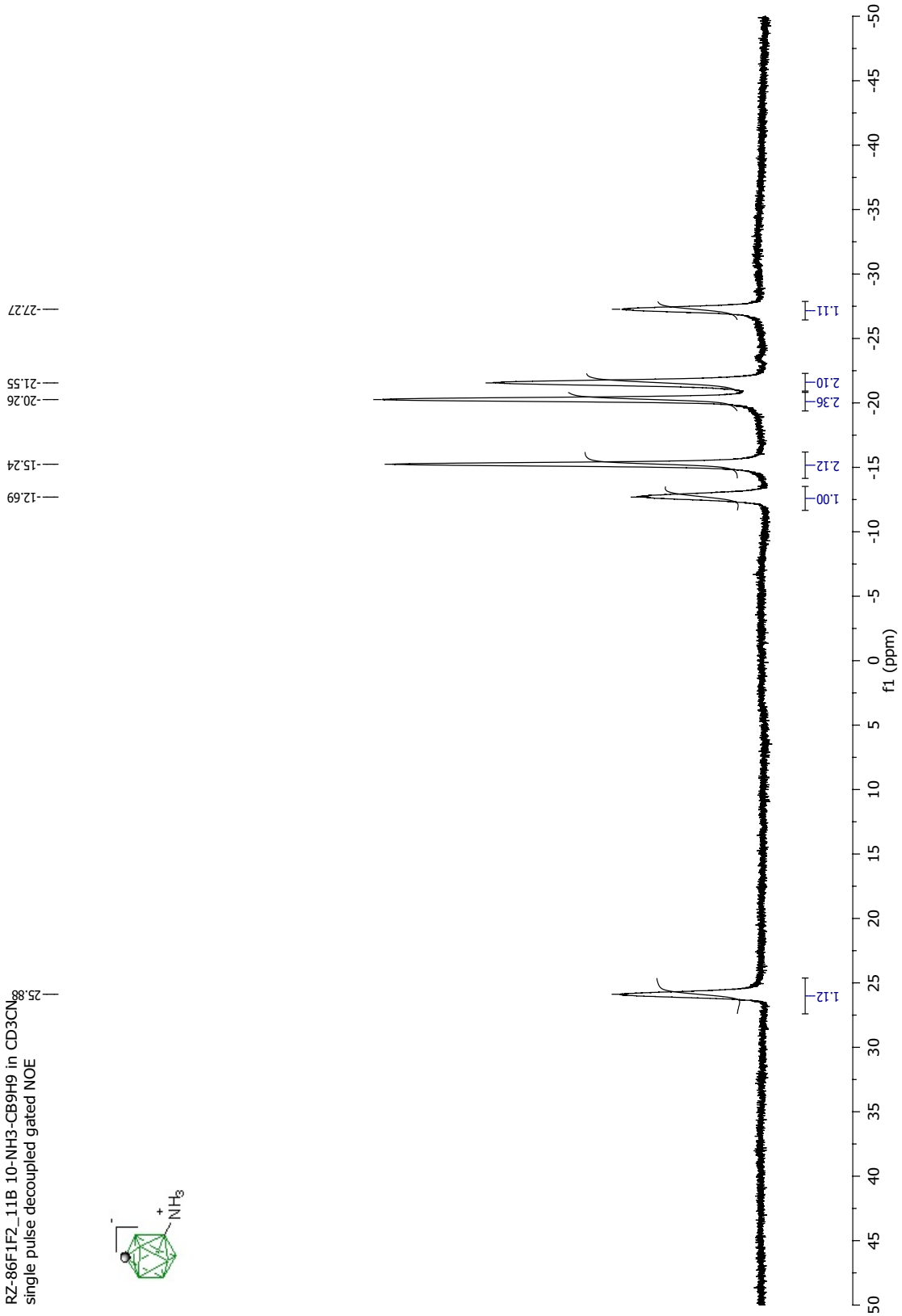


Figure S21. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NH_3] (**8[6]a**; CD_3CN, 160 MHz).

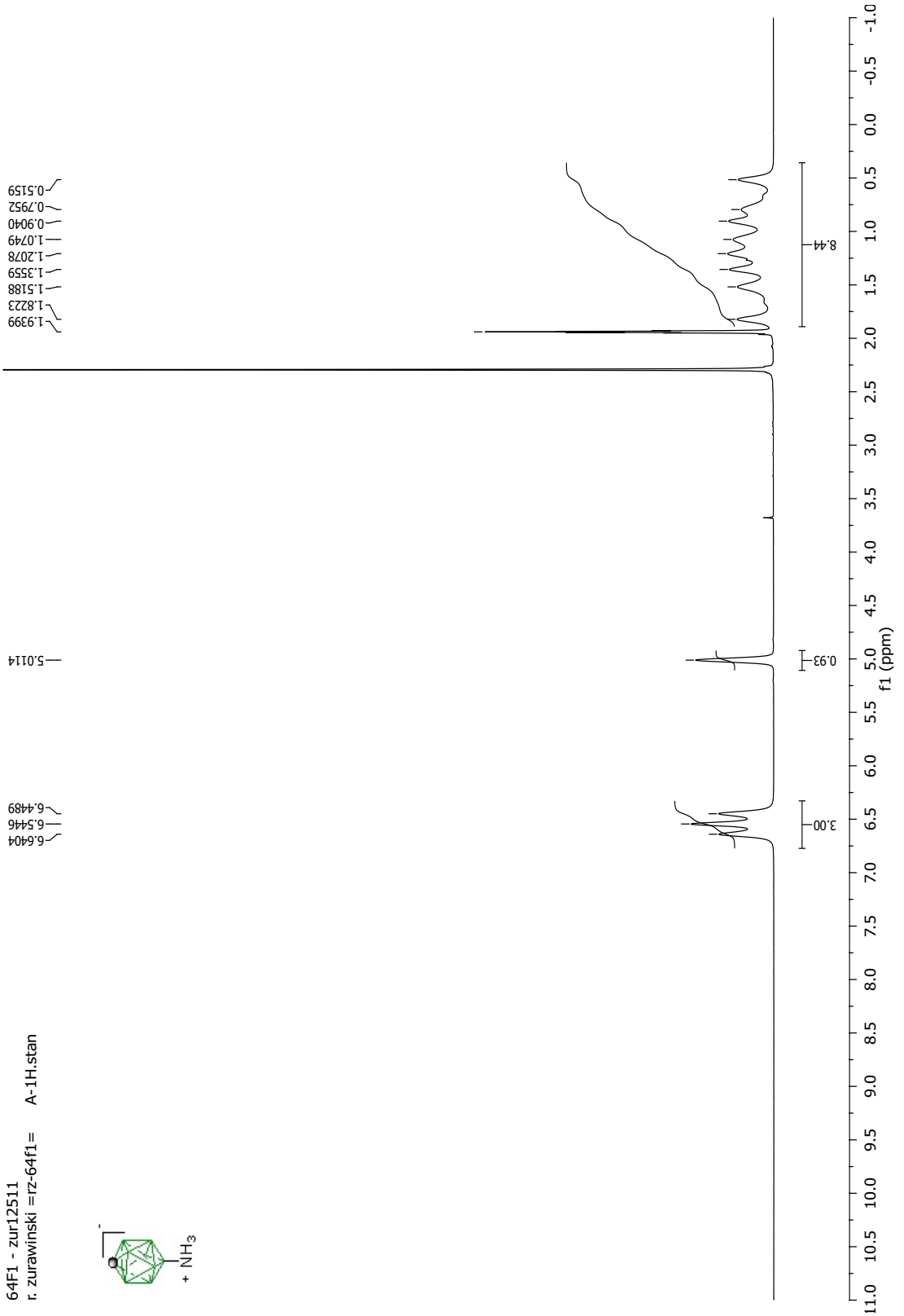


Figure S22. ^{1}H NMR of [*closo*-1-CB_9H_9-10-NH_3] (**8[10]a**; CD_3CN, 500 MHz).

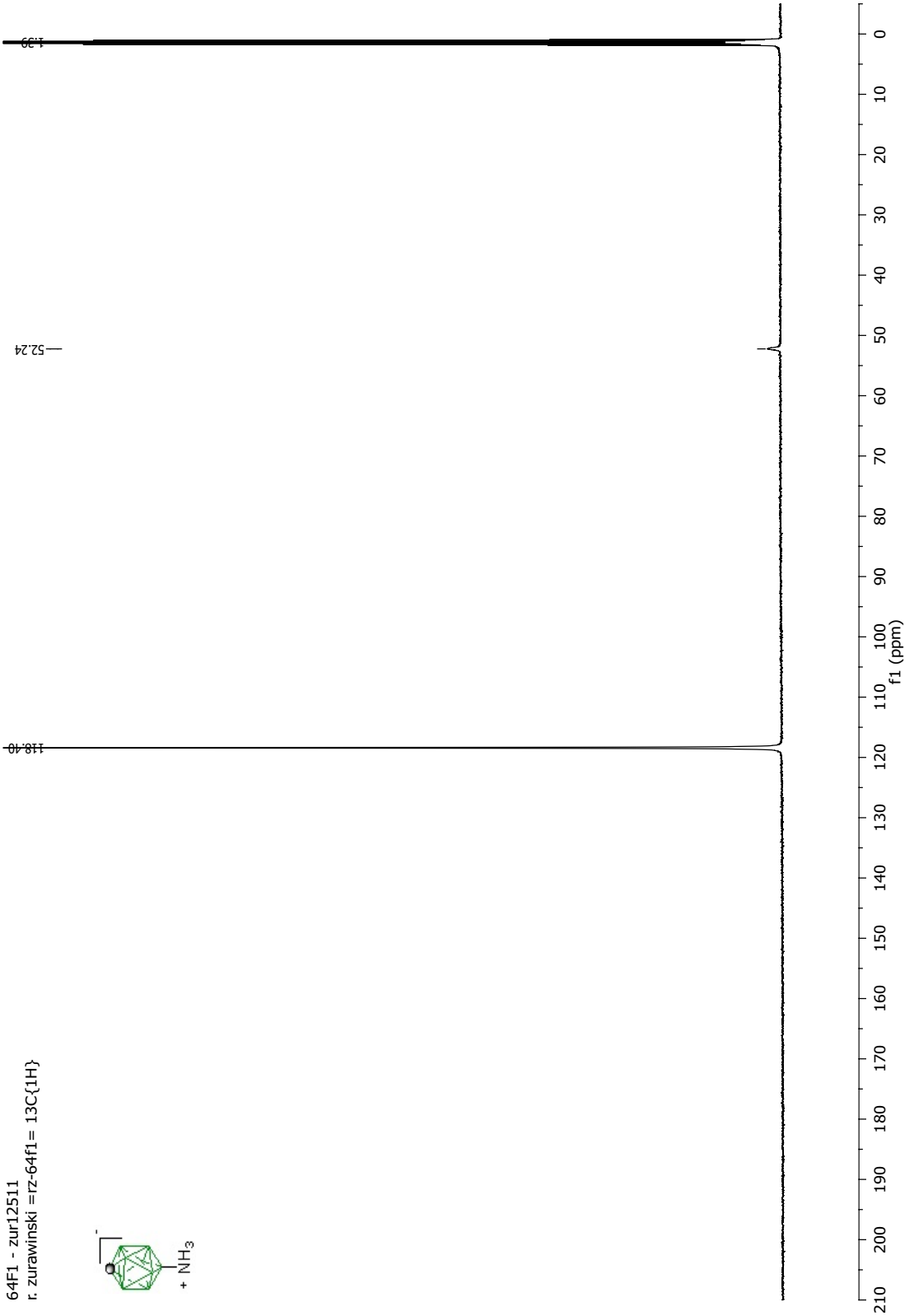


Figure S23. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-NH_3] (**8[10]a**; CD_3CN, 126 MHz)

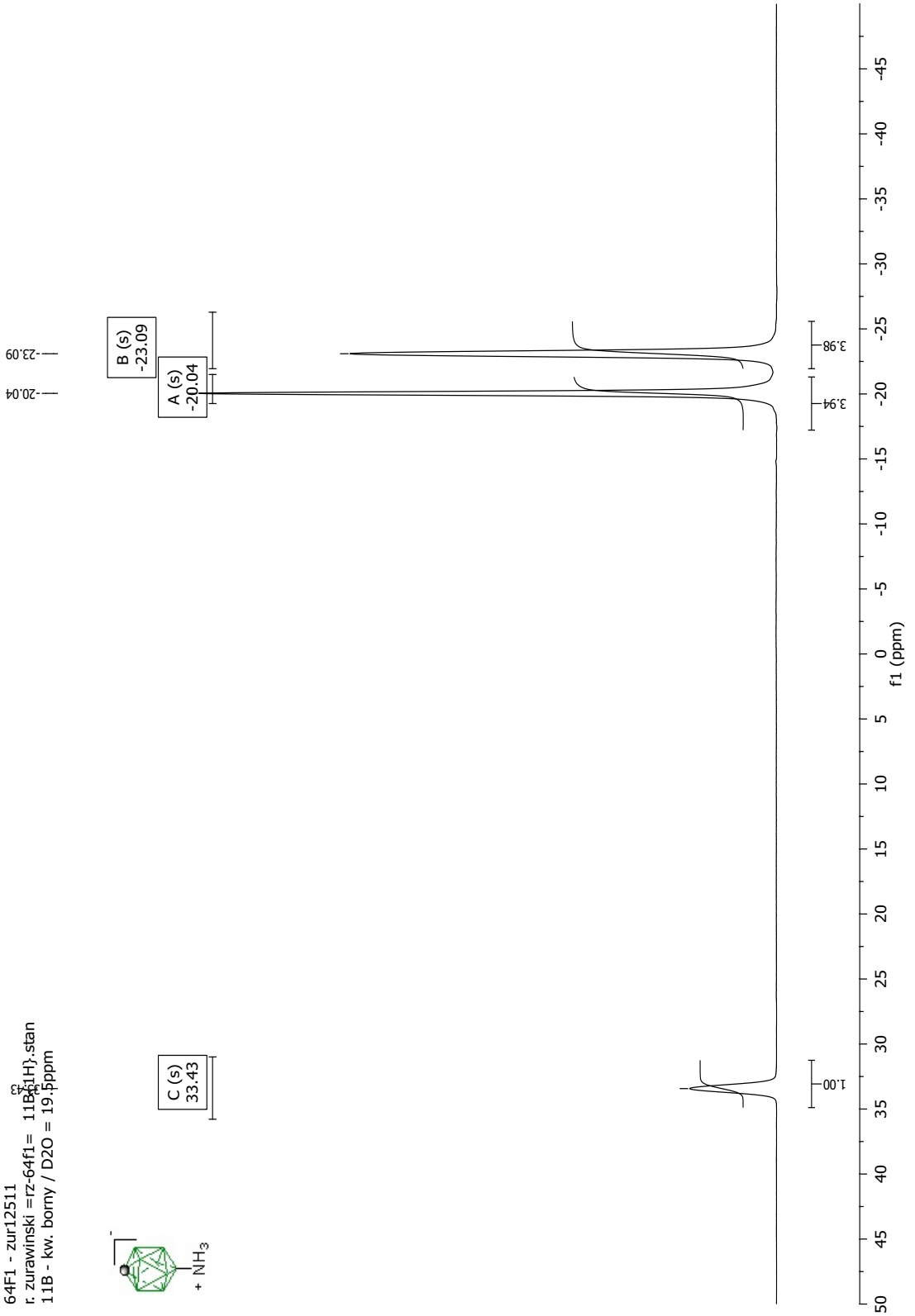


Figure S24. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-NH_3] (**8[10]a**; CD_3CN, 160 MHz).

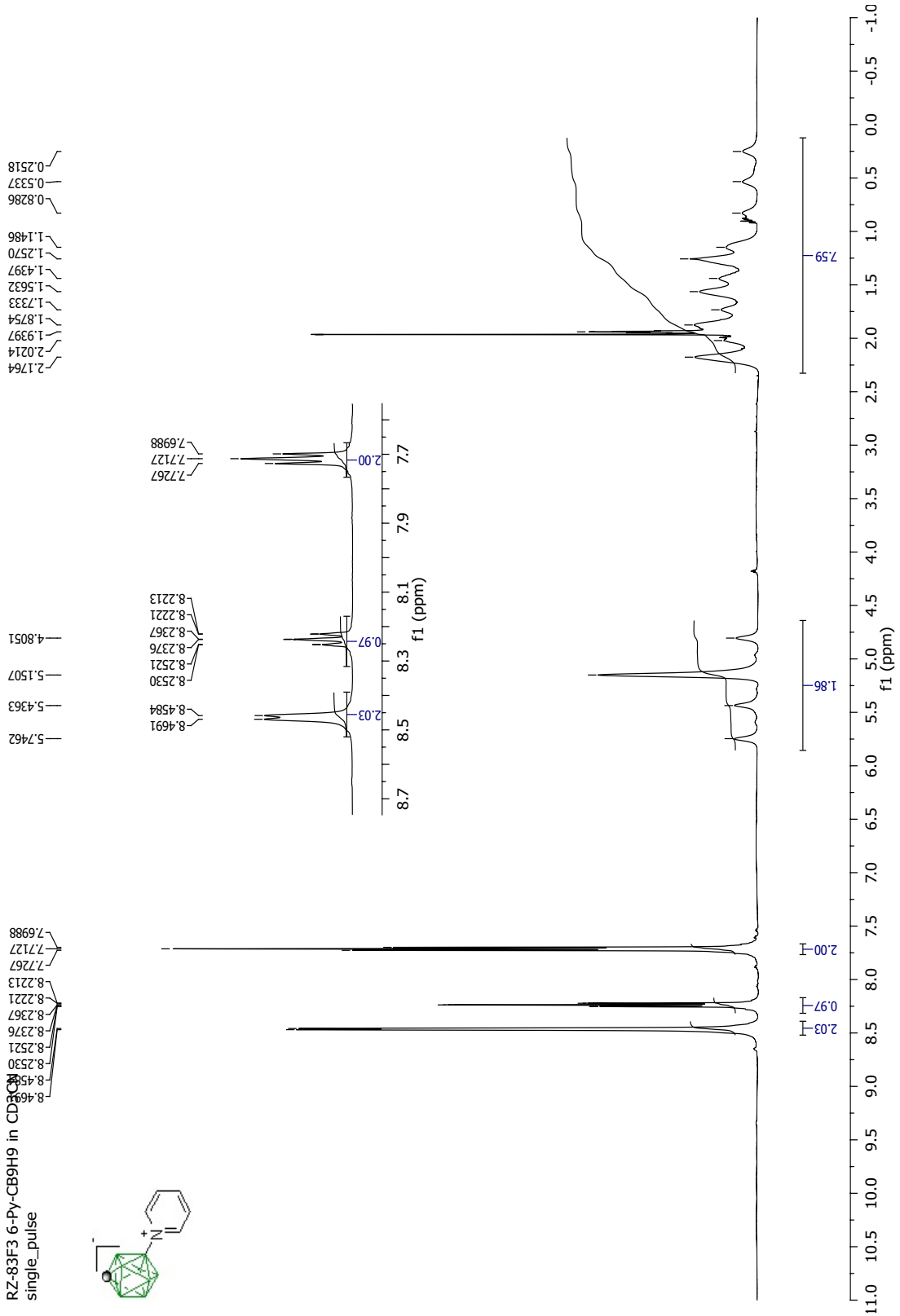


Figure S25. ^{1}H NMR of [*closo*-1-CB_9H_9-6-NC_5H_5] (**9[6]a**; CD_3CN, 500 MHz).

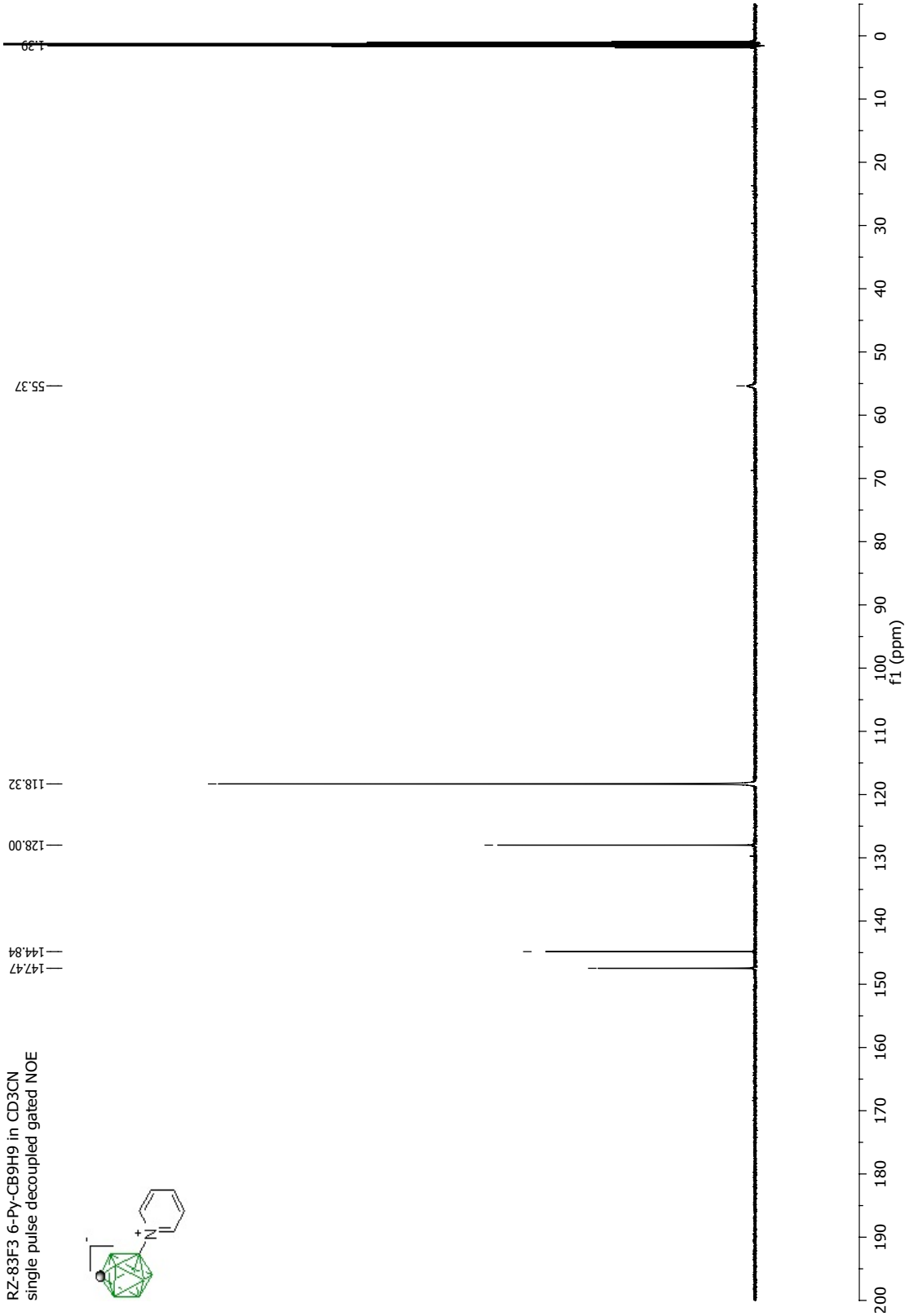


Figure S26. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NC_5H_5] (**9[6]a**; CD_3CN, 126 MHz)

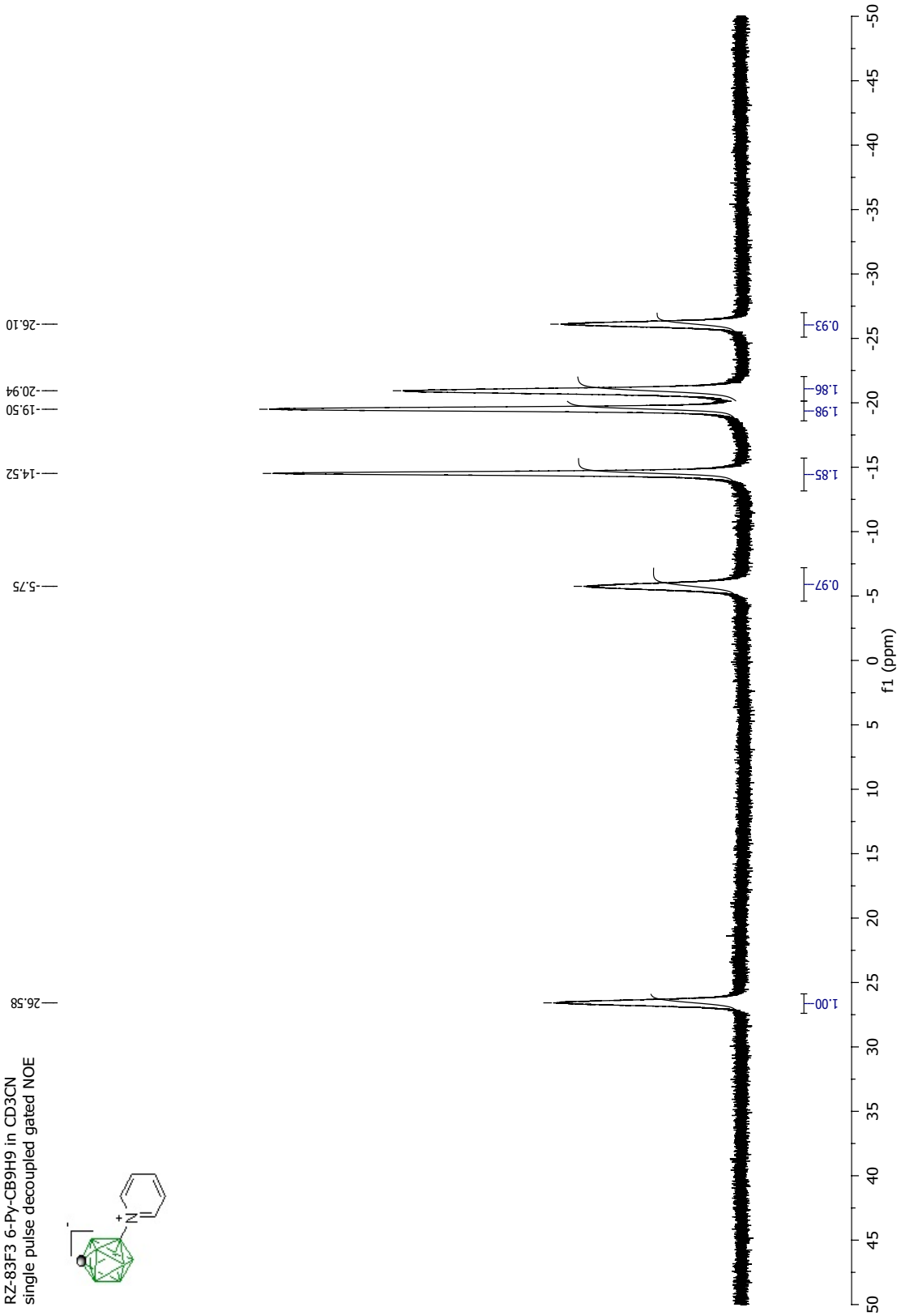


Figure S27. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NC_5H_5] (**9[6]a**; CD_3CN, 160 MHz).

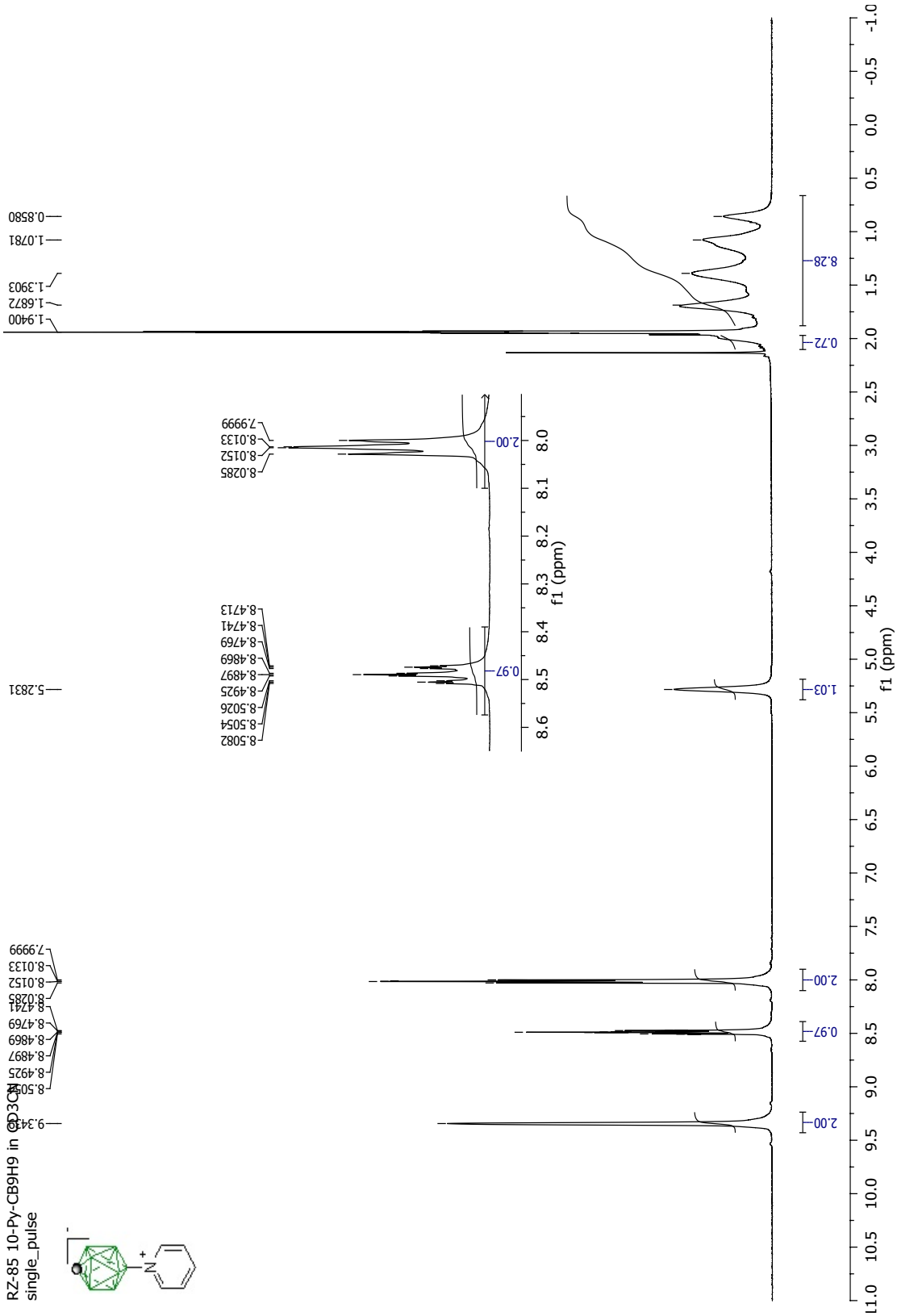


Figure S28. ^{1}H NMR of [*closo*-1-CB_9H_9-10-NC_5H_5] (**9[10]a**; CD_3CN, 500 MHz).

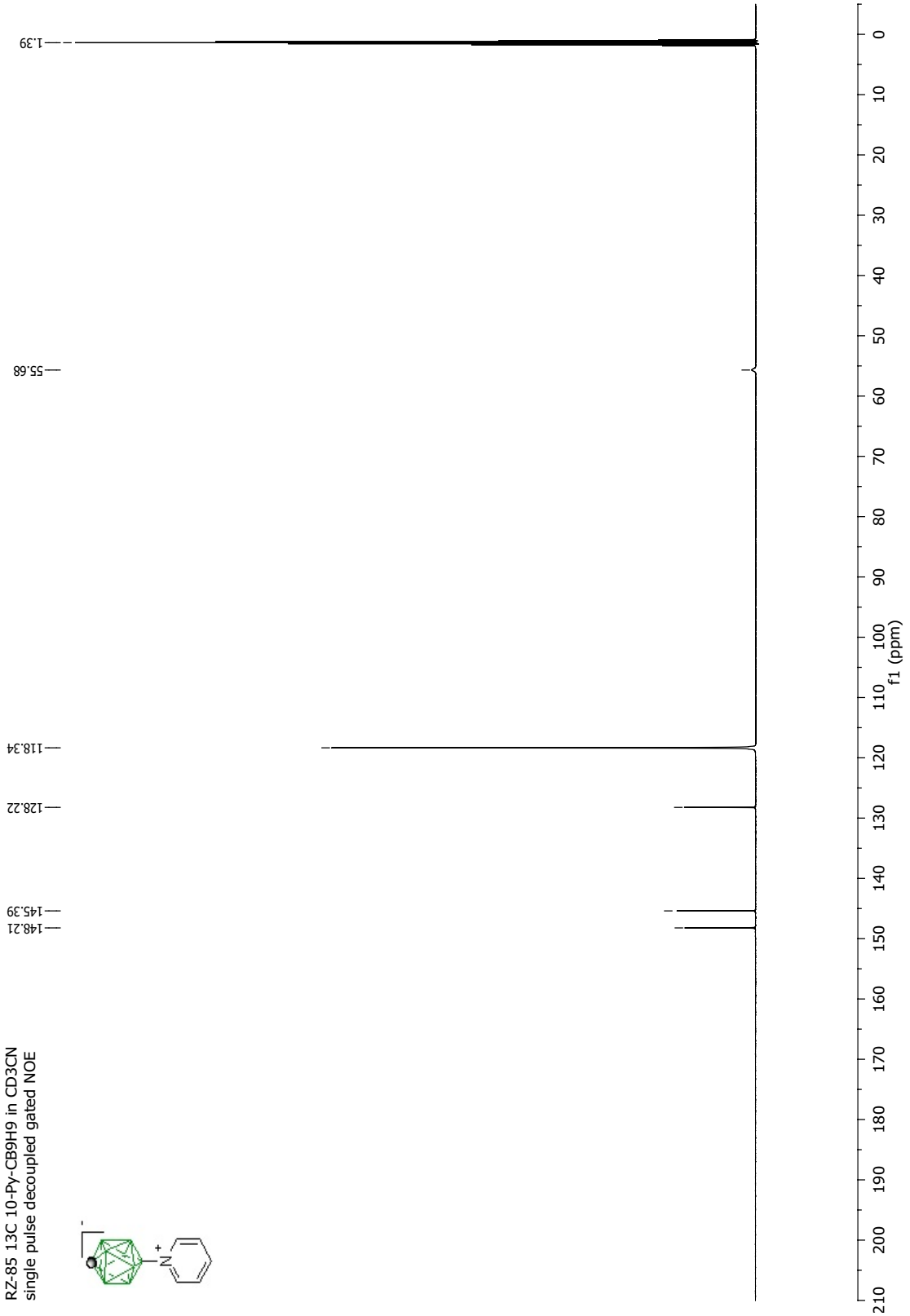


Figure S29. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-NC_5H_5] (**9[10]a**; CD_3CN, 126 MHz)

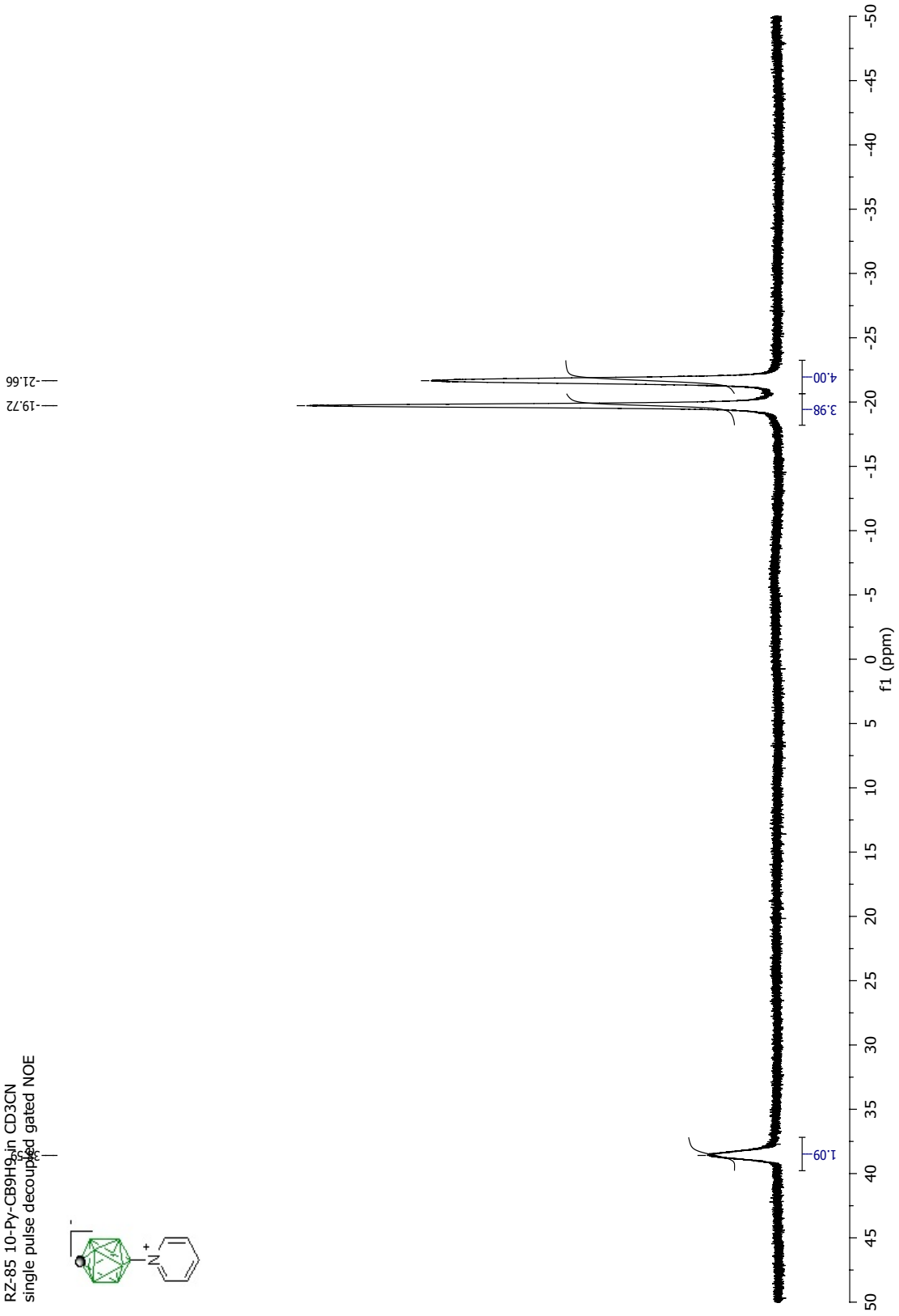


Figure S30. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-NC_5H_5] (**9[10]a**; CD_3CN, 160 MHz).

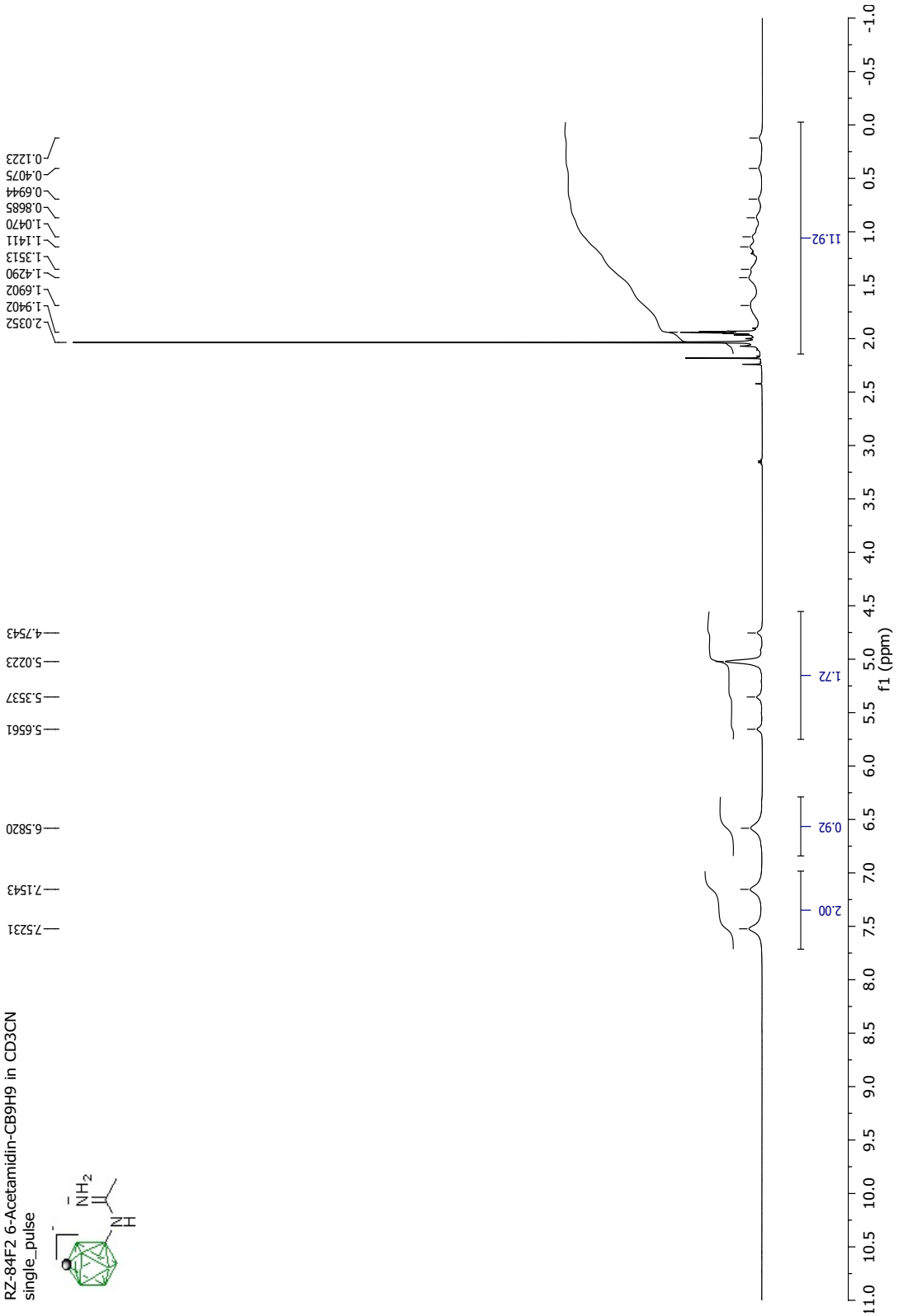


Figure S31. ^{1}H NMR of [*closo*-1-CB_9H_9-6-NHC(NH_2)Me] (**10[6]a**; CD_3CN, 500 MHz).

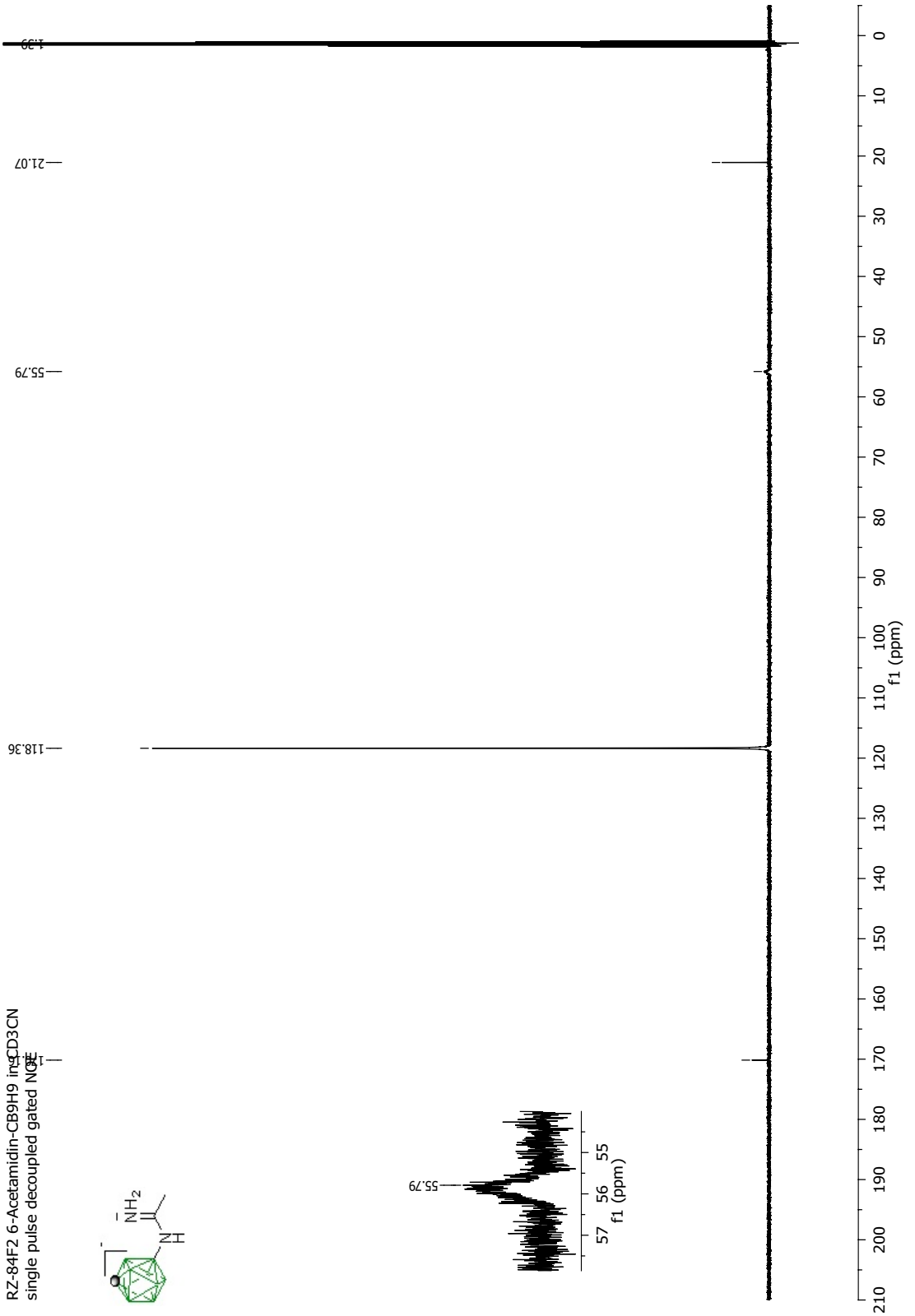


Figure S32. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NHC(NH_2)Me] (**10[6]a**; CD_3CN, 126 MHz)

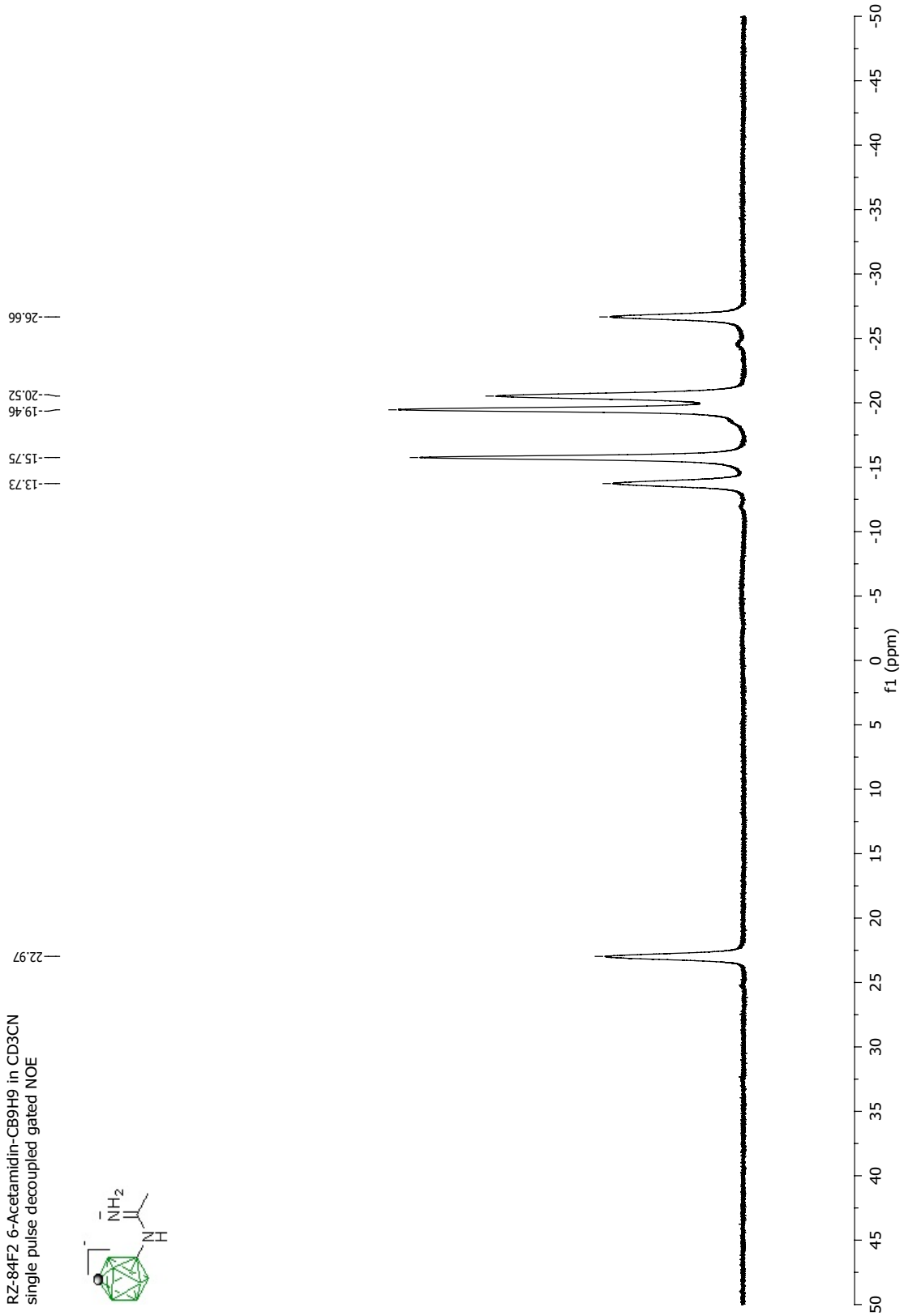


Figure S33. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NHC(NH_2)Me] (**10[6]a**; CD_3CN, 160 MHz).

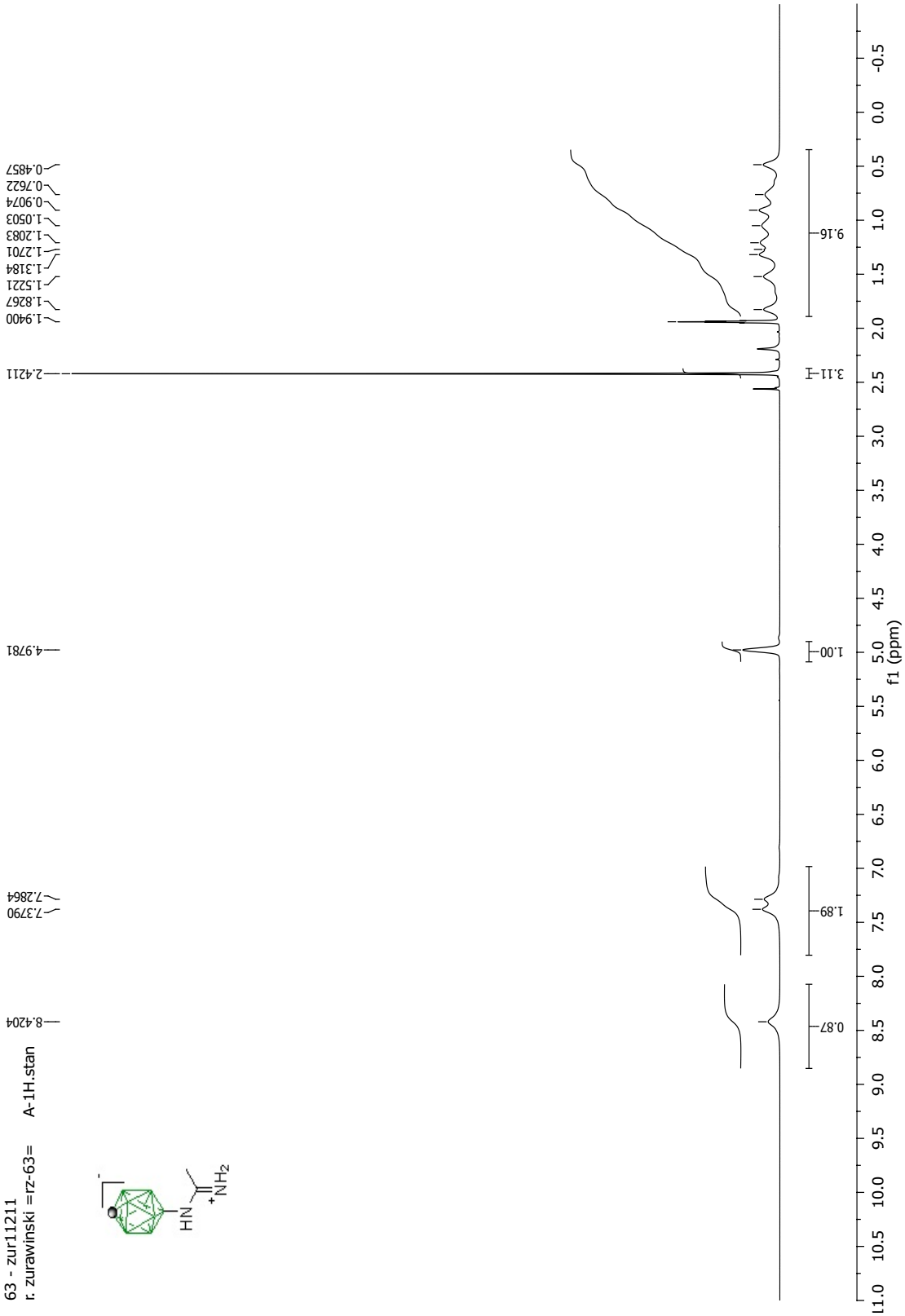


Figure S34. ^{1}H NMR of [*closo*-1-CB_9H_9-10-NHC(NH_2)Me] (**10[10]a**; CD_3CN, 500 MHz).

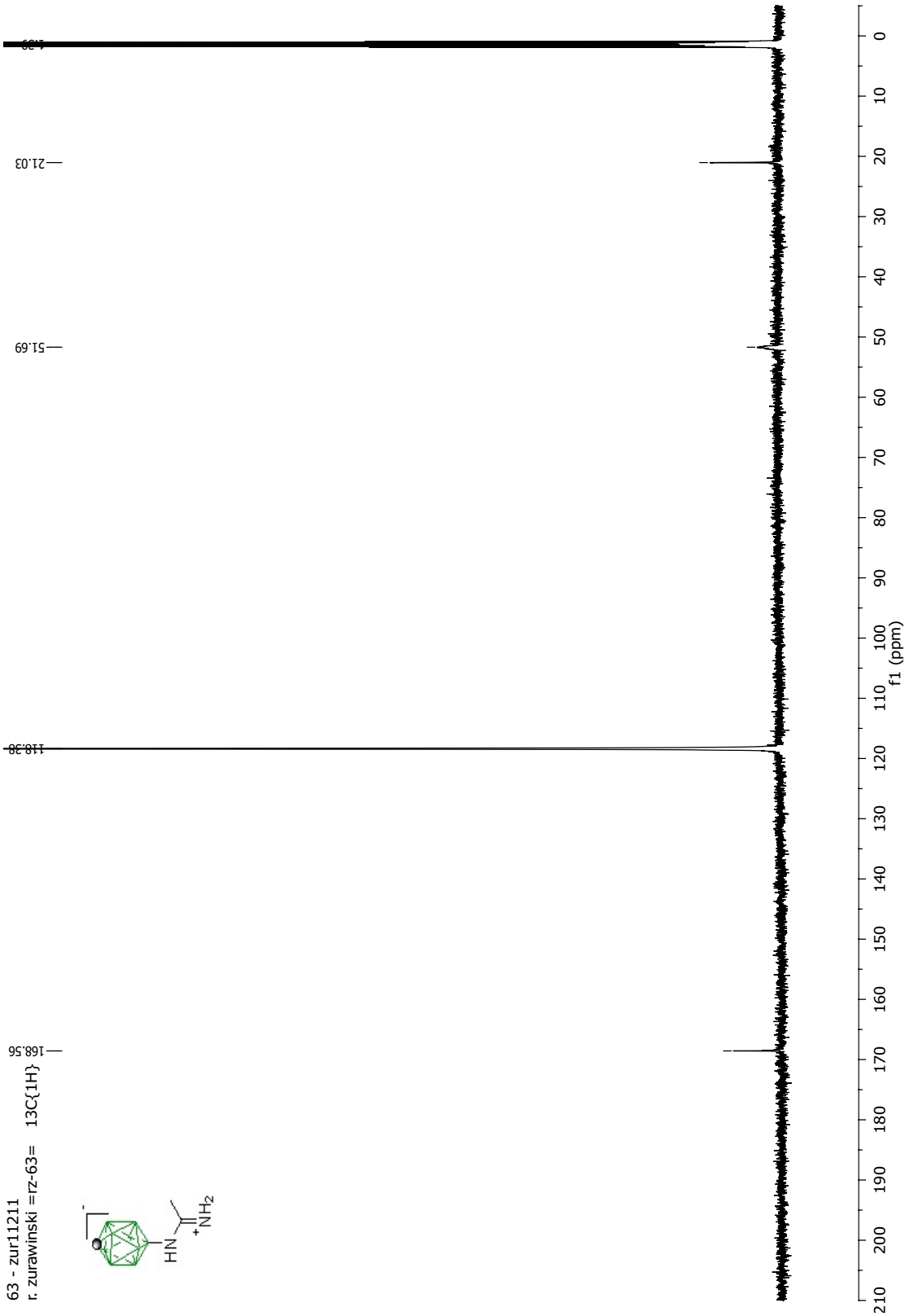


Figure S35. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-$NHC(NH_2)Me$] (**10[10]a**;CD_3CN, 126 MHz)

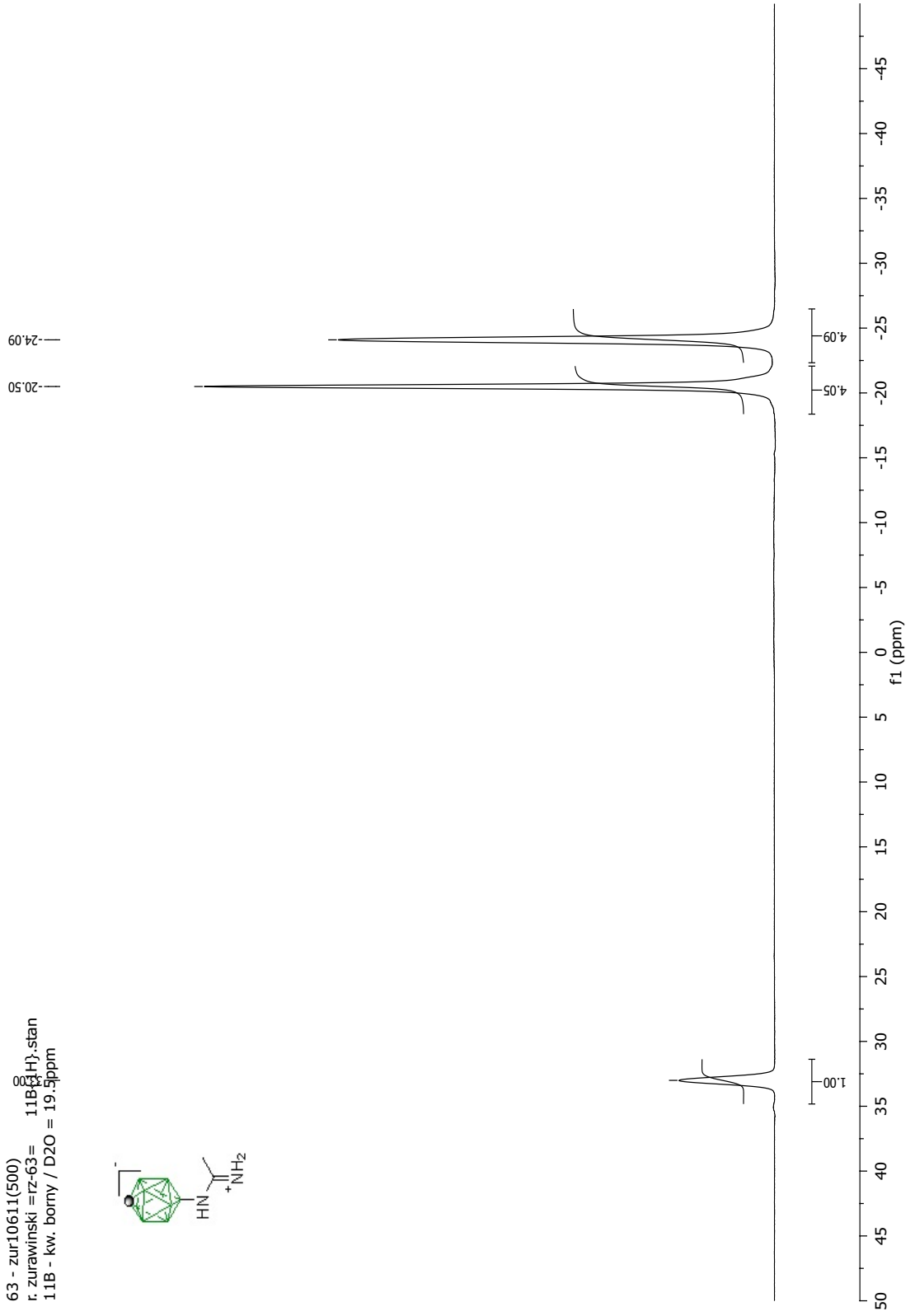


Figure S36. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-NHC(NH_2)Me] (**10[10]a**; CD_3CN, 160 MHz).

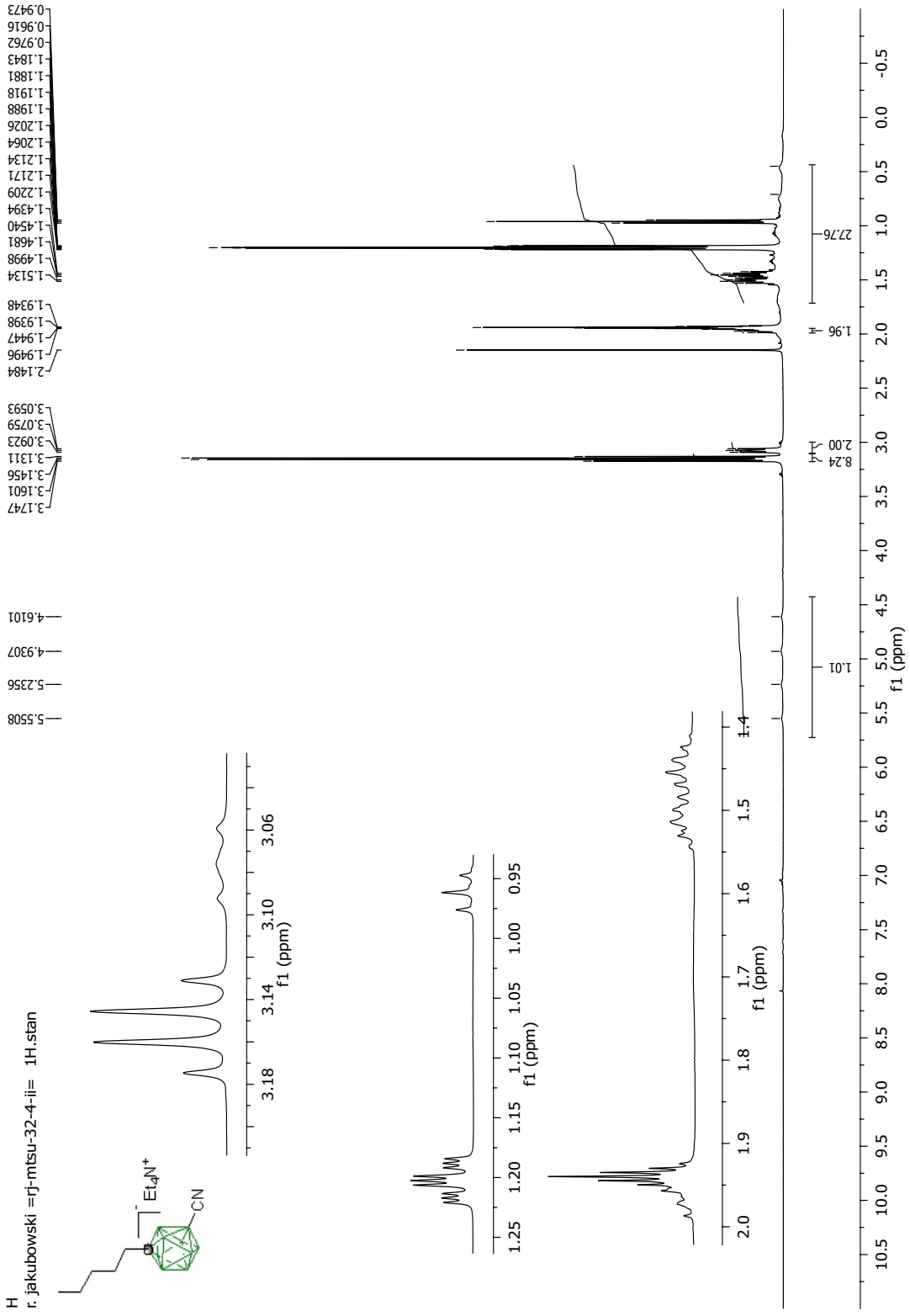


Figure S37. ^{1}H NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-CN]$^{-}$[Et_4N]$^{+}$ (**11[6]c[Et$_4$N]**; CD_3CN, 500 MHz).

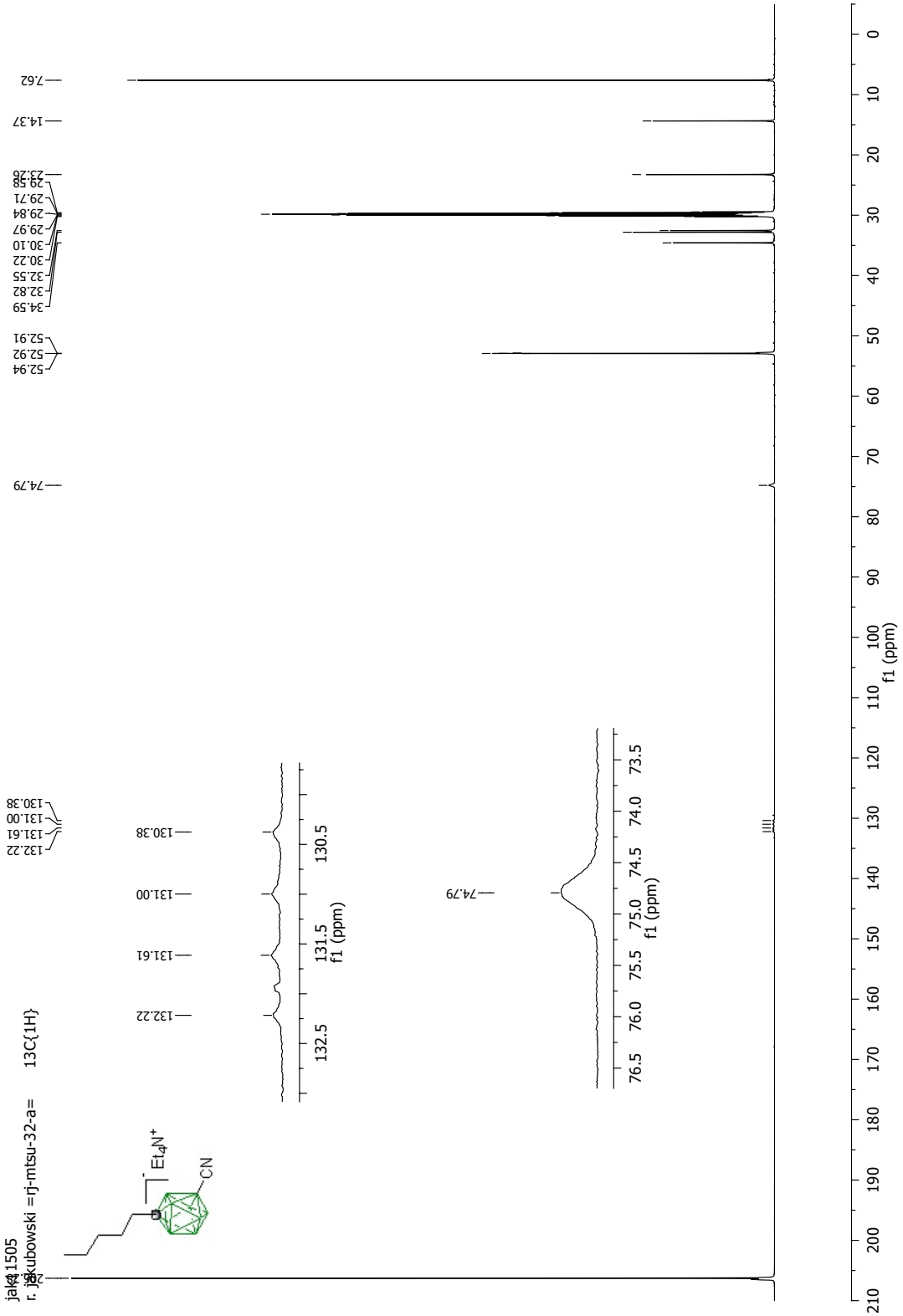


Figure S38. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-CN]$^-$[Et_4N]$^+$ (**11[6]c[Et$_4$N]**; acetone-d_6, 151 MHz).

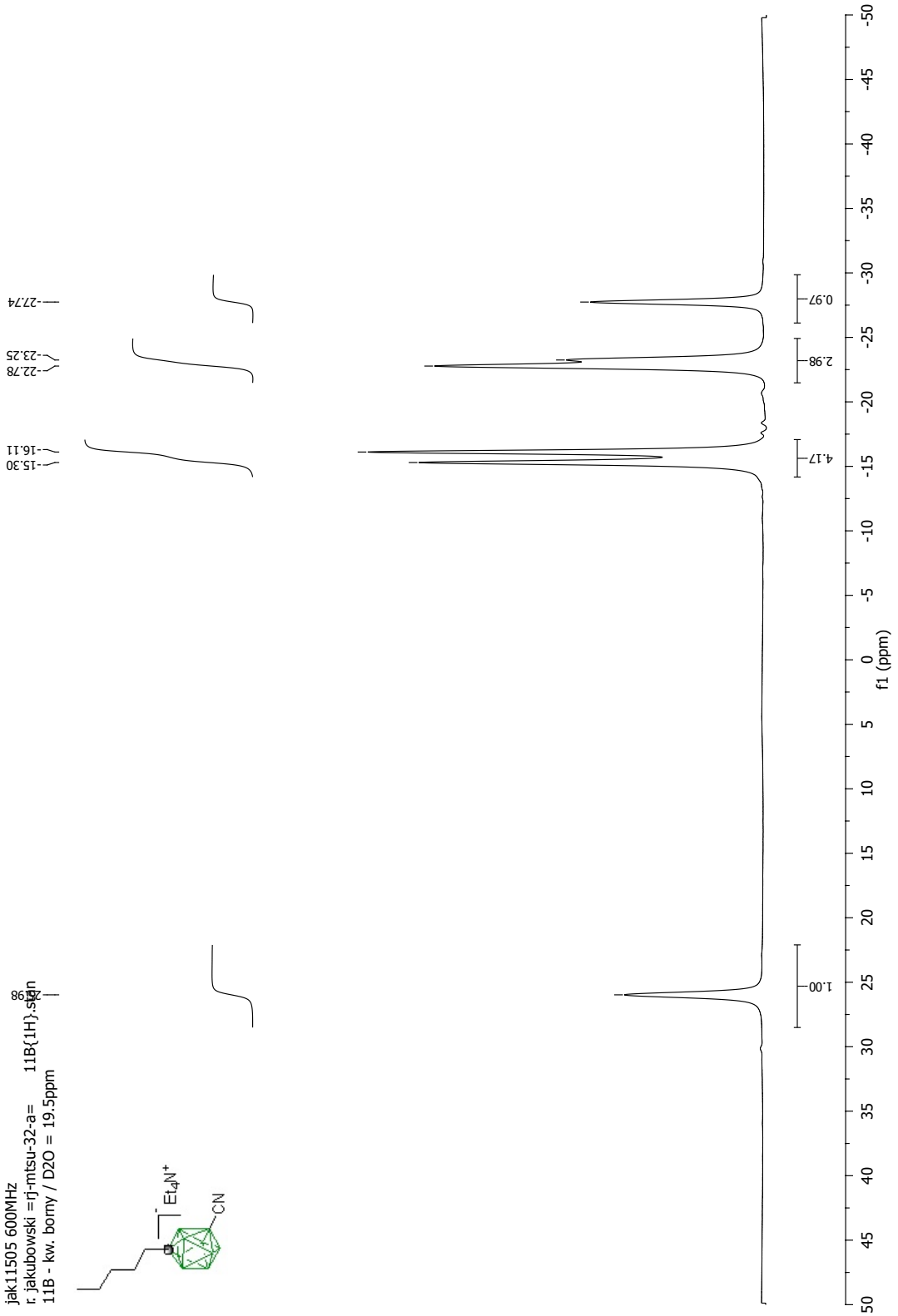


Figure S39. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_8-1-C_5H_{11}-10-CN]$^-$[$Et_4N]^+$ (**11[6]c[Et$_4$N]**; acetone-d_6, 193 MHz).

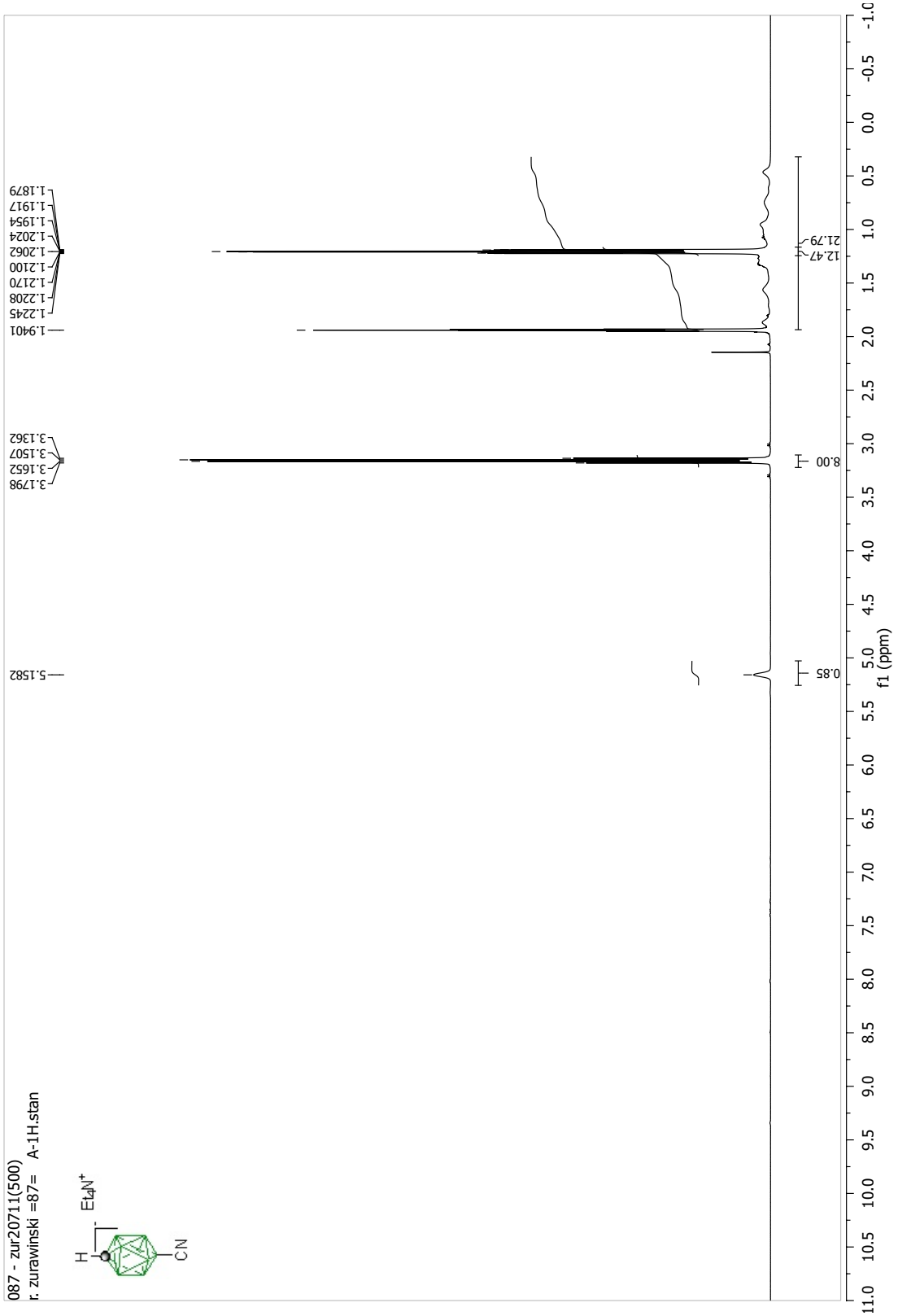


Figure S40. ^{1}H NMR of [*closo*-1-CB_9H_9-10-CN]$^{-}$[Et_4N]$^{+}$ (**11[10]a[Et$_4$N]**; CD_3CN, 500 MHz).

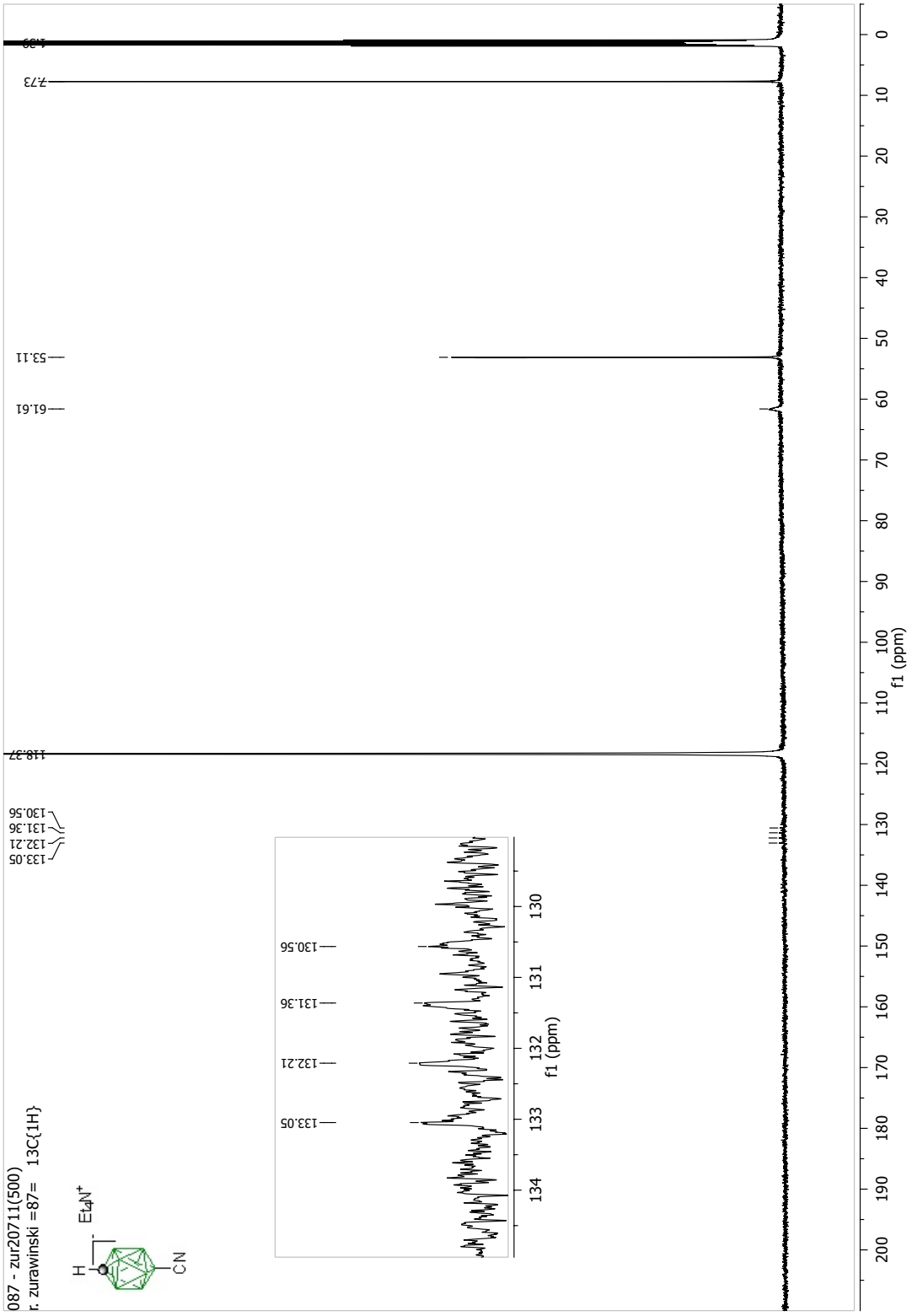


Figure S41. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-CN]$^-$[Et_4N]$^+$ (**11[10]a[Et_4N]**; CD_3CN, 126 MHz)

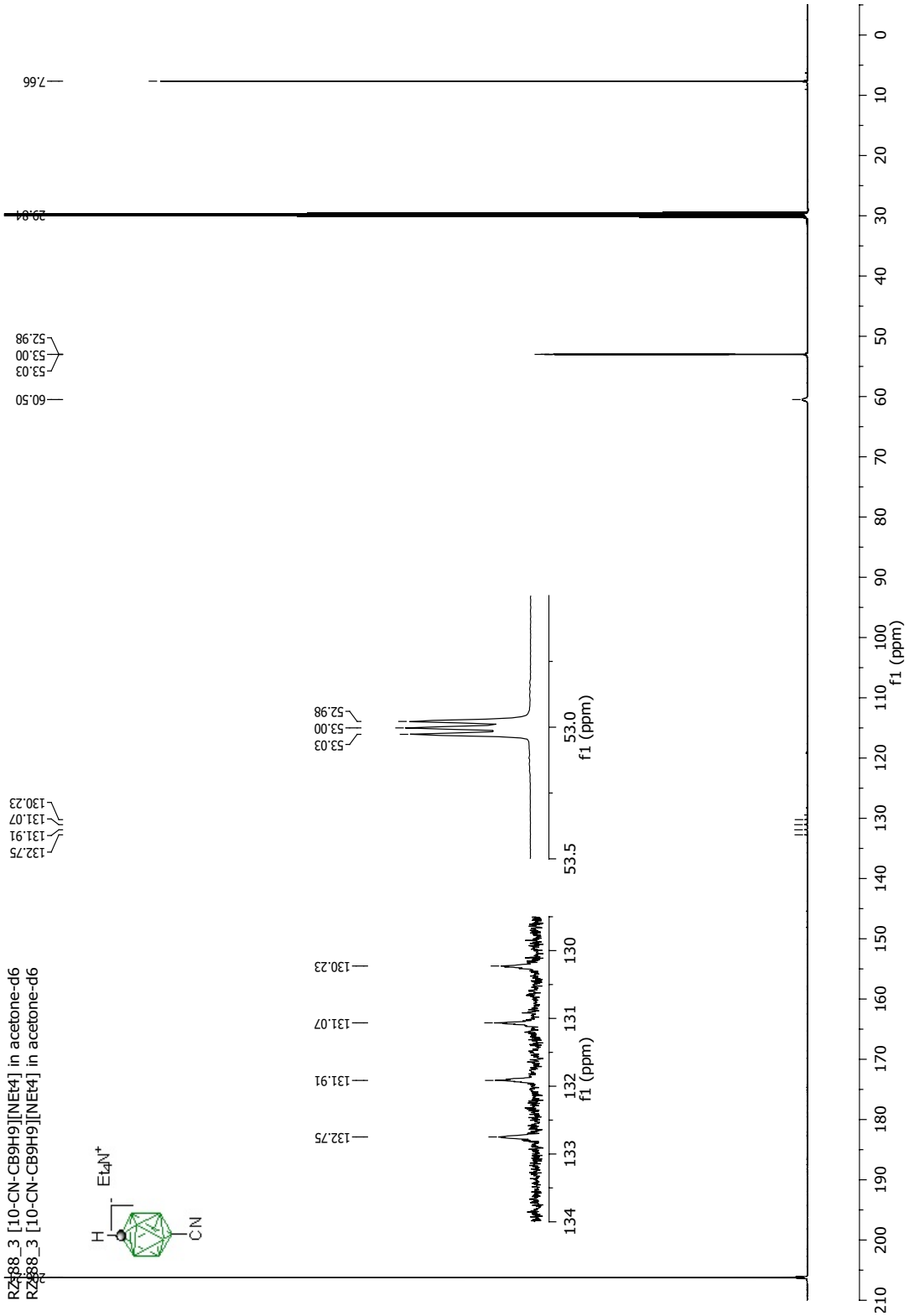


Figure S42. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-CN]$^-$[Et_4N]$^+$ (**11[10]a[Et_4N]**; acetone-d_6, 126 MHz)

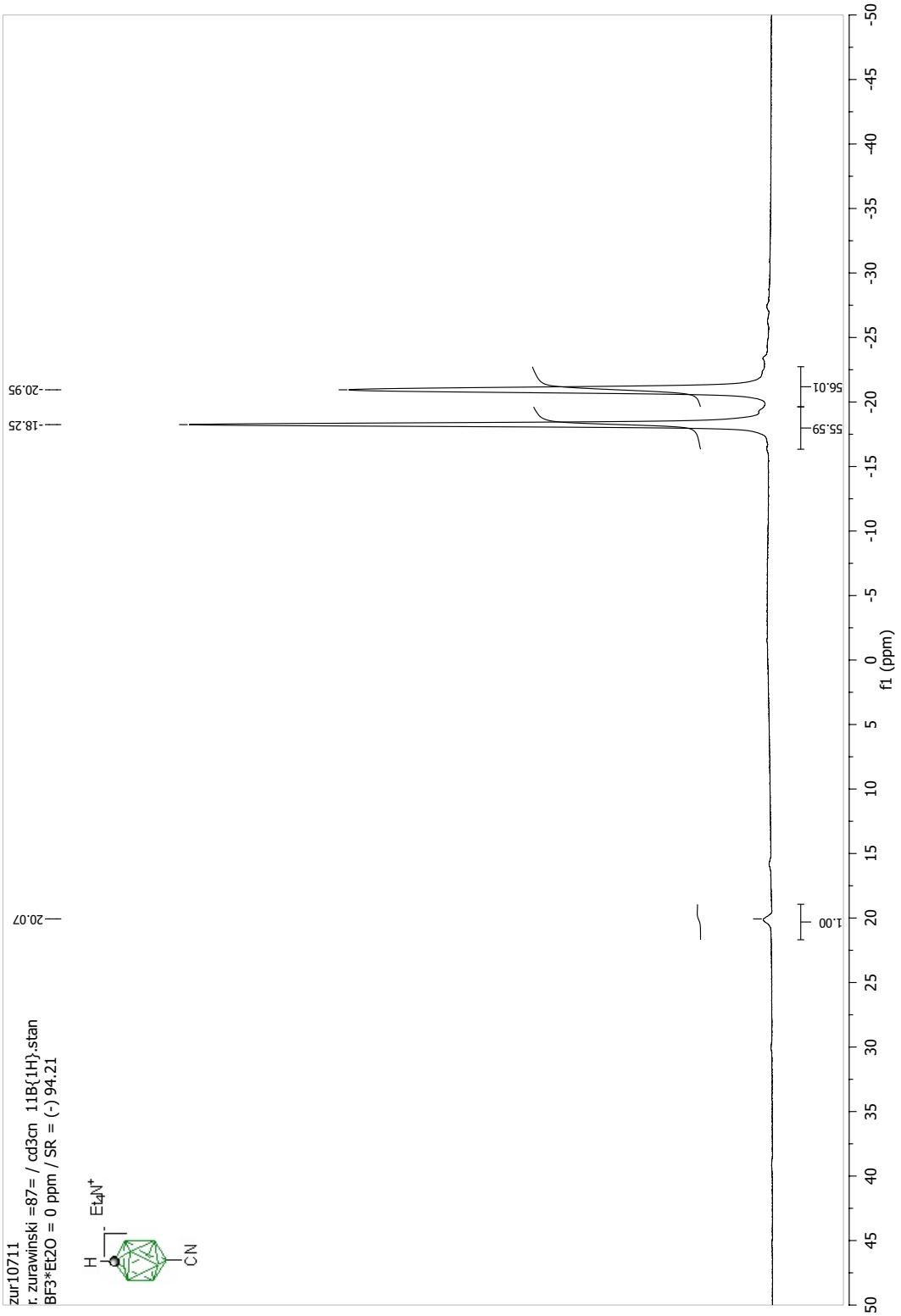


Figure S43. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-CN]$^-$[Et_4N]$^+$ (**11[10]a[Et_4N]**; CD_3CN, 160 MHz).

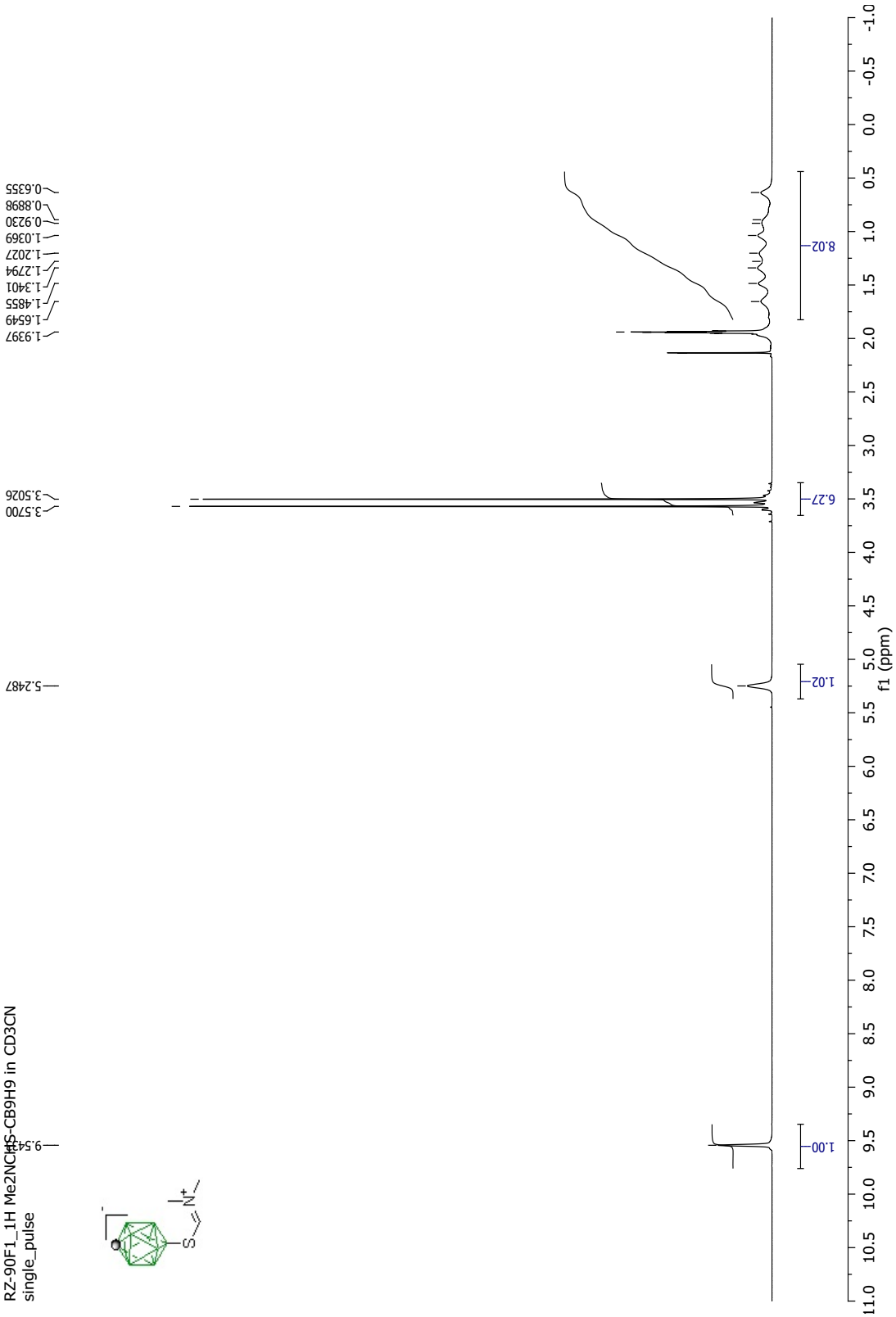


Figure S44. ^{1}H NMR of [*closo*-1-CB_9H_9-10-$SCHNMe_2$] (**12[10]a**; CD_3CN, 500 MHz).

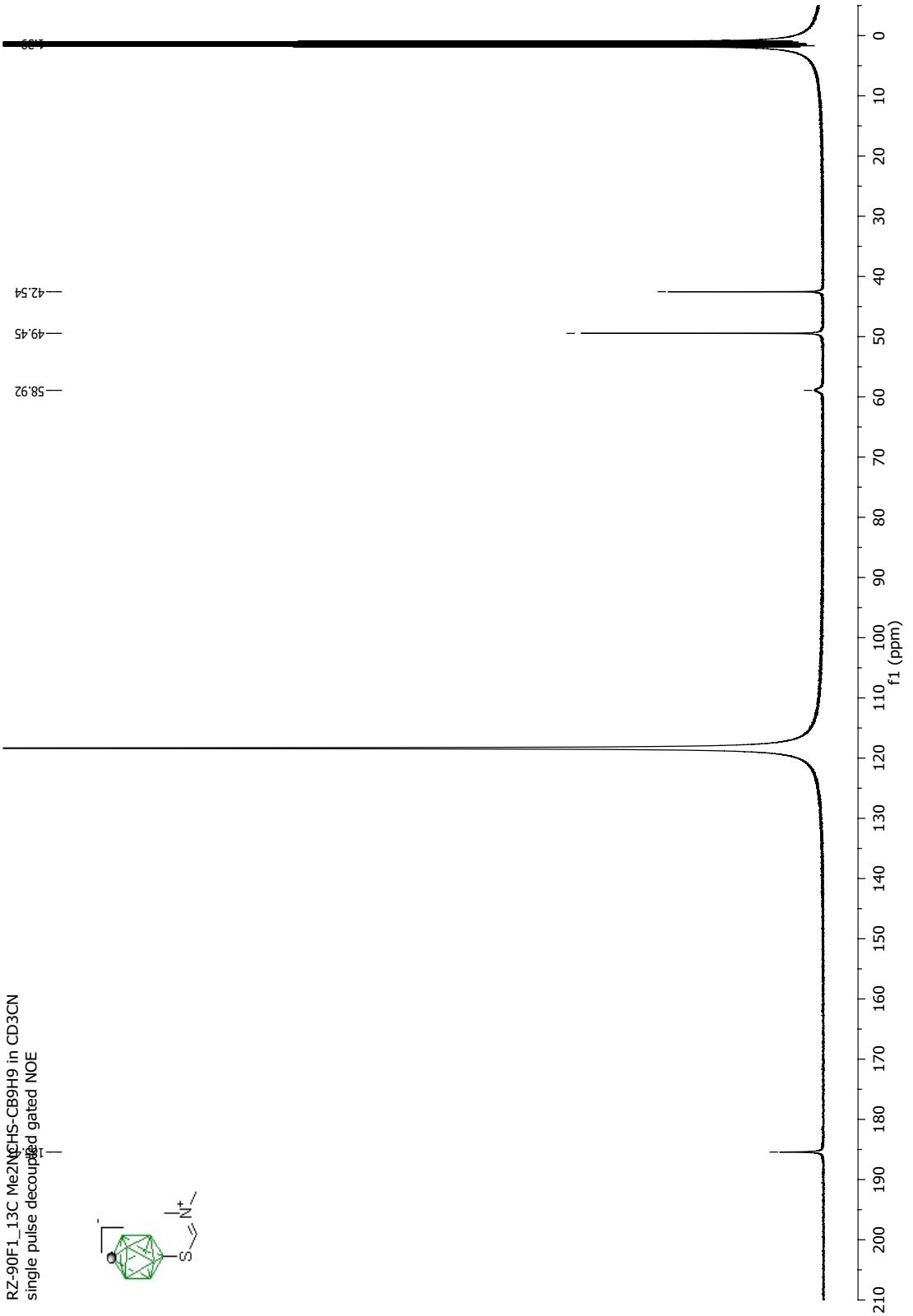


Figure S45. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-$SCHNMe_2$] (**12[10]a**; CD_3CN, 126 MHz)

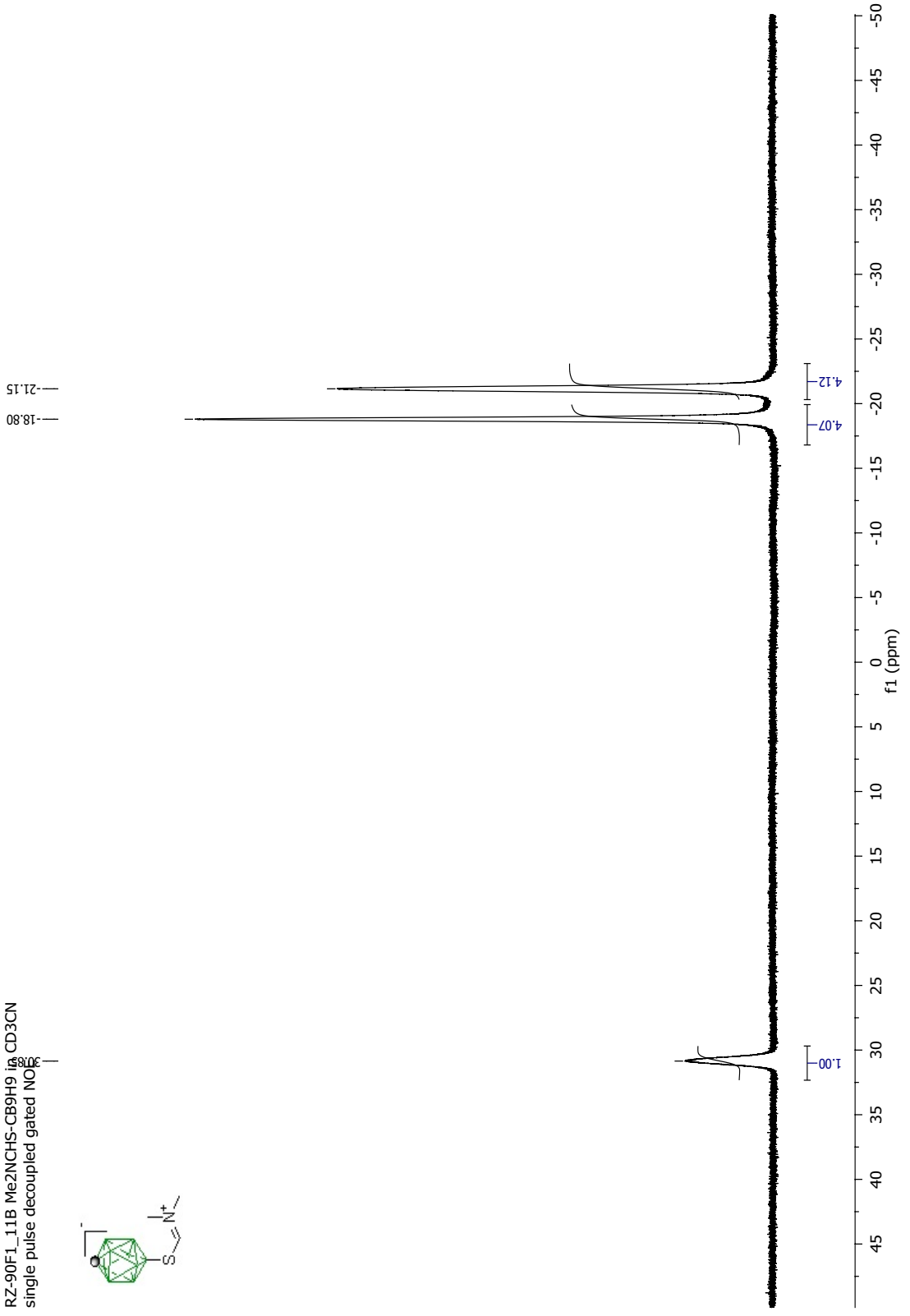


Figure S46. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-$SCHNMe_2$] (**12[10]a**; CD_3CN, 160 MHz).

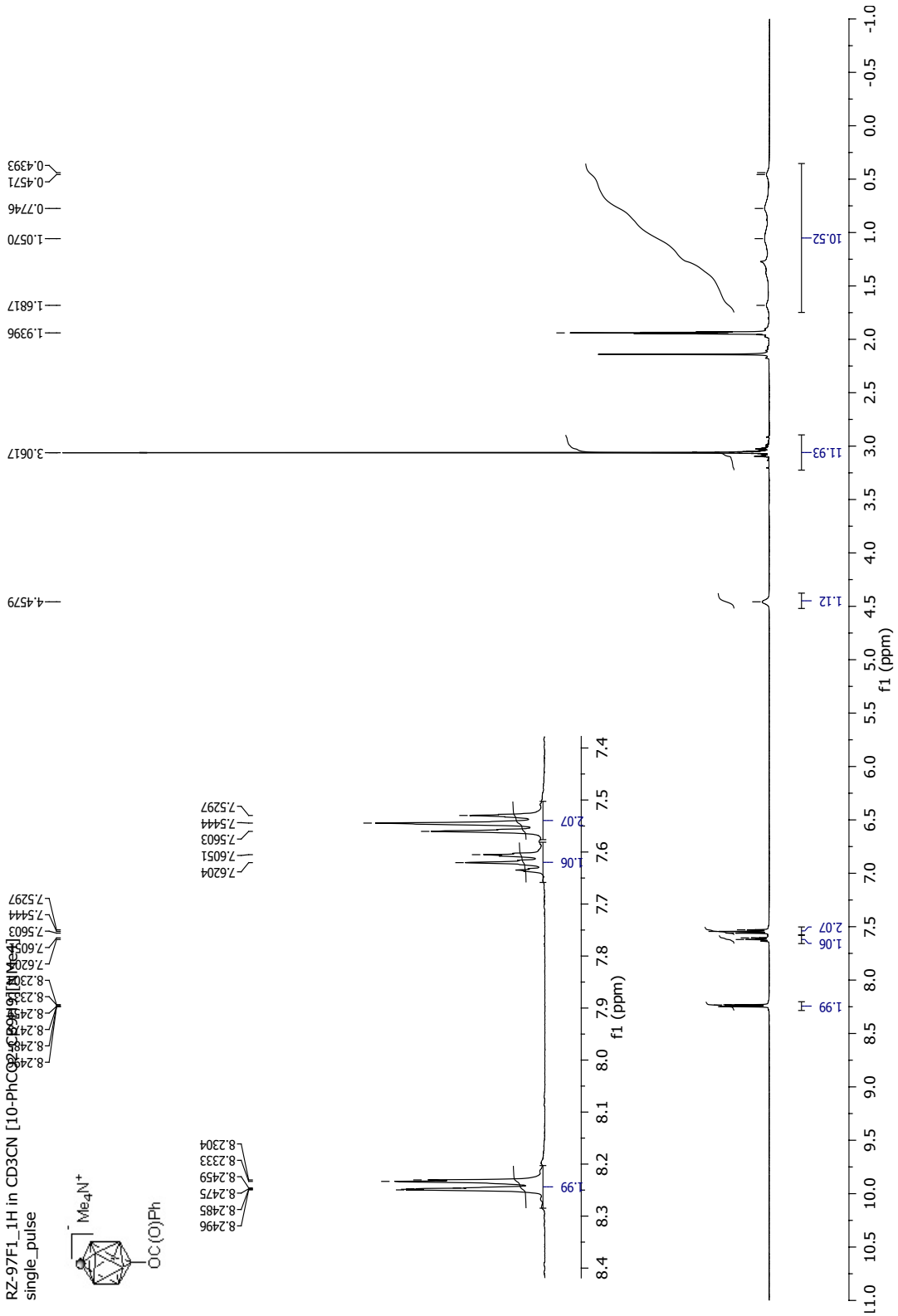


Figure S47. ^{1}H NMR of [*closo*-1-CB_9H_9-10-OCOPh]$^-$[Me_4N]$^+$ (**13[10]a[Me$_4$N]**; CD_3CN, 500 MHz)

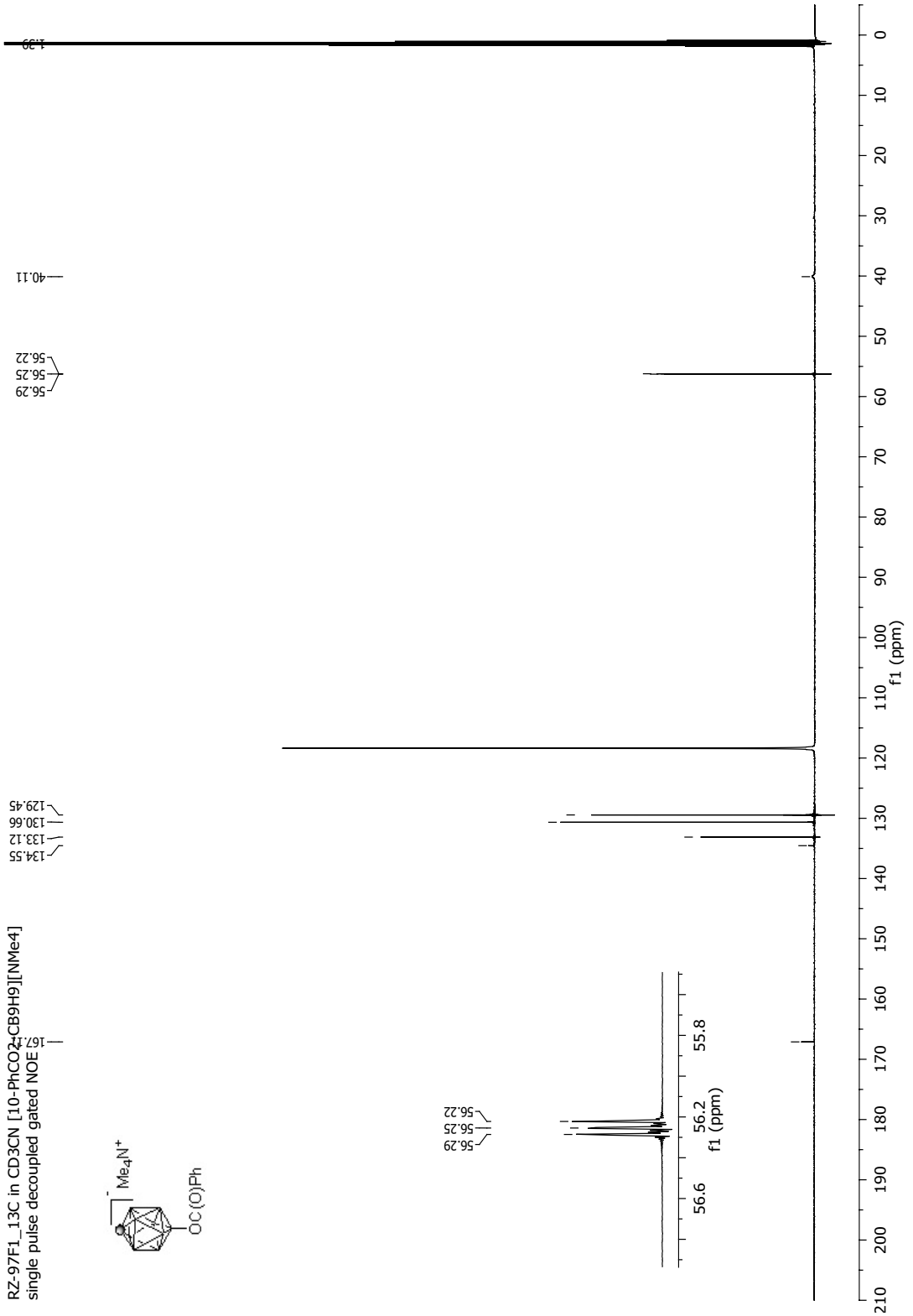


Figure S48. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-OCOPh]$^-$[Me_4N]$^+$ (**13[10]a[Me_4N]**; CD_3CN, 126 MHz)

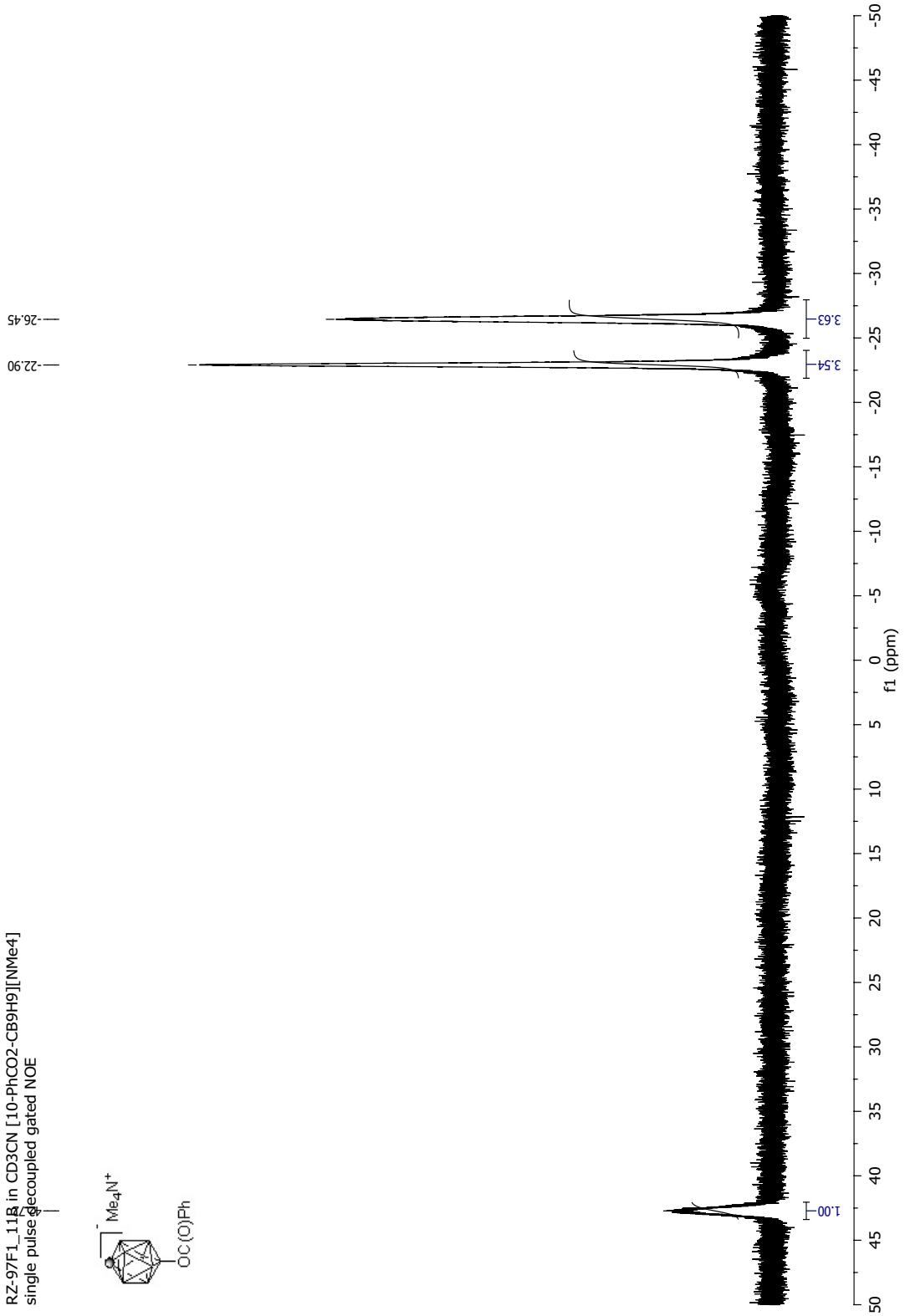


Figure S49. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-OCOPh]$^-$[Me_4N]$^+$ (**13[10]a[Me_4N]**; CD_3CN, 160 MHz)

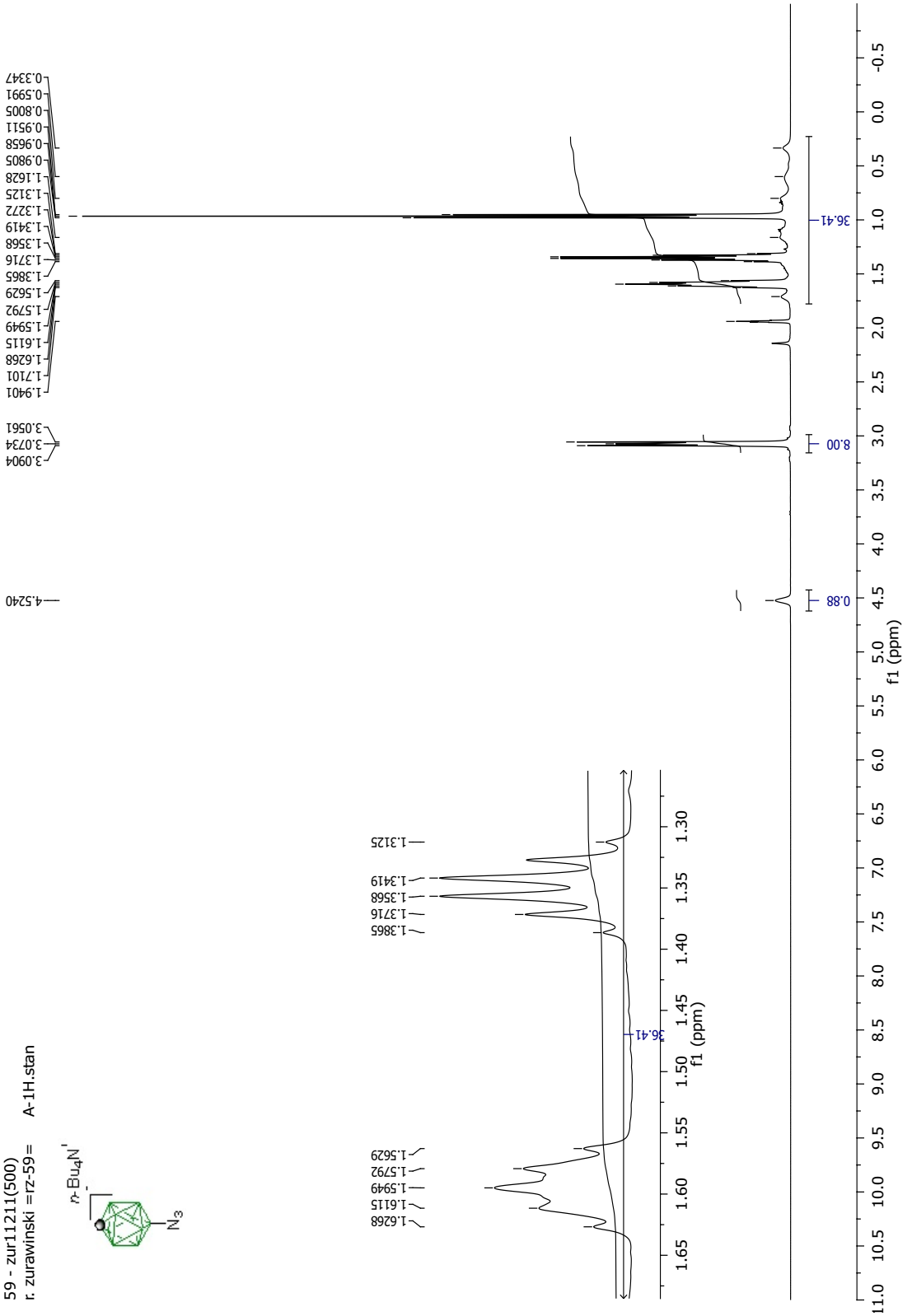


Figure S50. ^{1}H NMR of [*closo*-1-CB_9H_9-10-N_3]$^-$[Bu_4N]$^+$ (**14[10]a[Bu$_4$N]**; CD_3CN, 500 MHz)

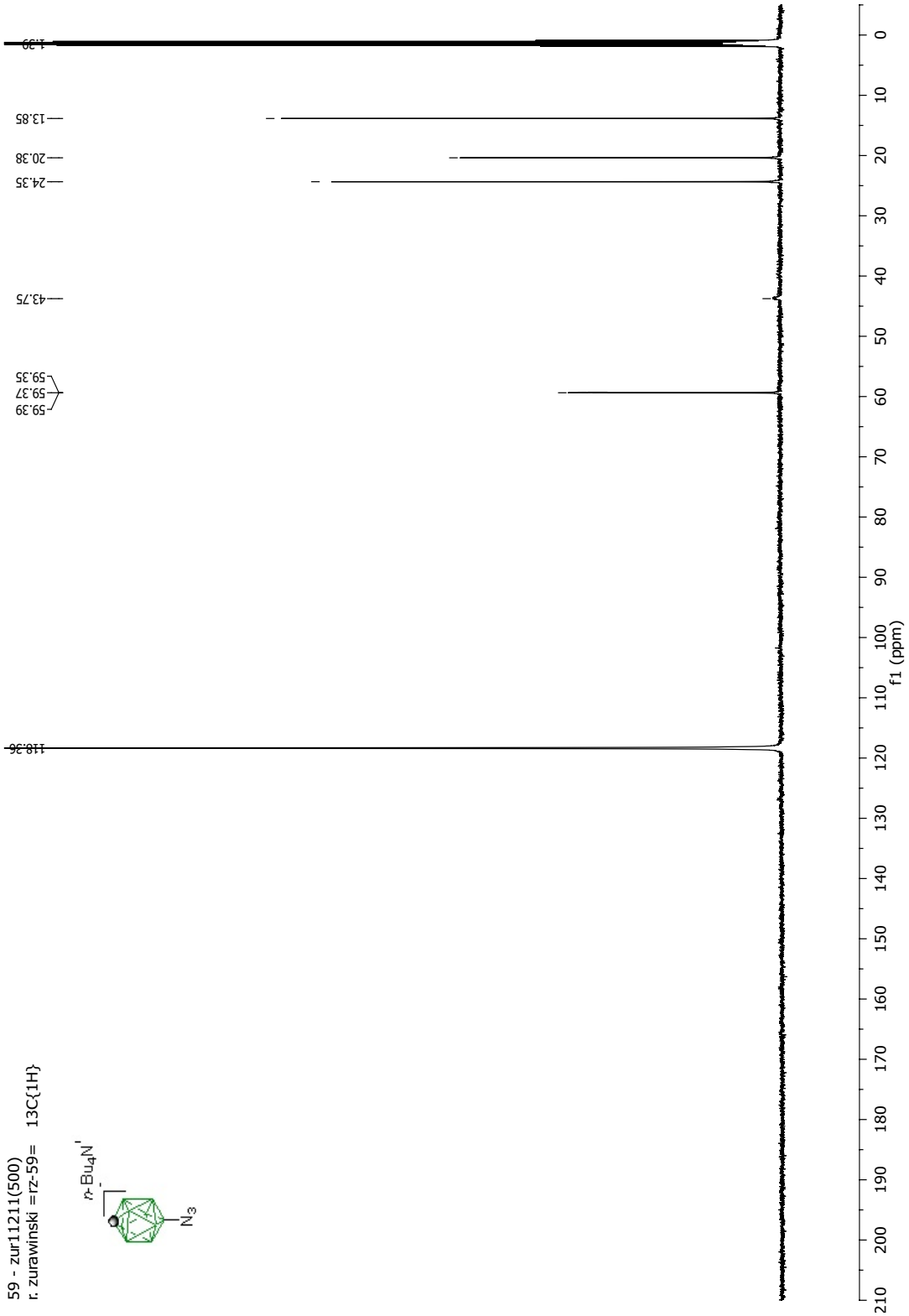


Figure S51. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-N_3]$^-$[Bu_4N]$^+$ (**14[10]a[Bu_4N]**; CD_3CN, 126 MHz)

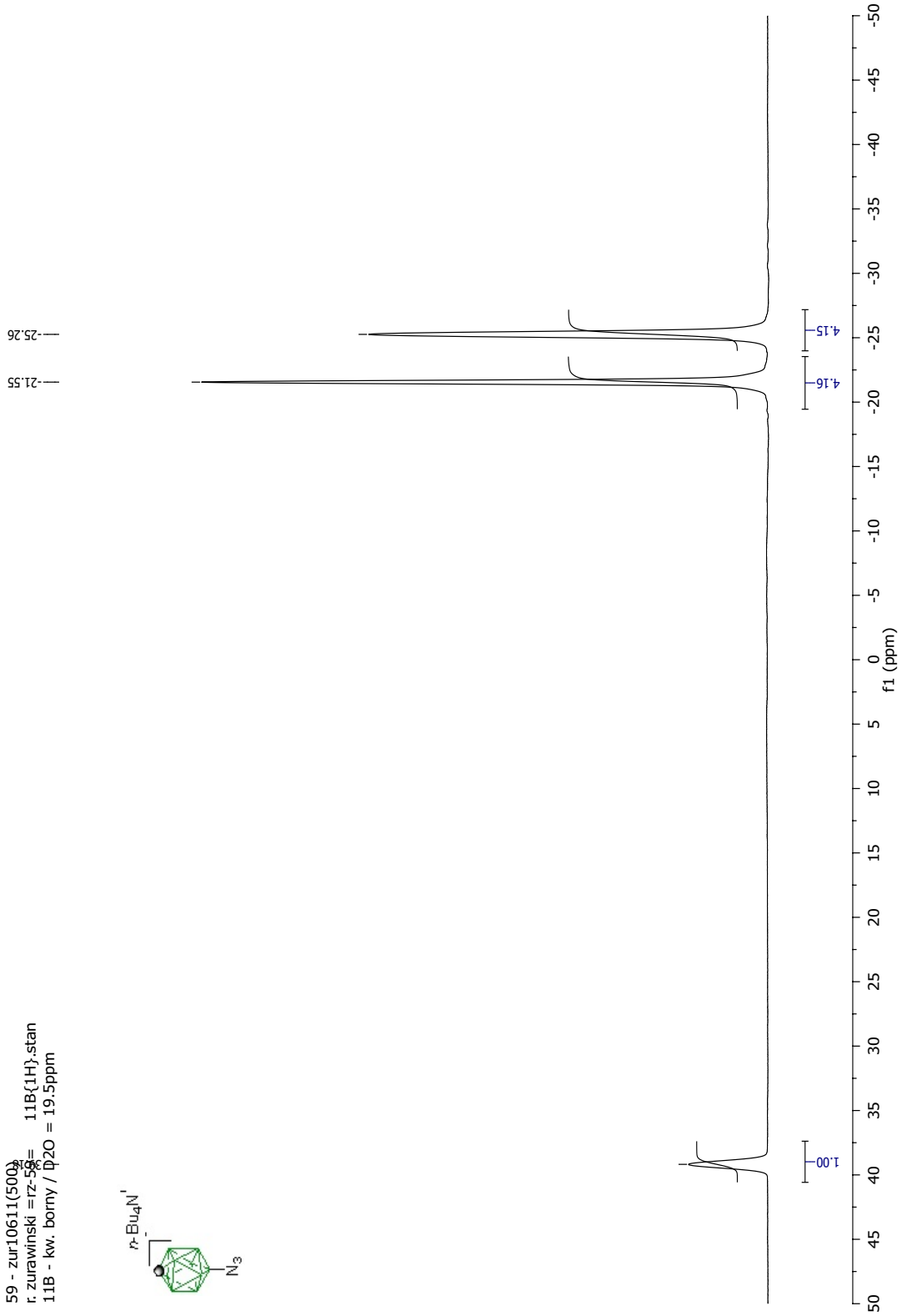


Figure S52. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-N_3]$^-$[Bu_4N]$^+$ (**14[10]a[Bu_4N]**; CD_3CN, 160 MHz)

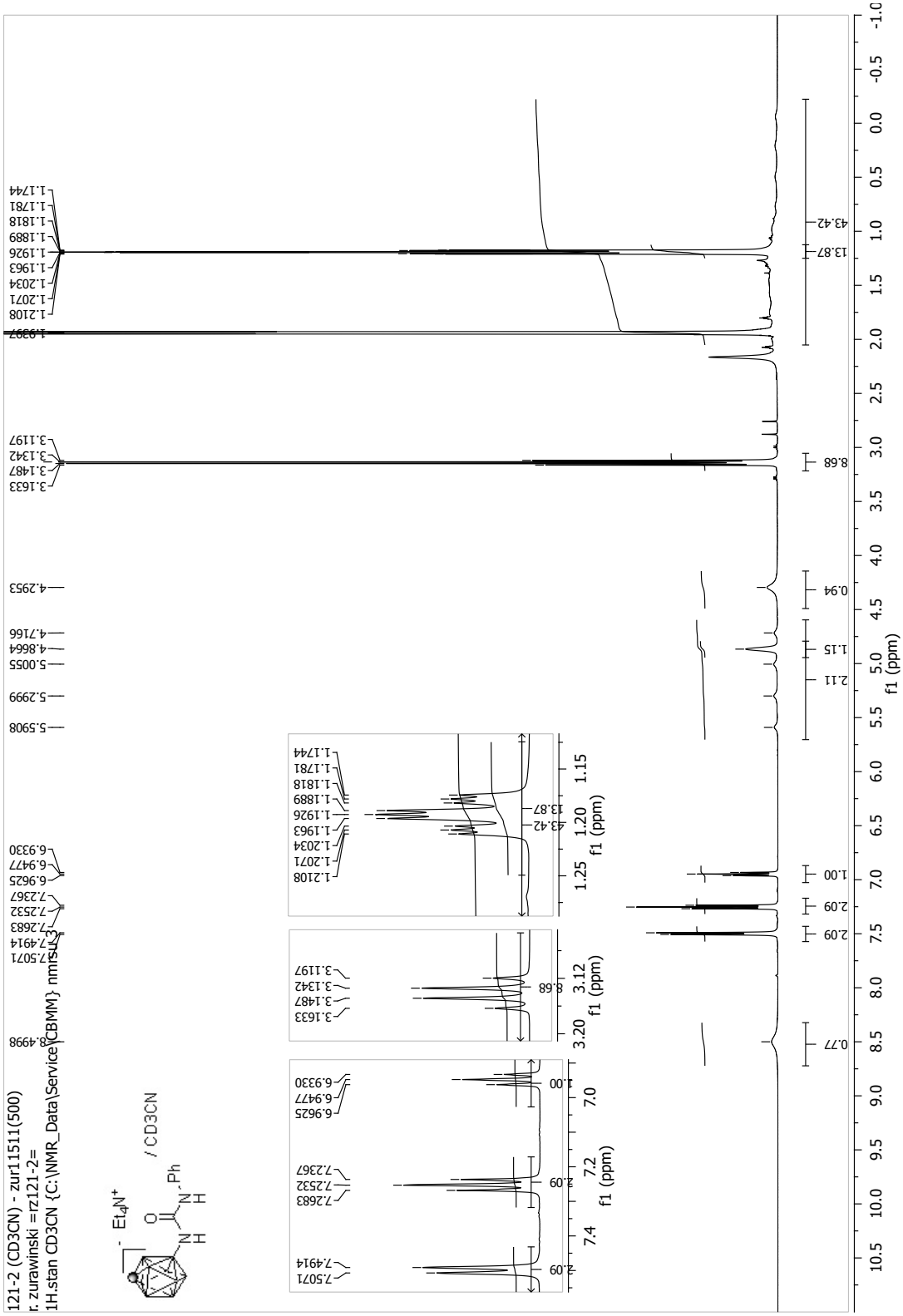


Figure S53. ^{1}H NMR of [*closo*-1-CB_9H_9-6-NHCONHPh]$^{-}$[Et_4N]$^{+}$ (**15[6]a[Et_4N]**; CD_3CN, 500 MHz)

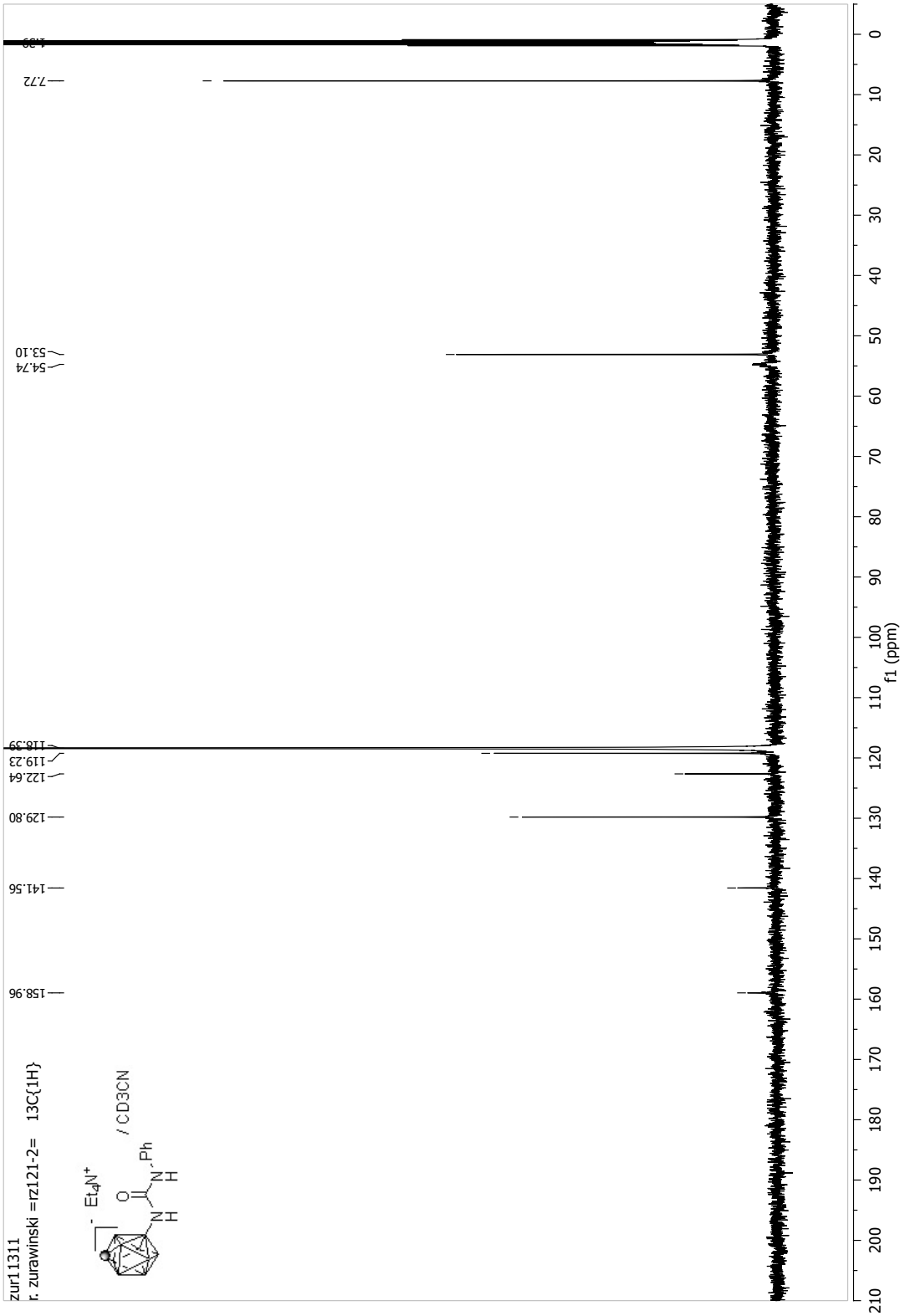


Figure S54. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NHCONHPh]$^-$[Et_4N]$^+$ (**15[6]a[Et_4N]**; CD_3CN, 126 MHz)

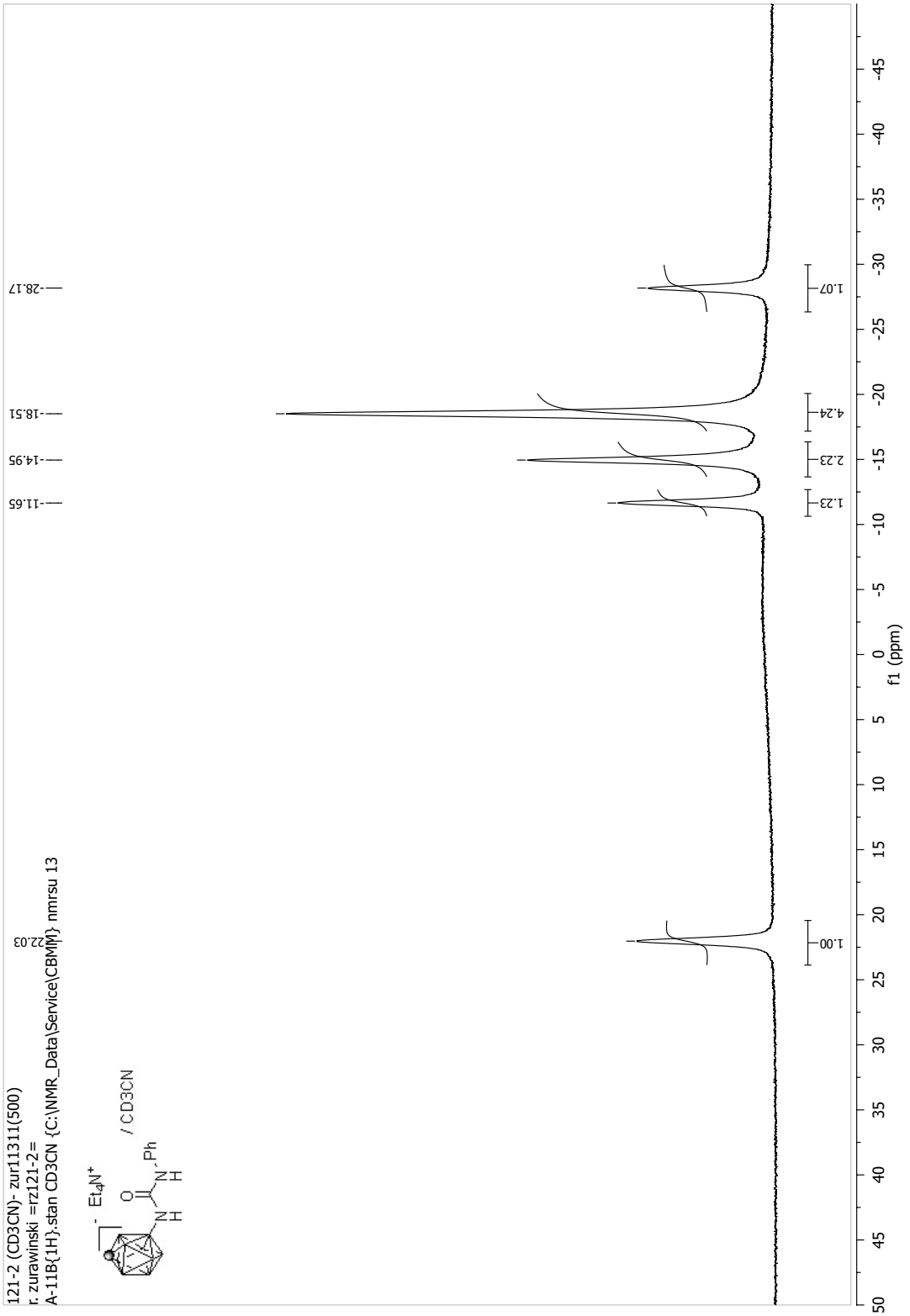


Figure S55. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-NHCONHPh]$^-$[Et_4N]$^+$ (**15[6]a[Et_4N]**; CD_3CN, 160 MHz)

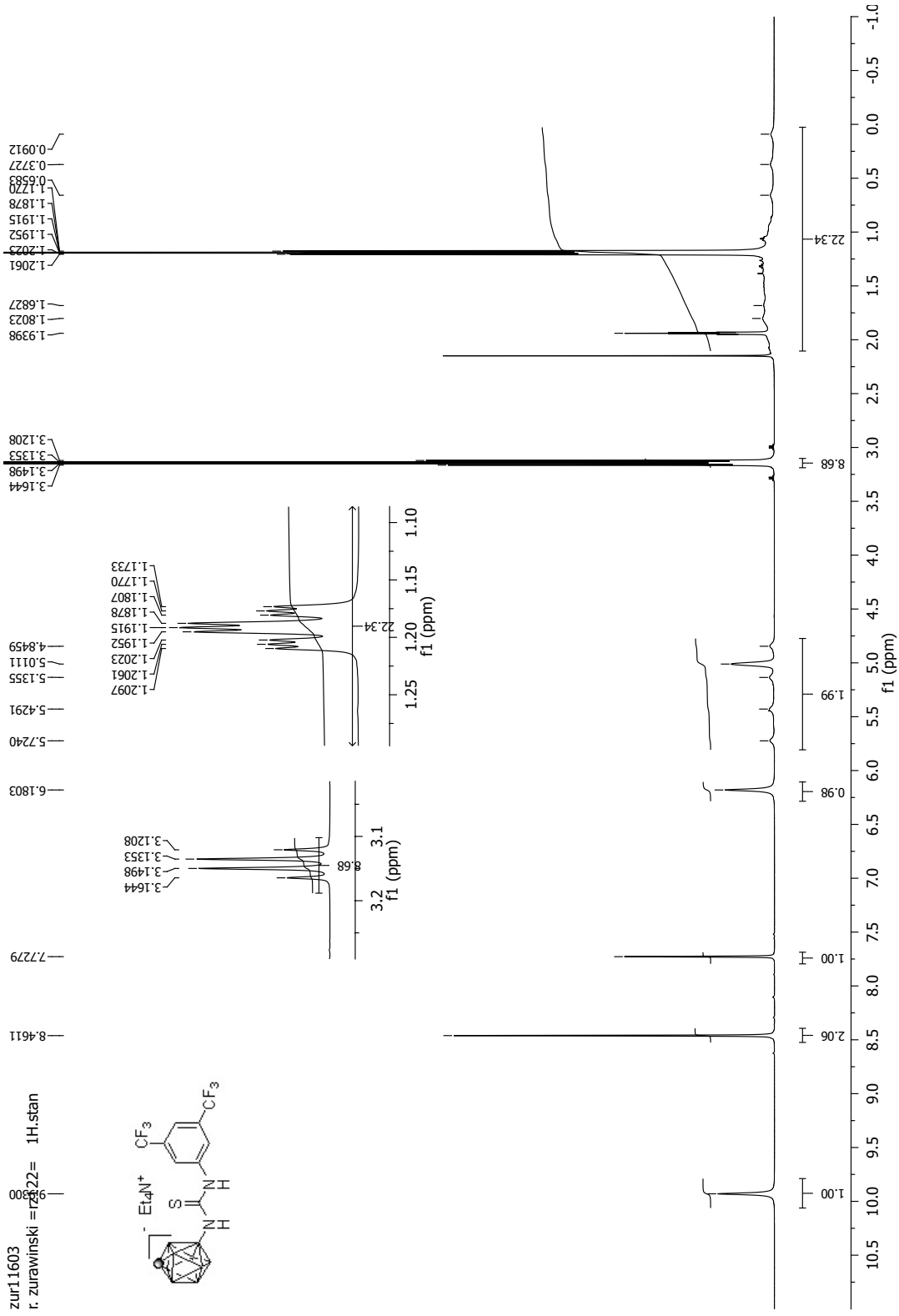


Figure S56. ^{1}H NMR of [*closo*-1-CB_9H_9-6-$NHCSNHC_6H_3(CF_3)_2$]$^-$[Et_4N]$^+$ (**16[6]a[Et_4N]**; CD_3CN, 500 MHz)

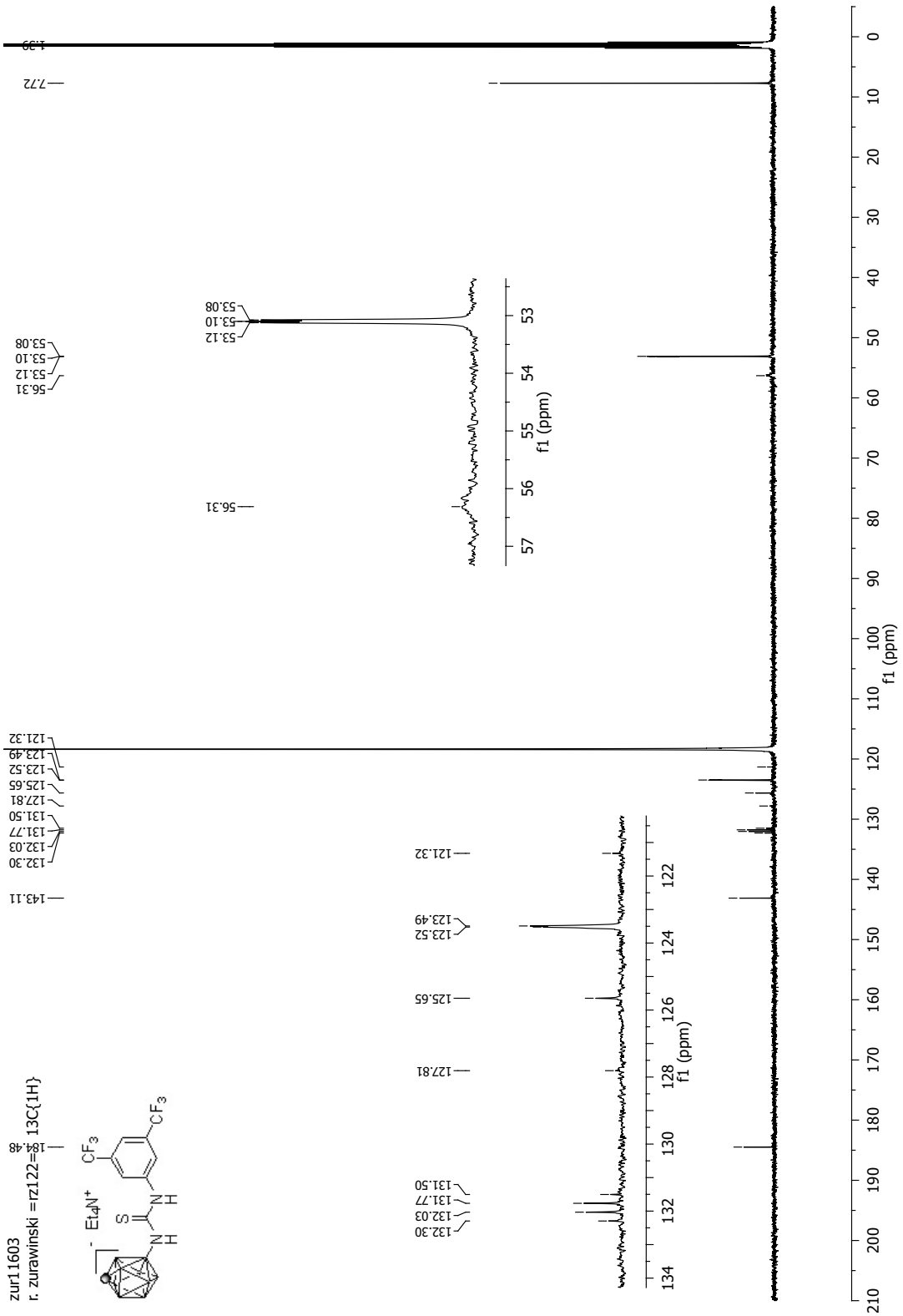


Figure S57. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-$NHCSNHC_6H_3(CF_3)_2$]$^-$[Et_4N]$^+$ (**16[6]a[Et$_4$N]**; CD_3CN, 126 MHz)

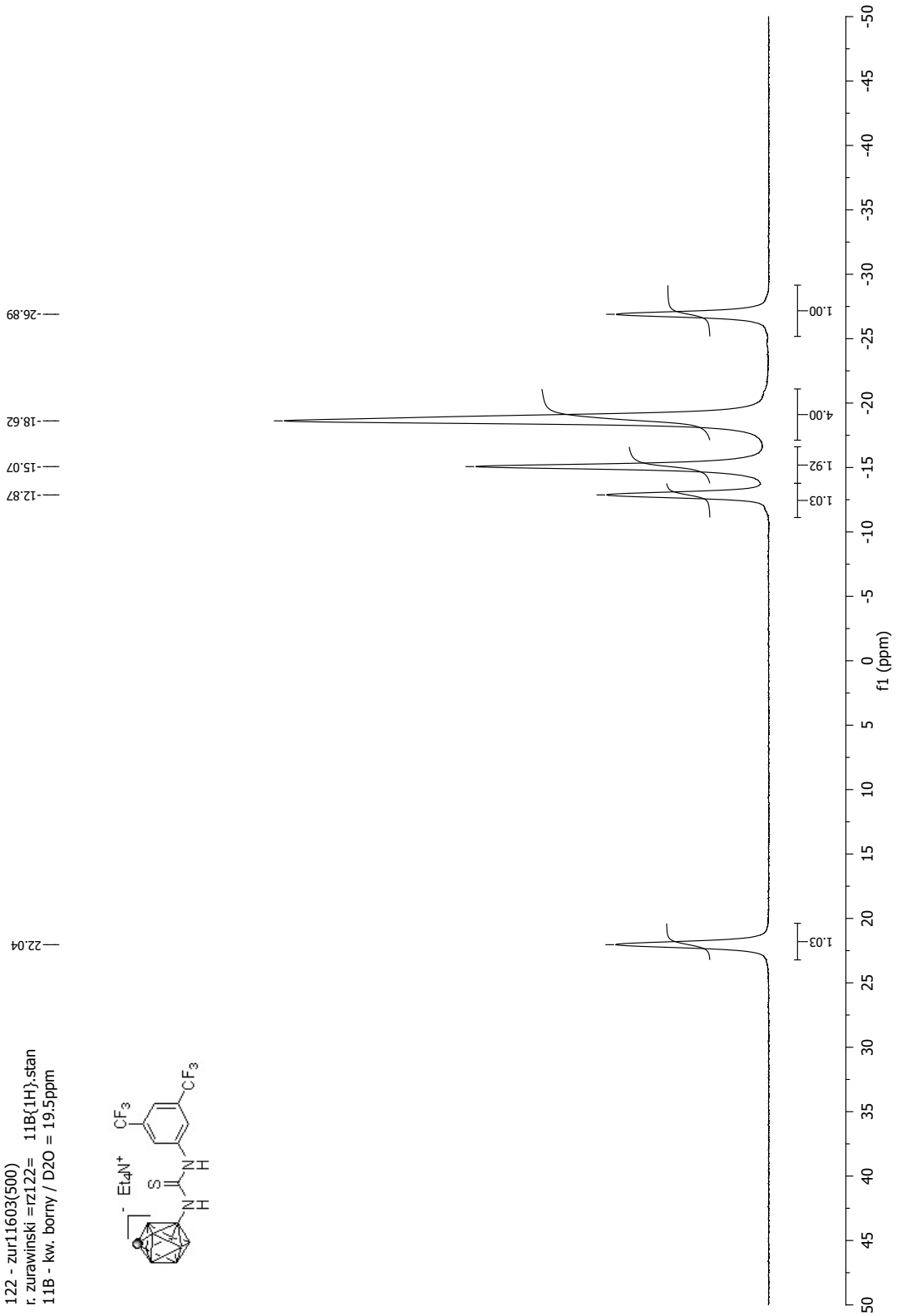


Figure S58. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-$NHCSNHC_6H_3(CF_3)_2$]$^-$[Et_4N]$^+$ (**16[6]a[Et$_4$N]**; CD_3CN, 160 MHz)

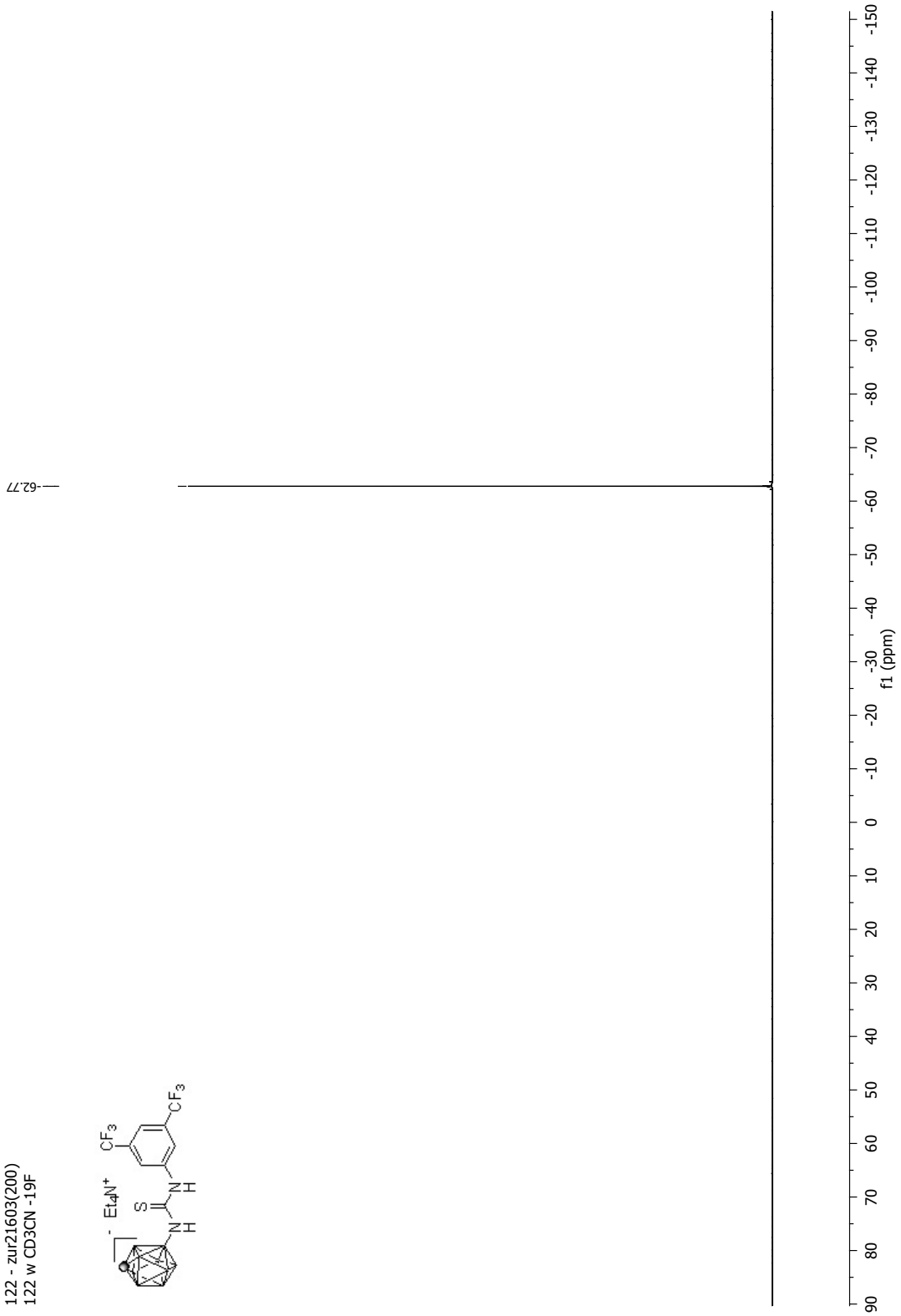


Figure S59. $^{19}F\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-$NHCSNHC_6H_3(CF_3)_2$]$^-$[Et_4N]$^+$ (**16[6]a[Et$_4$N]**; CD_3CN, 188 MHz)

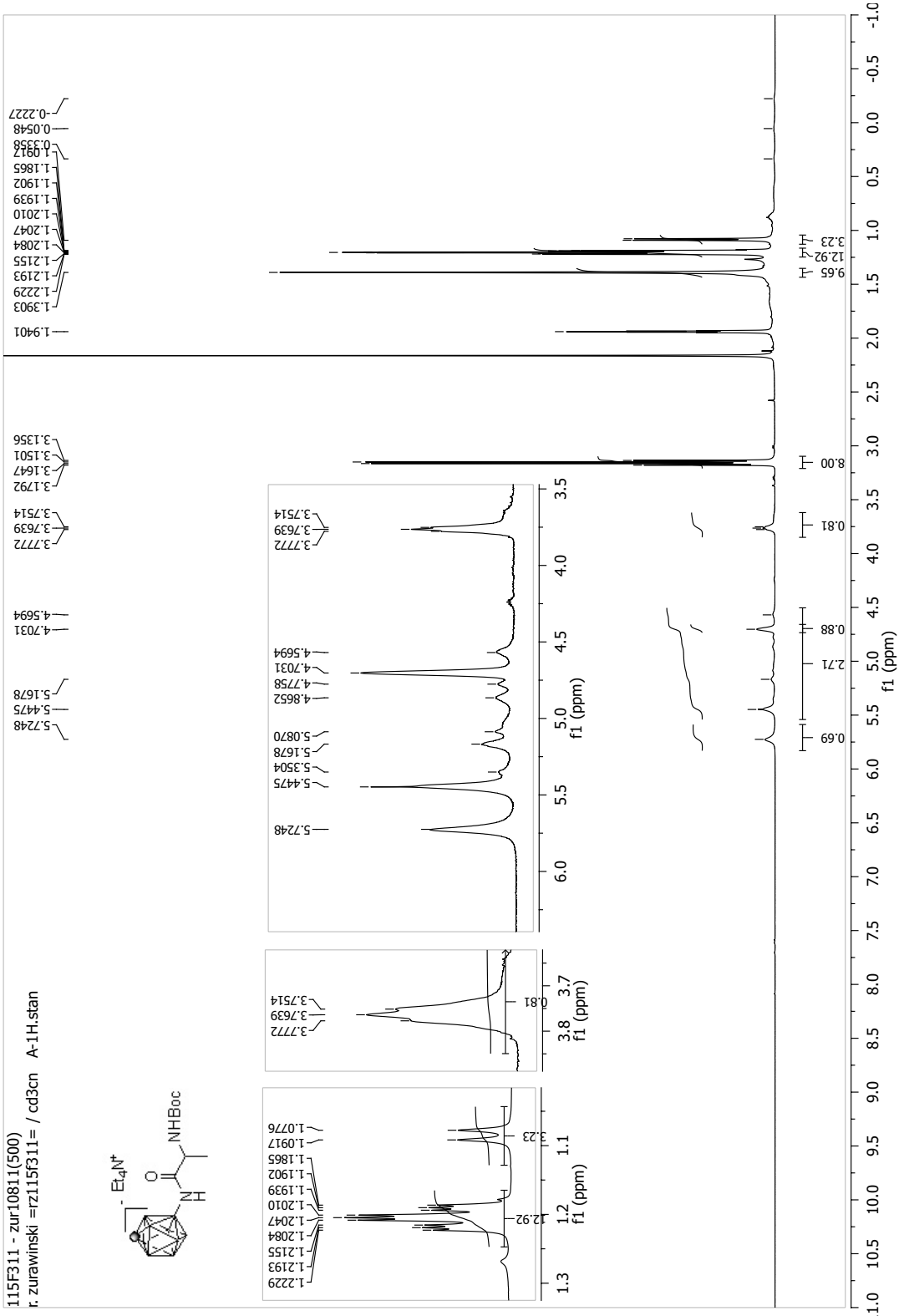


Figure S60. ^{1}H NMR of [*closo*-1-CB_9H_9-6-AlaBoc]$^{-}$[Et_4N]$^{+}$ (**17[6]a[Et_4N]**; CD_3CN, 500 MHz)

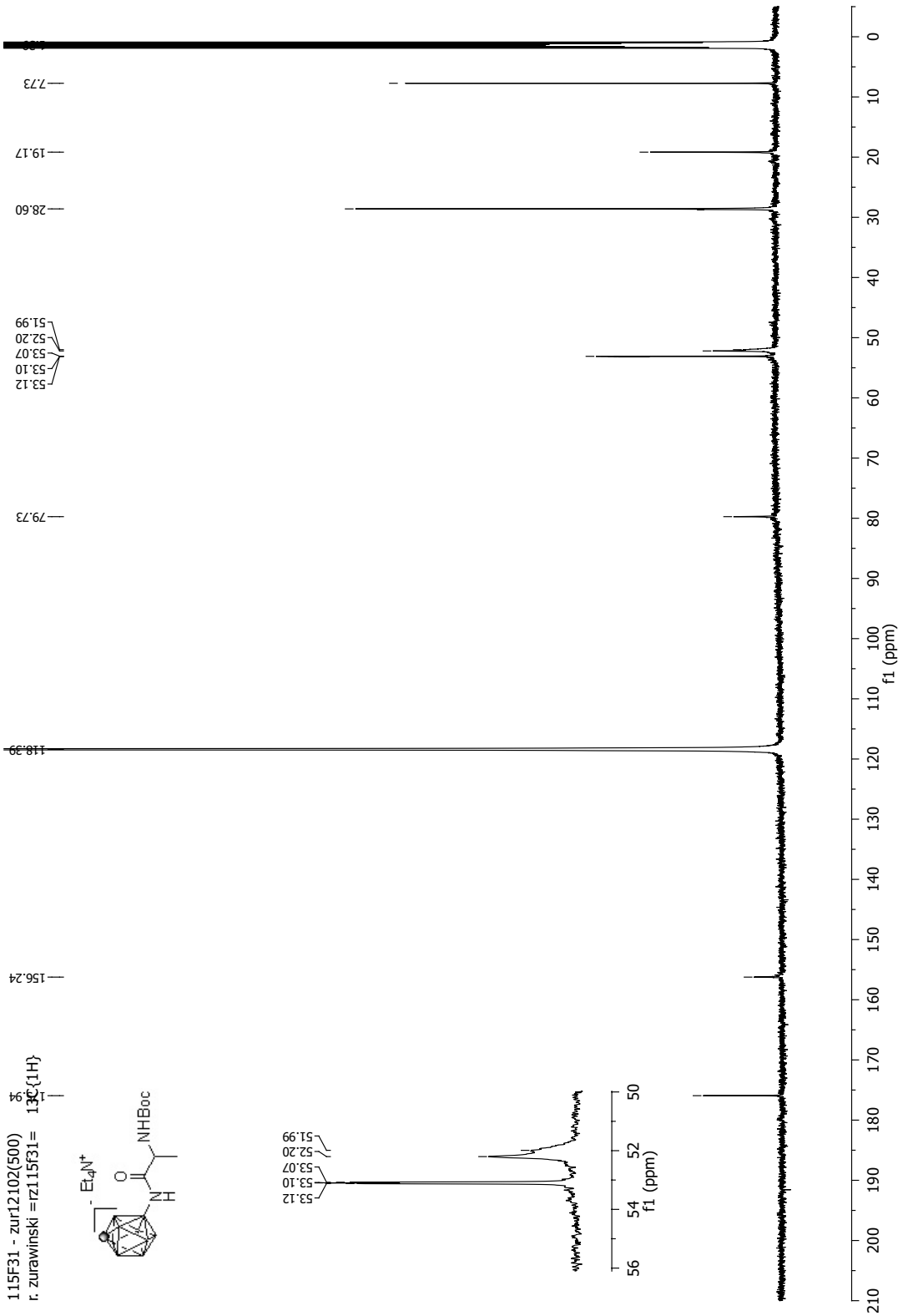


Figure S61. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-AlaBoc]$^-$[Et_4N]$^+$ (**17[6]a[Et_4N]**; CD_3CN, 126 MHz)

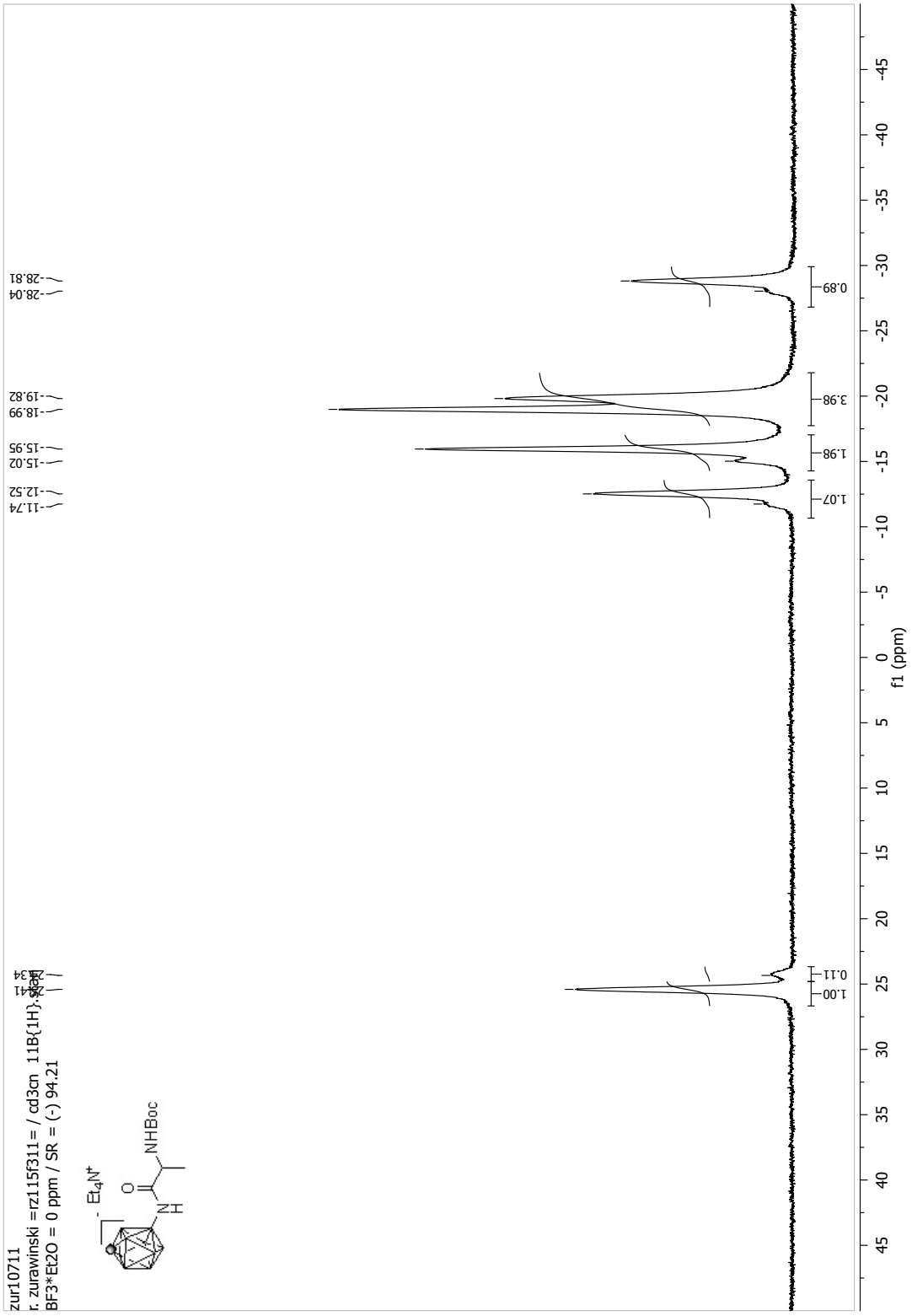


Figure S62. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-6-AlaBoc]$^-$[Et_4N]$^+$ (**17[6]a[Et_4N]**; CD_3CN, 160 MHz)

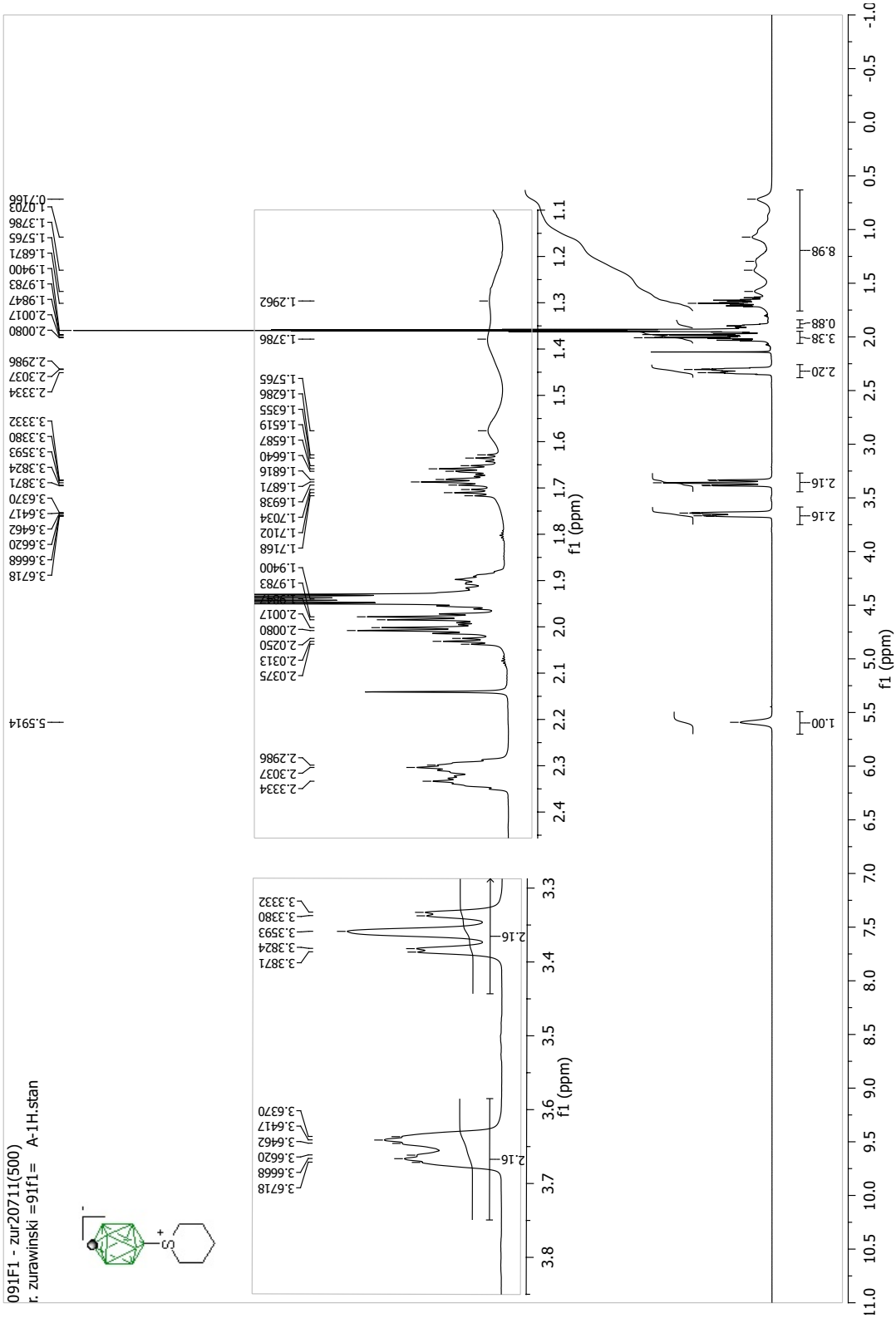


Figure S63. ^{1}H NMR of [*closo*-1-CB_9H_9-10-$(CH_2)_5S$] (**18[10]a**; CD_3CN, 500 MHz)

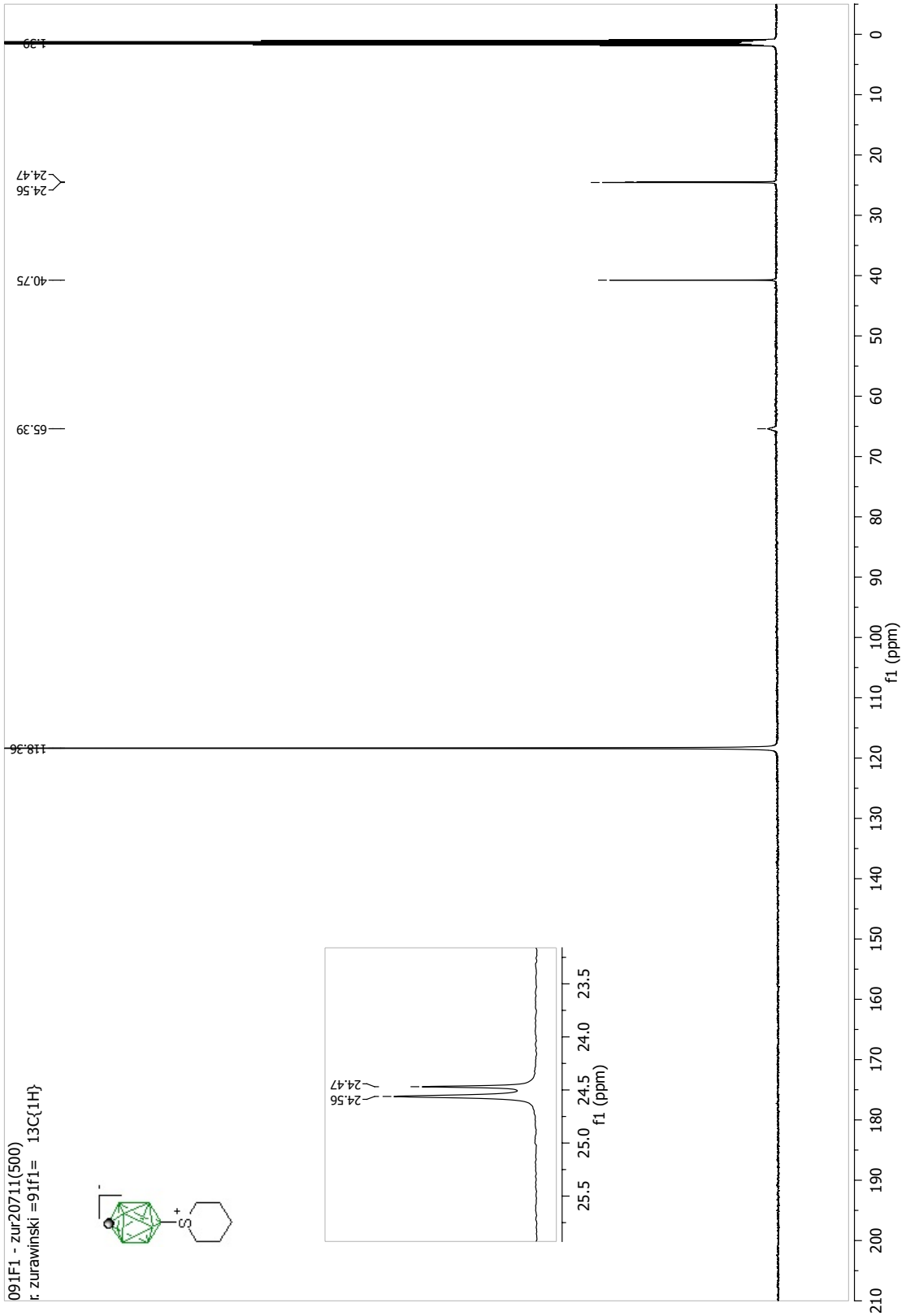


Figure S64. $^{13}C\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-$(CH_2)_5S$] (**18[10]a**; CD_3CN, 126 MHz)

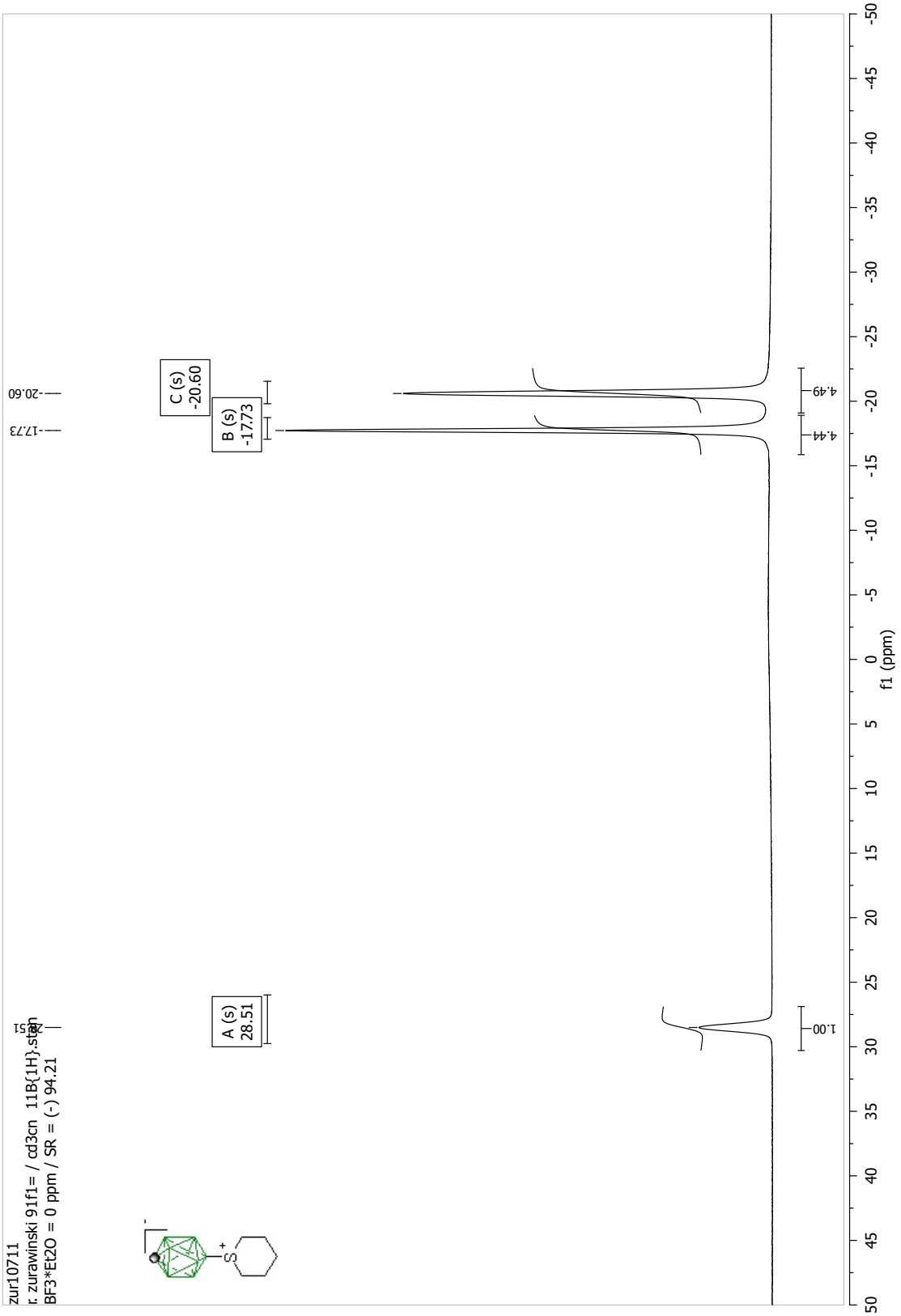


Figure S65. $^{11}B\{^{1}H\}$ NMR of [*closo*-1-CB_9H_9-10-$(CH_2)_5S$] (**18[10]a**; CD_3CN, 160 MHz)

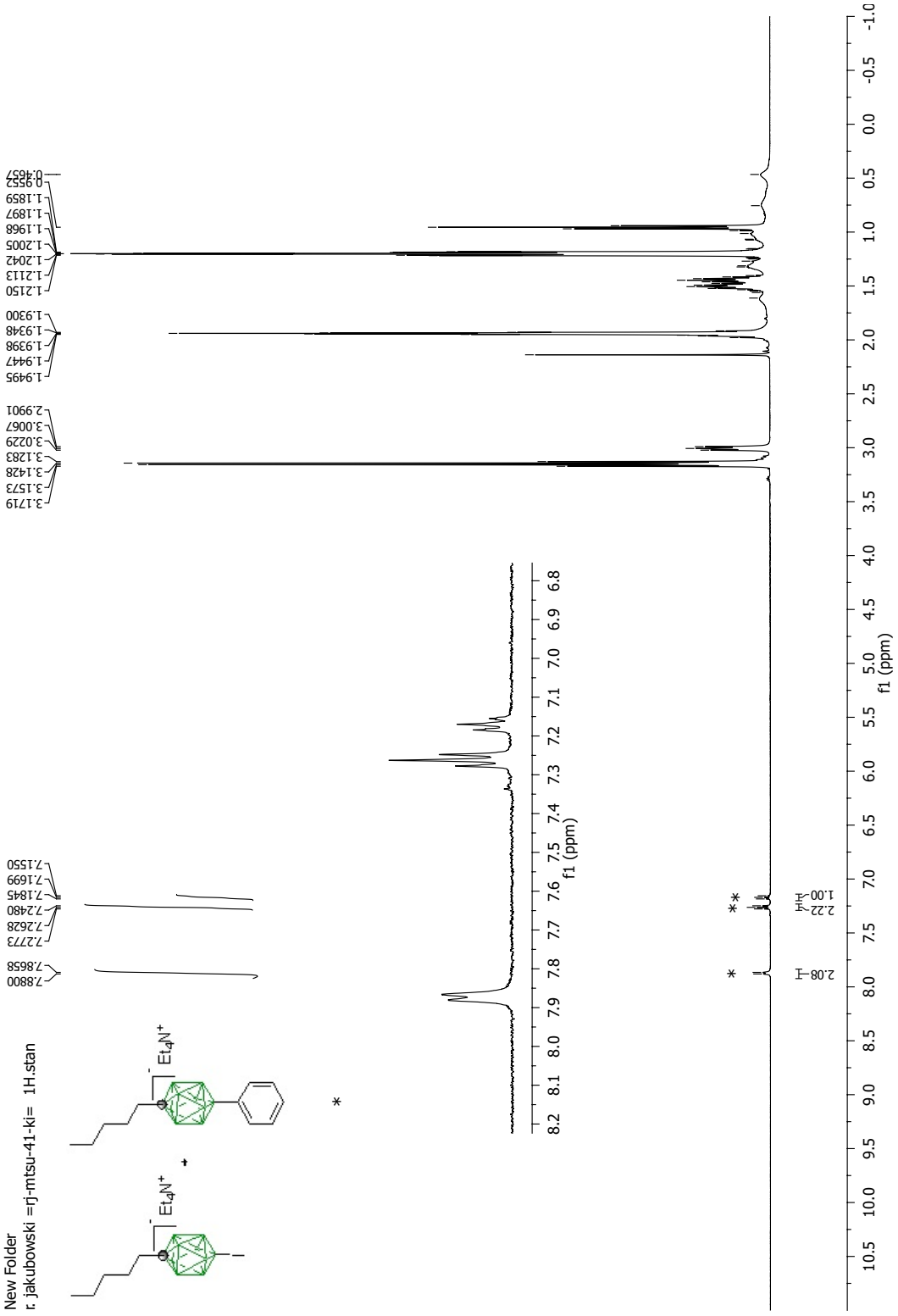


Figure S66. ^{1}H NMR of a crude mixture of **3[10]c[Et$_4$N]** and [*closo*-1-CB_9H_9-1-C_5H_{11}-10-Ph] (CD_3CN, 500 MHz). Signals characteristic for the latter are denoted with asterisks.

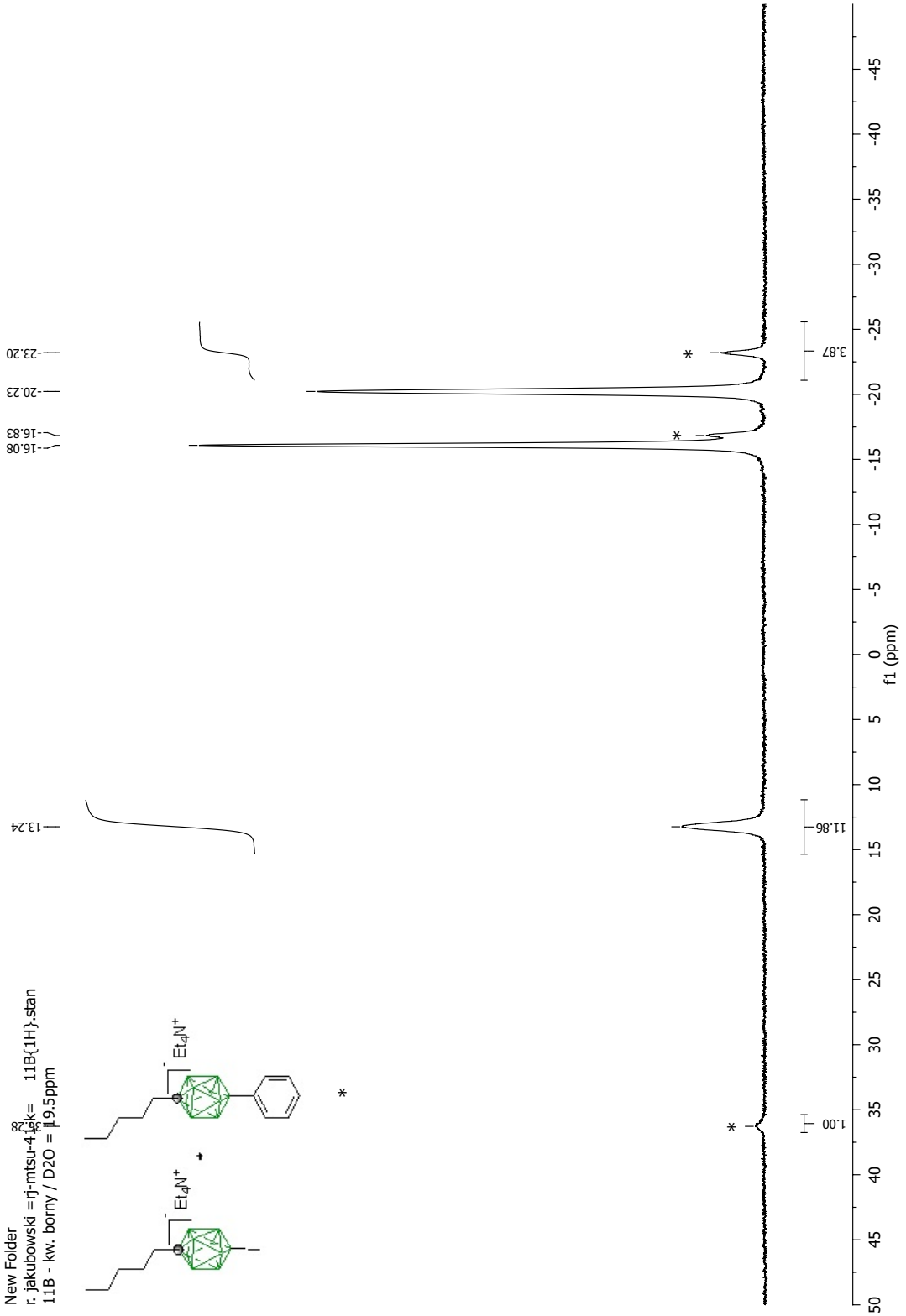


Figure S67. $^{11}B\{^{1}H\}$ NMR of a crude mixture of **3[10]c[Et$_4$N]** and [*closo*-1-CB_9H_9-1-C_5H_{11}-10-Ph] (CD_3CN, 160 MHz). Signals characteristic for the latter are denoted with asterisks.

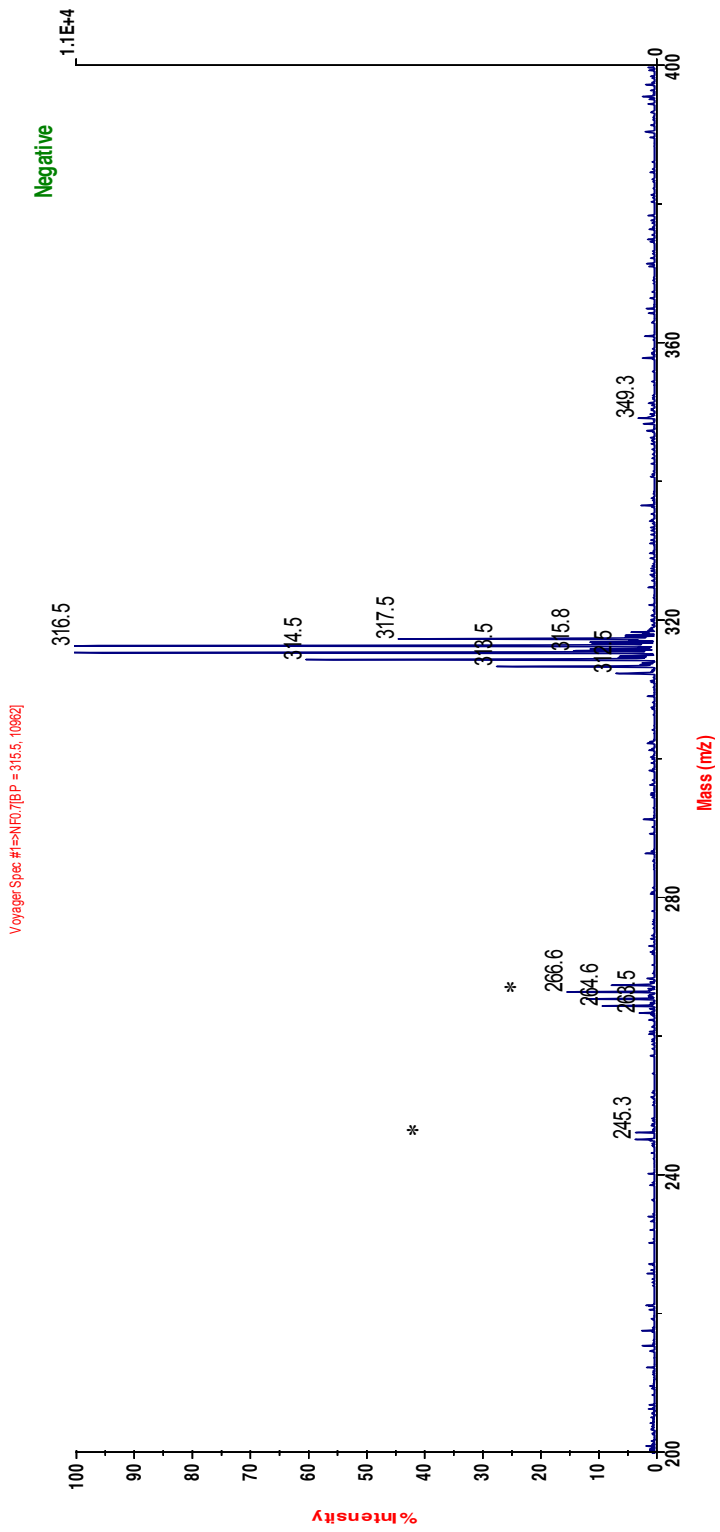


Figure S68. EI MS spectra of a crude mixture of **3[10]c[Et$_4$N]** and [*closo*-1-CB_9H_9-1-C_5H_{11}-10-Ph]. Signals characteristic for the latter are denoted with asterisks.

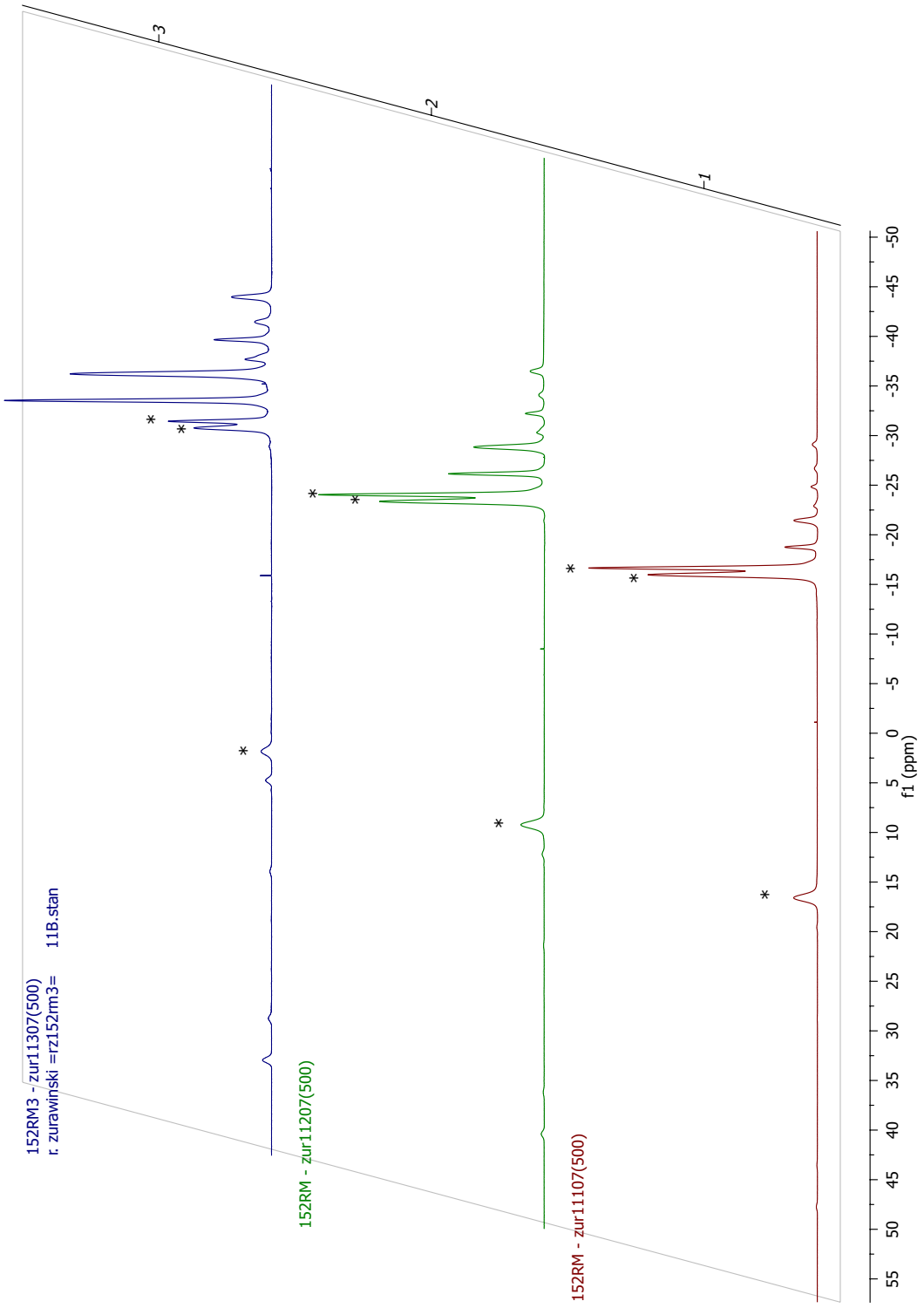


Figure S69. $^{11}B\{^{1}H\}$ NMR of a reaction mixture of **4[10]a** with $[Et_4N]^+$ CN^- in CD_3CN at three time intervals [*closo*-1-CB_9H_9-1-C_5H_{11}-10-Ph] (CD_3CN, 160 MHz). Signals characteristic for **4[10]a** are denoted with asterisks.

8. Archive data for DFT calculations

M06-2x/6-31G(2d,p)

4[1]a


```
1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C1H9B9N2\PIOTR\11-Nov-2017\
 0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck #
 P freq(noraman, readIso)\\1-CB9-1-N2, C4v\\0,1\B,-1.3295669735,0.,-0.0
 827685524\B,0.,1.3295669735,-0.0827685524\B,1.3295669735,0.,-0.0827685
 524\B,0.,-1.3295669735,-0.0827685524\B,-0.9186420602,-0.9186420602,1.3
 909985097\B,-0.9186420602,0.9186420602,1.3909985097\B,0.9186420602,0.9
 186420602,1.3909985097\B,0.9186420602,-0.9186420602,1.3909985097\B,0.,
 0.,2.4950672987\C,0.,0.,-0.9991756277\N,0.,0.,-2.3543325129\N,0.,0.,-3
 .4560169079\H,0.,0.,3.6725590529\H,-2.3732974104,0.,-0.6359534667\H,0.
 ,2.3732974104,-0.6359534667\H,2.3732974104,0.,-0.6359534667\H,0.,-2.37
 32974104,-0.6359534667\H,-1.7077617537,-1.7077617537,1.7845617148\H,-1
 .7077617537,1.7077617537,1.7845617148\H,1.7077617537,1.7077617537,1.78
 45617148\H,1.7077617537,-1.7077617537,1.7845617148\\Version=ES64L-G09R
 evD.01\State=1-A1\HF=-376.6343929\RMSD=9.111e-09\RMSF=2.052e-06\Dipole
 =0.,0.,-2.4979273\Quadrupole=-1.7010024,-1.7010024,3.4020047,0.,0.,0.\
 PG=C04V [C4(H1B1C1N1N1),2SGV(H2B2),2SGD(H2B2)]\\@
```


4[10]a


```
1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C1H9B9N2\PIOTR\10-Nov-2017\
 0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck #
 P freq(noraman, readIso)\\1-CB9-10-B2, C4v\\0,1\B,-1.3162137069,0.,-0.
 0863097039\B,0.,1.3162137069,-0.0863097039\B,1.3162137069,0.,-0.086309
 7039\B,0.,-1.3162137069,-0.0863097039\B,-0.9215849014,-0.9215849014,1.
 4080071204\B,-0.9215849014,0.9215849014,1.4080071204\B,0.9215849014,0.
 9215849014,1.4080071204\B,0.9215849014,-0.9215849014,1.4080071204\C,0.
 ,0.,2.3277324438\B,0.,0.,-1.1103008518\N,0.,0.,-2.5828509555\N,0.,0.,-
 3.6795549549\H,0.,0.,3.4046196095\H,-2.4194987129,0.,-0.5153989184\H,0
 .,2.4194987129,-0.5153989184\H,2.4194987129,0.,-0.5153989184\H,0.,-2.4
 194987129,-0.5153989184\H,-1.6803464513,-1.6803464513,1.9005531421\H,-
 1.6803464513,1.6803464513,1.9005531421\H,1.6803464513,1.6803464513,1.9
 005531421\H,1.6803464513,-1.6803464513,1.9005531421\\Version=ES64L-G09
 RevD.01\State=1-A1\HF=-376.7182882\RMSD=9.120e-09\RMSF=2.361e-06\Dipol
 e=0.,0.,-1.1223702\Quadrupole=-4.4201108,-4.4201108,8.8402216,0.,0.,0.
 \PG=C04V [C4(H1C1B1N1N1),2SGV(H2B2),2SGD(H2B2)]\\@
```


5[6]a


```
1\1\GINC-OCTOPUS\FOpt\RM062X\Gen\C7H14B9I1\PIOTR\16-Nov-2014\0\\#P M06
 2x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(noraman, r
 eadIso) Pseudo=Read\\6-PhI-CB9, C1 orientation syn\\0,1\B,1.3215390149
 ,1.6817110753,0.6912110741\B,1.2990355439,0.0474574886,-0.0212937609\B
 ,3.0241350926,-0.2621426474,0.3060172848\B,3.0980659039,1.4183541251,1
 .0124718881\B,2.554629384,2.450005789,-0.3694897084\B,1.2204391428,1.4
 459362772,-1.1052177138\B,2.4350611262,0.0592021044,-1.380013043\B,3.7
 51080254,1.0840175135,-0.6401740941\B,1.927023758,0.2953055404,1.50373
 09337\I,-0.3878718034,-1.4091596069,-0.1268883686\C,2.6827397214,1.596
 1384126,-1.7204867745\C,-0.8383055456,-1.3965746602,-2.1817665429\C,-0
 .1725428058,-2.2860196094,-3.0163701136\C,-1.7608640858,-0.4725299158,
 -2.6571006223\C,-0.4509401949,-2.2441739295,-4.3788459376\C,-2.0239806
 314,-0.4481302135,-4.0230330078\C,-1.3726057492,-1.3301855977,-4.87900
 80352\H,2.9154098655,1.9929891181,-2.6947394289\H,0.4769105882,2.34111
```

12778,1.1976188765\H,3.6336724432,-1.2629630164,0.4834357929\H,3.82101
66983,1.8907330803,1.8241609203\H,2.7119441421,3.6216522801,-0.4011523
672\H,0.2554725552,1.7355241657,-1.7297479517\H,2.4505276453,-0.770571
4603,-2.2263557119\H,4.9048778408,1.1179794277,-0.8972805948\H,1.64036
28966,-0.1641762033,2.5554026104\H,0.5537310616,-2.9854898818,-2.61980
75887\H,-2.2535583837,0.2197689337,-1.9848142629\H,0.0606280889,-2.927
1316983,-5.0473634544\H,-2.7376268565,0.2678161813,-4.4144138869\H,-1.
5814695607,-1.3023931503,-5.9426793305\\Version=EM64L-G09RevD.01\State
=1-A\HF=-510.1074404\RMSD=5.771e-09\RMSF=9.788e-06\Dipole=-2.377431,-1
.6385843,-2.2397981\Quadrupole=-3.6269355,-1.5009106,5.127846,-3.38758
29,-2.6431296,-3.1648698\PG=C01 [X(C7H14B9I1)]\\@

5[1O]a

1\1\GINC-OCTOPUS\FOpt\RM062X\Gen\C7H14B9I1\PIOTR\16-Nov-2014\0\\#P M06
2x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(noraman, r
eadIso) Pseudo=Read\\10-PhI-CB9, C1\\0,1\B,0.2596782168,0.2621393187,-
0.223922862\B,0.0167512036,0.4555441131,1.6091991426\B,1.8151171573,0.
1346513855,1.8785637756\B,2.0556954744,-0.0725480718,0.0479002087\B,0.
9198198001,-1.413593357,-0.3320718815\B,-0.5167855495,-1.03551451,0.76
10029295\B,0.5793171116,-1.1332196712,2.2331369177\B,2.0171621926,-1.4
992292345,1.1392434083\B,1.2323586078,1.2018186845,0.7431891331\I,1.68
78926676,3.333938832,0.6041199427\C,0.5729935552,-2.1727707203,1.02578
0469\C,-0.0013723519,4.0300648349,-0.4541521143\C,0.1791821887,5.05100
84227,-1.3762972124\C,-0.9414327665,5.5267216803,-2.0511392941\C,-2.19
44768918,4.9770238599,-1.8034692417\C,-2.3401419463,3.9491143207,-0.87
7636638\C,-1.2372533322,3.4630887376,-0.1819905899\H,0.3666300789,-3.2
267231366,1.1131875962\H,-1.3387782345,2.6581434825,0.537369868\H,-3.3
161629577,3.5170635405,-0.6884045923\H,-3.0612026237,5.348962687,-2.33
80680403\H,-0.825975863,6.323802233,-2.7767723671\H,1.1616857062,5.462
0323607,-1.5783612417\H,-0.3317322776,0.7212890737,-1.1467711192\H,-0.
7742242105,1.0832637792,2.2379452106\H,2.5573221457,0.4783378911,2.739
8818896\H,3.0019534244,0.1150102568,-0.6437879011\H,0.9622087892,-2.01
04911048,-1.3523592902\H,-1.6577581562,-1.3252953444,0.642223301\H,0.3
478050521,-1.4995301866,3.3335310277\H,2.9683097896,-2.1725161574,1.34
10835651\\Version=EM64L-G09RevD.01\State=1-A\HF=-510.1045935\RMSD=8.24
8e-09\RMSF=4.352e-06\Dipole=-0.5733335,2.8801619,-0.8604044\Quadrupole
=2.4202112,1.796345,-4.2165562,0.8933996,3.1099878,-4.5471122\PG=C01 [
X(C7H14B9I1)]\\@

5[6]a-CN

1\1\GINC-LOCALHOST\FOpt\RM062X\Gen\C8H14B9I1N1(1-)\PIOTR\08-Dec-2017\0
\\#P M062x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(no
raman, readIso) Pseudo=Read\\6-PhI....CN-CB9, C1 orientation anti\\-1,
1\B,-1.5387360639,-1.4460212974,-1.2823371981\B,-1.210807657,-0.269665
3517,0.034418289\B,-1.6302669649,-1.4561208147,1.3181579133\B,-1.99548
13287,-2.6608619135,-0.0017032459\B,-3.2703306802,-1.8184592707,-0.958
3001674\B,-2.6875909226,-0.0872920502,-0.9451626641\B,-2.7525450098,-0
.0942085778,0.9115580277\B,-3.3343162977,-1.8243771773,0.8715755362\B,
-0.5335081884,-1.8048020421,0.0542837729\I,0.1271938364,1.5329925485,0
.0711100002\C,-3.8894001565,-0.6477163408,-0.0599623804\C,1.9125876579
,0.2904488418,0.0276459291\C,2.4257671949,-0.1584152599,-1.1876429129\
C,2.574368824,-0.0282153365,1.2108306648\C,3.5875992975,-0.9237826412,
-1.2187199797\C,3.7371836566,-0.7936789466,1.1807357292\C,4.2449475714
,-1.2420551423,-0.034160235\H,-4.9054878889,-0.2918511095,-0.094165208
5\H,-1.1157109907,-1.5448324761,-2.3883490549\H,-1.2865190884,-1.56414
8361,2.4500096916\H,-1.9695879597,-3.8494706783,-0.0053715361\H,-3.956
9689413,-2.3751934682,-1.7491149944\H,-2.8539753055,0.7983934048,-1.71
04846048\H,-2.9716848216,0.7850551769,1.670125831\H,-4.0743196512,-2.3

868390634,1.6083417857\H,0.58512822,-2.1845856204,0.092949563\H,1.9030
279227,0.0699268513,-2.1126235989\H,2.1717541574,0.3054639836,2.163476
336\H,3.975768845,-1.2791003088,-2.1683121757\H,4.2425110603,-1.046183
6611,2.107929757\H,5.1483168996,-1.8429461166,-0.0578029781\C,-1.88435
82565,2.9589668605,0.0995276432\N,-2.7173124699,3.7711731487,0.1020721
849\\Version=ES64L-G09RevD.01\State=1-A\HF=-602.9741017\RMSD=8.269e-09
\RMSF=2.268e-06\Dipole=3.4802063,-0.6916809,-0.0492617\Quadrupole=0.85
69331,-16.6386298,15.7816966,6.262725,0.5602884,-0.2014775\PG=C01 [X(C
8H14B9I1N1)]\\@

5[1O]a-CN

1\1\GINC-LOCALHOST\FOpt\RM062X\Gen\C8H14B9I1N1(1-)\PIOTR\05-Nov-2017\0
\\#P M062x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(no
raman, readIso) Pseudo=Read\\10-PhI...CN-CB9, C1\\-1,1\B,-1.2299794721
,0.8733773575,-1.0889787694\B,-1.4338235342,1.0030409629,0.7381092202\
B,-2.3897448751,-0.5734545104,0.7461735418\B,-2.1852970093,-0.70350942
06,-1.0864712866\B,-2.9376730625,0.8318063829,-1.6567591096\B,-2.40416
79351,2.0329118737,-0.3727455093\B,-3.2248720353,1.0145322057,0.917709
4733\B,-3.752789932,-0.1894280471,-0.3654794387\B,-0.9250887178,-0.390
263379,-0.0357726001\I,0.9659374213,-1.4578971559,0.2509622699\C,-3.86
62605806,1.4000548984,-0.4909427917\C,2.0596928888,0.4370327938,0.2384
654352\C,2.5700468509,0.9474939566,-0.9541231164\C,3.3144801379,2.1238
526563,-0.9555409649\C,3.5556340365,2.7972555258,0.2377669727\C,3.0482
300864,2.2933119102,1.4311637102\C,2.3040058805,1.1168217508,1.4307321
643\H,-4.7798609057,1.9536679556,-0.6321541332\H,1.8998505677,0.733303
2872,2.3637246714\H,3.2279146432,2.8195339068,2.3636835373\H,4.1348034
814,3.715308389,0.237194451\H,3.7024378629,2.5175144351,-1.8900508792\
H,2.3743997324,0.4312746806,-1.8901477608\H,-0.3858036109,1.2847879442
,-1.8193330838\H,-0.7640277386,1.5253622393,1.5710949214\H,-2.53561562
2,-1.4004891936,1.5849304332\H,-2.1565447892,-1.6416322292,-1.81302332
5\H,-3.2409652924,1.0142853522,-2.788570134\H,-2.2703559811,3.20931370
26,-0.4413266446\H,-3.7660947938,1.3483587612,1.9186681234\H,-4.735335
1472,-0.8491346015,-0.4282706714\C,-0.304974758,-3.5341664722,0.256545
2879\N,-0.710219937,-4.6233348693,0.2886615255\\Version=ES64L-G09RevD.
01\State=1-A\HF=-602.9712104\RMSD=5.939e-09\RMSF=1.179e-06\Dipole=2.87
89784,2.8417678,0.1194455\Quadrupole=3.3887998,-18.8452765,15.4564767,
-4.4911378,-1.0560294,1.9519949\PG=C01 [X(C8H14B9I1N1)]\\@

5[6]a-Pyr

1\1\GINC-LOCALHOST\FOpt\RM062X\Gen\C12H19B9I1N1\PIOTR\07-Dec-2017\0\\#
P M062x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(noram
an, readIso) Pseudo=Read\\6-PhI...Pyr-CB9, C1 orientation acros\\0,1\B
,-1.5258695627,-1.7204662064,-0.2505146586\B,-0.0146484682,-0.89891491
97,0.221785172\B,1.0114904464,-2.3095629294,-0.1669668486\B,-0.5175639
082,-3.1925098642,-0.6267110527\B,-1.4922619014,-3.1120675946,0.892853
5982\B,-1.1261877601,-1.4272314661,1.4981535111\B,0.6745423391,-1.8470
655681,1.5564503787\B,0.2949528204,-3.5274418798,0.9510368968\B,-0.141
8749721,-1.6677022546,-1.2587958955\I,0.416015476,1.3319683482,0.20043
55573\C,-0.5069605153,-2.765227945,2.1061653072\C,-1.5692694319,1.8942
94103,0.6254373924\C,-1.8672128217,2.4871227959,1.8472122838\C,-2.5524
730736,1.6422643742,-0.3252179372\C,-3.1854242901,2.8419519137,2.11564
33157\C,-3.8672533232,1.9938047293,-0.0368990223\C,-4.182071322,2.5942
002077,1.1774289811\H,-0.6197612453,-3.1010952873,3.1234700347\H,-2.57
19590239,-1.3217387319,-0.6426411522\H,2.1464272314,-2.4233609585,-0.4
926420015\H,-0.7020449715,-4.0992203279,-1.3685405713\H,-2.4431249254,
-3.7892654754,1.0839611994\H,-1.7511949284,-0.6774881493,2.1701532308\
H,1.5206066026,-1.4379749698,2.2796940759\H,0.8378978262,-4.5515700571
,1.188341174\H,-0.0114750253,-1.2558388763,-2.3608716645\H,-1.09060548

77,2.6595759459,2.5840836183\H,-2.3022611403,1.162211496,-1.2649469294
\H,-3.4313435103,3.3052835964,3.0647680717\H,-4.6442450697,1.792672155
3,-0.7657488907\H,-5.208625651,2.8667041903,1.3956059407\N,2.952486981
2,0.3237745029,-0.4668392081\C,3.7838178513,-0.1937783036,0.4377308544
\C,3.1120818211,-0.0246573723,-1.743828697\C,4.8121165279,-1.066764698
8,0.1071676631\C,4.1118606476,-0.8868769473,-2.1734400466\C,4.97768823
48,-1.4181453273,-1.2262402291\H,3.6101530266,0.097950657,1.4702812091
\H,2.3982240906,0.3963483893,-2.4476522327\H,5.4563329953,-1.465602876
8,0.8811205047\H,4.1952982177,-1.1424714742,-3.2226224919\H,5.76472835
3,-2.1033533434,-1.5220148212\\Version=ES64L-G09RevD.01\State=1-A\HF=-
758.3052126\RMSD=8.208e-09\RMSF=2.804e-06\Dipole=0.9581029,2.2394866,0
.3835534\Quadrupole=13.2788241,-14.0096386,0.7308145,-12.6505326,-5.09
56251,0.760358\PG=C01 [X(C12H19B9I1N1)]\\@

5[10]a-Pyr

1\1\GINC-LOCALHOST\FOpt\RM062X\Gen\C12H19B9I1N1\PIOTR\07-Nov-2017\0\\#
P M062x/Gen FOpt(tight) geom(noangle, nodistance) fcheck #P freq(noram
an, readIso) Pseudo=Read\\10-PhI...Pyridine-CB9, C1\\0,1\B,-1.05766488
21,1.0669919639,-0.7389483025\B,-1.3850519068,0.6547459512,1.036264334
7\B,-1.8264108469,-1.0667866224,0.5596532234\B,-1.509573024,-0.6535721
37,-1.2222676576\B,-2.6521151895,0.7066178677,-1.5023475265\B,-2.55699
79473,1.6314547878,0.0842933863\B,-3.1041207306,0.1300863287,0.9922785
042\B,-3.1866755462,-0.7995085383,-0.5963706264\B,-0.453385579,-0.2904
109638,0.0193753619\I,1.6553949957,-0.8572924632,0.2141886216\C,-3.757
5309863,0.6729741761,-0.3556467711\C,2.4772198846,1.0833163711,0.06404
92421\C,3.5620818546,1.2712705567,-0.7832564098\C,4.1306258765,2.53891
69379,-0.8727046213\C,3.6088784046,3.5924741292,-0.1308332237\C,2.5173
650108,3.384899072,0.7064841988\C,1.9431442093,2.1229707816,0.81547514
33\H,-4.7859768657,0.9723183153,-0.4720743448\H,1.0846385412,1.9593648
815,1.457440183\H,2.1050239181,4.2078063924,1.2795016401\H,4.050663304
7,4.5795156395,-0.2093109843\H,4.9759500453,2.6994560249,-1.5326399996
\H,3.9540283679,0.451902016,-1.3762791981\H,-0.3366894479,1.8655011419
,-1.24309025\H,-0.9485768259,1.0970263743,2.0502016517\H,-1.7758806201
,-2.0877912756,1.1629416576\H,-1.1659086973,-1.3229896236,-2.143176391
6\H,-2.9325281534,1.0839494312,-2.5881828821\H,-2.7667206023,2.7740602
243,0.3098742139\H,-3.7595744338,0.0257091419,1.9716158247\H,-3.917808
6102,-1.6694519714,-0.9285375024\N,0.6803734575,-3.5329445524,0.383825
1401\C,-0.3385887514,-4.0374721555,-0.3139644848\C,1.3373881185,-4.340
8879272,1.2147343282\C,-0.7363562267,-5.3649341375,-0.2109565375\C,1.0
135993502,-5.6801232071,1.3887312014\C,-0.0472959557,-6.2006727767,0.6
584310583\H,-0.8574459634,-3.3445244952,-0.9707713799\H,2.1589293494,-
3.8927222461,1.7702701512\H,-1.5717779429,-5.725576684,-0.7985401932\H
,1.5784201094,-6.2919414453,2.0817654213\H,-0.3335611131,-7.241253175,
0.7672841193\\Version=ES64L-G09RevD.01\State=1-A\HF=-758.3024793\RMSD=
8.217e-09\RMSF=5.239e-06\Dipole=2.4641993,-1.3004221,0.3069321\Quadrup
ole=-4.963474,15.9527371,-10.989263,8.2260717,-0.2751925,-1.5984133\PG
=C01 [X(C12H19B9I1N1)]\\@

5[6]a-TS

1\1\GINC-OCTOPUS\FTS\RM062X\Gen\C7H14B9I1\PIOTR\20-Aug-2015\0\\#P M062
x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noraman, read
Iso) Pseudo=Read\\beginning: 6-PhI-CB9, C1 TS to the CB9-adduct\\0,1\B
,-2.2757001643,-0.3857641929,1.158192492\B,-0.9747664882,0.2095700405,
0.1823515339\B,-1.2522742184,1.9129850977,0.3006647022\B,-2.6996317039
,1.3777626492,1.2638394087\B,-3.6022596617,0.2844776152,0.1259419134\B
,-2.2328438561,-0.6301699811,-0.677228193\B,-1.5191554223,0.9807517769
,-1.278182581\B,-2.889055149,1.8845993671,-0.4714099714\B,-1.132441513
3,0.8313332314,1.6664006692\I,1.3364121321,-2.1499832951,-0.002519677\

C,-3.057121802,0.5574454417,-1.3560414948\C,1.8938311285,-0.1204230153
,-0.0373919857\C,2.2181308219,0.5182028921,1.1573288694\C,1.8949120648
,0.5637818593,-1.2497627338\C,2.5357079299,1.8706642573,1.1302408348\C
,2.2142412265,1.9187485542,-1.2577173033\C,2.5310990198,2.5718347404,-
0.0724256735\H,-3.6421648055,0.4826122417,-2.2575017741\H,-2.487633890
6,-1.3258482499,1.8410770345\H,-0.6151843359,2.9077708749,0.2660679903
\H,-3.2873317381,1.9565436166,2.1146344355\H,-4.7265455996,-0.04358241
82,0.2826156679\H,-2.1558434928,-1.712371388,-1.142199139\H,-0.8694523
154,1.2100952006,-2.2374333706\H,-3.423012591,2.8827274466,-0.81058828
96\H,-0.5003447742,0.9168770657,2.6572097493\H,2.1985079866,-0.0259345
439,2.0940842577\H,1.6398206537,0.0517719222,-2.1705238118\H,2.7771906
92,2.378130875,2.0574257655\H,2.2069831653,2.4605728141,-2.1969600201\
H,2.7703357012,3.6291205039,-0.0833443053\\Version=EM64L-G09RevD.01\St
ate=1-A\HF=-510.0762815\RMSD=6.405e-09\RMSF=1.258e-05\Dipole=1.0578797
,0.216557,-0.7485835\Quadrupole=-3.1220751,1.2258104,1.8962647,6.03528
51,5.4941139,-1.3492018\PG=C01 [X(C7H14B9I1)]\\@

5[10]a-TS

1\1\GINC-OCTOPUS\FTS\RM062X\Gen\C7H14B9I1\PIOTR\14-Aug-2015\0\\#P M062
x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noraman, read
Iso) Pseudo=Read\\beginning: 10-PhI-CB9, C1 TS to the CB9-adduct\\0,1\
B,1.6371318876,1.1862191396,0.0066024569\B,1.6930899573,-0.1209747267,
-1.3186249581\B,1.7834625207,-1.4476449817,-0.0144983412\B,1.686915871
5,-0.1424286201,1.3106167152\B,3.1408164469,0.8663512268,0.9273766287\
B,3.1451696476,0.8813043426,-0.9120822814\B,3.248331662,-0.9635011857,
-0.9249822443\B,3.2440264811,-0.9783835986,0.9107878177\B,0.6924389957
,-0.1812663794,-0.0067614743\I,-1.6657403987,-1.49329218,-0.0212905443
\C,4.1111707855,0.0042223396,0.0028542223\C,-1.445967069,0.6171632995,
-0.0049613949\C,-1.4764674619,1.2865491184,1.2218750443\C,-1.503933270
3,2.6731459327,1.2197366923\C,-1.5164917606,3.372339552,0.0154040138\C
,-1.4971411557,2.6912195984,-1.1991197065\C,-1.469591883,1.304781084,-
1.2218084174\H,5.1868549618,0.0642868471,0.0058348053\H,-1.4385085835,
0.7608099765,-2.1583593334\H,-1.4991599916,3.2393270432,-2.1340460348\
H,-1.5348247093,4.4563761562,0.0234518557\H,-1.5113788194,3.2072260427
,2.1627211228\H,-1.4508642185,0.7286333782,2.1503524389\H,1.1622931062
,2.273314034,0.0142676422\H,1.2897361642,-0.1288490978,-2.4357239768\H
,1.4339092323,-2.5796826991,-0.0243861152\H,1.2778832323,-0.1684750038
,2.425378312\H,3.5899573109,1.6430148714,1.6979967196\H,3.5979240317,1
.6703950329,-1.6678248063\H,3.7839855783,-1.686286243,-1.692774757\H,3
.7760874479,-1.7136342998,1.6691818983\\Version=EM64L-G09RevD.01\State
=1-A\HF=-510.0637215\RMSD=4.529e-09\RMSF=1.066e-05\Dipole=-2.0724091,0
.9702809,0.0028582\Quadrupole=-3.5648901,5.0311549,-1.4662648,-1.75007
46,-0.0213371,0.0444613\PG=C01 [X(C7H14B9I1)]\\@

5[6]aCN-TS

1\1\GINC-LOCALHOST\FTS\RM062X\Gen\C8H14B9I1N1(1-)\PIOTR\06-Nov-2017\0\
\#P M062x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noram
an, readIso) Pseudo=Read\\beginning: 6-(syn)PhI...CN-CB9, C1 TS\\-1,1\
B,-1.149533267,-1.3821470354,1.0539175019\B,-1.5077809432,-0.104234847
9,-0.1904592377\B,-3.2593478086,-0.0738867064,0.2551281777\B,-2.906159
3351,-1.3623618924,1.4898106384\B,-2.2236131025,-2.7073100889,0.498767
293\B,-1.195016286,-1.7960009415,-0.7075624566\B,-2.6926808454,-0.8701
524539,-1.2853170275\B,-3.7075714917,-1.7841356141,-0.0703272944\B,-1.
9916884543,0.068398765,1.3930942375\I,0.6374811654,1.0457806171,-0.770
0033593\C,-2.6124372421,-2.4456437889,-1.0319336571\C,2.4359458991,0.0
460814542,-0.1603647326\C,3.3917535881,-0.3391970847,-1.0993069115\C,2
.6295245612,-0.2571040353,1.1868518807\C,4.541788737,-1.0085558093,-0.

6908312763\C,3.7749962768,-0.9370275818,1.5902556274\C,4.734130585,-1.
3094475025,0.653875454\H,-2.8032190734,-3.204387514,-1.7725977371\H,-0
.1619342779,-1.6571115913,1.6576465758\H,-4.0940287738,0.7620236887,0.
1721557191\H,-3.4551461028,-1.6291355633,2.5103370577\H,-2.1123201114,
-3.8225538891,0.8890249541\H,-0.2244999579,-2.1294203723,-1.3008610714
\H,-2.9621378228,-0.4456942548,-2.354322186\H,-4.8389668028,-2.1298308
132,-0.1579119813\H,-1.7616596427,0.9067555445,2.1956601286\H,3.235012
3878,-0.1220296528,-2.1518850535\H,1.8781243952,0.028955746,1.91654719
12\H,5.2846635066,-1.302428151,-1.4259574775\H,3.9163091231,-1.1773595
292,2.6392030131\H,5.6277770986,-1.8372102744,0.9707251465\C,-1.692365
6625,1.9828046772,-1.3886247029\N,-2.3699393201,2.7939134958,-1.876498
4339\\Version=ES64L-G09RevD.01\State=1-A\HF=-602.942453\RMSD=8.815e-09
\RMSF=4.858e-06\Dipole=4.4134885,-1.4377707,0.0352133\Quadrupole=-8.25
17187,-2.2758809,10.5275995,5.6503911,-0.286964,10.613985\PG=C01 [X(C8
H14B9I1N1)]\\@

5[10]aCN-TS

1\1\GINC-LOCALHOST\FTS\RM062X\Gen\C8H14B9I1N1(1-)\PIOTR\06-Nov-2017\0\
\#P M062x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noram
an, readIso) Pseudo=Read\\beginning: 10-(syn)PhI...CN-CB9, C1 TS\\-1,1
\B,-1.3147314661,-1.2056336221,0.9047739575\B,-1.3259828714,-1.2009952
425,-0.9239406076\B,-2.7763294623,-0.0579571893,-0.9230405703\B,-2.763
8558776,-0.061903522,0.9270774054\B,-2.9550425339,-1.8110743323,1.2996
145114\B,-1.9554261053,-2.6199757058,-0.0086020923\B,-2.9717483954,-1.
8051203557,-1.3004288965\B,-3.9878486788,-1.0151972148,0.0076403697\B,
-1.3978975026,0.2188334574,-0.0061324509\I,0.7797935761,1.3002687136,-
0.0071841899\C,-3.543061071,-2.5435582631,0.0016359704\C,2.4724456565,
-0.0204467318,-0.0000282924\C,3.0029734545,-0.4706925474,1.2084053509\
C,4.0674538662,-1.3668639077,1.2120315514\C,4.6014513864,-1.821903528,
0.0105434576\C,4.0658914965,-1.3828434758,-1.1961480704\C,3.0014353139
,-0.4866257405,-1.2030907257\H,-4.2125482092,-3.3874325205,0.004002857
2\H,2.5735953532,-0.1556989215,-2.144503736\H,4.4725962855,-1.74416486
88,-2.1354206724\H,5.4294789828,-2.5233917797,0.0146934776\H,4.4752916
884,-1.715773579,2.1555005741\H,2.5762079187,-0.1274600527,2.145884393
2\H,-0.4260986173,-1.3783419009,1.6774969925\H,-0.4477223062,-1.370704
0007,-1.7090228125\H,-3.1591661609,0.7417408861,-1.7099299382\H,-3.136
304171,0.7343517718,1.7226386376\H,-3.258761108,-2.2051581707,2.376625
7242\H,-1.4094013233,-3.6733792253,-0.0145080349\H,-3.2889619096,-2.19
46287536,-2.3751732908\H,-5.1394866227,-0.7343406414,0.0154115187\C,-1
.4742035345,2.5673965334,-0.0122942677\N,-2.1028270515,3.5471324312,-0
.012110101\\Version=ES64L-G09RevD.01\State=1-A\HF=-602.9353387\RMSD=3.
755e-09\RMSF=8.552e-06\Dipole=4.2762456,-1.7746796,0.0083542\Quadrupol
e=-5.4724823,-9.1258881,14.5983705,6.9343567,-0.0250757,0.0708475\PG=C
01 [X(C8H14B9I1N1)]\\@

5[6]aPyr-TS

1\1\GINC-LOCALHOST\FTS\RM062X\Gen\C12H19B9I1N1\PIOTR\07-Dec-2017\0\\#P
 M062x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noraman,
 readIso) Pseudo=Read\\beginning: 6-(anti)PhI...Pyr-CB9, C1 TS second
attempt\\0,1\B,0.7026843741,1.9919346217,-0.8392434621\B,-0.6898614814
,1.048035104,-0.219135949\B,-1.9009047089,2.2392551051,-0.7738427583\B
,-0.5089836806,3.2275695757,-1.384361261\B,0.4829907163,3.5043956146,0
.1059852265\B,0.3561647381,1.8853237108,0.9471777578\B,-1.48410322,2.0
589959735,0.9974509174\B,-1.3506014141,3.6773432661,0.1540803616\B,-0.
6763583546,1.5811633056,-1.780570313\I,0.4446083607,-1.4378502899,0.02
35890325\C,-0.4377247957,3.1985966584,1.3796312538\C,2.4836701801,-0.9
755678693,-0.059062946\C,3.1690279253,-0.6847663628,1.1158396569\C,3.1
08383667,-0.9207564456,-1.3007382854\C,4.5135577812,-0.3354508422,1.03

80759607\C,4.4532959501,-0.5723857886,-1.3598279688\C,5.1543591041,-0.
2798579061,-0.194567952\H,-0.3666258194,3.6876957192,2.33687925\H,1.79
03227496,1.701198353,-1.2105832575\H,-3.0431502413,2.1581373659,-1.080
426158\H,-0.4519532701,4.018373787,-2.2659771486\H,1.336387383,4.31995
46856,0.1847144857\H,1.0865596049,1.3390604949,1.7022830471\H,-2.26420
84704,1.6557066386,1.7905932244\H,-2.0347945175,4.6346942364,0.2764823
587\H,-0.7461584434,1.0249798351,-2.8231479541\H,2.6621380661,-0.72202
7314,2.0730268972\H,2.551806536,-1.1288097656,-2.2070610169\H,5.056278
9864,-0.1027429723,1.9474618959\H,4.9486236428,-0.5214513042,-2.322993
3949\H,6.2014852721,-0.0036251373,-0.2475900171\N,-2.4560373603,-0.606
4514322,-0.0146253574\C,-2.9451084828,-1.1051826158,1.1203265311\C,-3.
1136482224,-0.8267286811,-1.152335695\C,-4.1157991117,-1.850794844,1.1
683191538\C,-4.2900020245,-1.5635503891,-1.203109865\C,-4.7987540443,-
2.0841527228,-0.0194208873\H,-2.3739814215,-0.8886375977,2.0202806587\
H,-2.6765745117,-0.3828538035,-2.0437692562\H,-4.4786366346,-2.2336651
931,2.1143650239\H,-4.7916840465,-1.7186668347,-2.1504663272\H,-5.7167
227601,-2.6618789392,-0.0216604628\\Version=ES64L-G09RevD.01\State=1-A
\HF=-758.275768\RMSD=5.396e-09\RMSF=9.350e-06\Dipole=-0.2306162,-2.468
4397,0.8643099\Quadrupole=17.7974529,-16.9265079,-0.8709449,10.4477253
,-0.8113508,5.2608118\PG=C01 [X(C12H19B9I1N1)]\\@

5[1O]aPyr-TS

1\1\GINC-LOCALHOST\FTS\RM062X\Gen\C12H19B9I1N1\PIOTR\09-Nov-2017\0\\#P
M062x/gen Opt(QST3) geom(noangle, nodistance) fcheck #P freq(noraman,
readIso) Pseudo=Read\\beginning: 10-(syn)PhI...Pyr-CB9, C1 TS\\0,1\B,
-0.2574362313,1.7095710528,0.8909768319\B,-0.1446142861,1.8147548656,-
0.9425775561\B,1.6982039908,1.8871637366,-0.8301006009\B,1.5849578045,
1.7809534286,1.0129131543\B,0.5739971756,3.2118767756,1.4115469933\B,-
0.639199326,3.2479363172,0.0328557216\B,0.7332207988,3.3610358062,-1.1
828655652\B,1.9498595002,3.3475938608,0.1971869095\B,0.7746336507,0.75
00121138,-0.0240795202\I,-0.5110987266,-1.4865828169,-0.2275695226\C,0
.6159667512,4.2137582732,0.1653517417\C,-2.487818236,-0.806492808,-0.2
922625969\C,-3.1895009522,-0.6549047678,0.8989604545\C,-4.4957760587,-
0.1798050395,0.8494546873\C,-5.0809467775,0.1383273992,-0.3714279771\C
,-4.3623914273,-0.014950869,-1.5521626093\C,-3.0550277506,-0.489066740
6,-1.5217979389\H,0.5728206494,5.288476894,0.2244372248\H,-2.485273033
8,-0.5978340638,-2.4370982975\H,-4.8135197545,0.2395659975,-2.50456587
87\H,-6.0984424029,0.5115851314,-0.4023636269\H,-5.0511176948,-0.05370
63243,1.7720201636\H,-2.7230900102,-0.890520392,1.8482605514\H,-1.0792
111914,1.2338311078,1.6058997038\H,-0.8698400545,1.4293508918,-1.80182
68641\H,2.5556089242,1.576137472,-1.5913528332\H,2.3453486136,1.379222
4261,1.8326263305\H,0.4879300687,3.6417284036,2.5109642084\H,-1.736613
9134,3.6890749456,-0.0091759186\H,0.7786743921,3.914204383,-2.22831034
75\H,3.0048556259,3.8747275106,0.2922781603\N,2.3956992314,-0.91164731
68,-0.0247708872\C,2.8932505051,-1.3428789748,1.1334916644\C,3.0304109
634,-1.2104888547,-1.1574624499\C,4.0557197775,-2.098399245,1.20829765
44\C,4.1985442856,-1.9605935208,-1.1797830423\C,4.7192567959,-2.410566
969,0.027667641\H,2.3383036329,-1.0572756142,2.0231281349\H,2.58336793
46,-0.8207936071,-2.0681262262\H,4.4294960195,-2.4257666035,2.17074221
7\H,4.6860657292,-2.1781878185,-2.1221915119\H,5.633215007,-2.99436044
65,0.0487116225\\Version=ES64L-G09RevD.01\State=1-A\HF=-758.2668667\RM
SD=6.378e-09\RMSF=5.948e-06\Dipole=0.0852393,-2.6577196,-0.1395861\Qua
drupole=16.1282569,-12.3458386,-3.7824183,-13.2613433,0.3303742,-1.310
9988\PG=C01 [X(C12H19B9I1N1)]\\@

9[1]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C6H14B9N1\PIOTR\10-Nov-2017

\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck\
\1-CB9 1-Pyridine, C2v, preopt at B3LYP/6-31G(d,p)\\0,1\B,-1.296525609
1,0.,-2.573836393\B,1.2965256091,0.,-2.573836393\B,0.,1.2953801226,-2.
5735381271\B,0.,-1.2953801226,-2.5735381271\B,-0.9258310458,-0.9224399
56,-1.0850846553\B,-0.9258310458,0.922439956,-1.0850846553\B,0.9258310
458,0.922439956,-1.0850846553\B,0.9258310458,-0.922439956,-1.085084655
3\B,0.,0.,-3.6730311589\C,0.,0.,-0.1677457355\N,0.,0.,1.2697957441\C,-
1.1982726079,0.,3.3098539051\C,1.1982726079,0.,3.3098539051\C,-1.17174
21693,0.,1.9310870793\C,1.1717421693,0.,1.9310870793\C,0.,0.,4.0126822
13\H,-2.4168984655,0.,-2.9611566995\H,2.4168984655,0.,-2.9611566995\H,
0.,2.4182567349,-2.9526788533\H,0.,-2.4182567349,-2.9526788533\H,-1.66
83460728,-1.6687453672,-0.5369633766\H,-1.6683460728,1.6687453672,-0.5
369633766\H,1.6683460728,1.6687453672,-0.5369633766\H,1.6683460728,-1.
6687453672,-0.5369633766\H,0.,0.,-4.852304693\H,-2.1541719993,0.,3.816
2754182\H,2.1541719993,0.,3.8162754182\H,-2.0546106383,0.,1.3057263218
\H,2.0546106383,0.,1.3057263218\H,0.,0.,5.0961465579\\Version=ES64L-G0
9RevD.01\State=1-A1\HF=-515.4207824\RMSD=6.547e-09\RMSF=2.035e-06\Dipo
le=0.,0.,5.7838969\Quadrupole=2.5449443,-6.6799481,4.1350038,0.,0.,0.\
PG=C02V [C2(H1B1C1N1C1H1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\@

9[6]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C6H14B9N1\PIOTR\09-Nov-2017
\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck
#P freq(noraman, readIso)\\1-CB9-6-Pyr, Cs\\0,1\B,-1.4411747676,0.8211
844936,-1.3059729601\B,-0.3337430907,0.2823015443,-0.0085333368\B,-1.4
278469258,0.8492154976,1.2885369881\B,-2.5962536538,1.3923797006,-0.00
84240267\B,-2.9128335074,-0.1401668001,-0.9096091532\B,-1.2723819145,-
0.9332680907,-0.9148190614\B,-1.2619715241,-0.9135343704,0.9296476513\
B,-2.9025340807,-0.1204511413,0.926542423\B,-0.9700367203,1.8412581618
,-0.0219780567\C,-2.4853994612,-1.3722589001,0.0188962559\N,1.20172874
91,0.1405246151,-0.0130739854\C,1.8668415726,0.1393281325,-1.178242803
6\C,1.8682834425,0.0500929121,1.1478444526\C,3.2436727603,0.0371135182
,-1.2165259427\C,3.2450292854,-0.0535018953,1.1765548294\C,3.946005400
9,-0.0621143817,-0.0224367581\H,-1.2361783456,1.1466410134,-2.42964383
49\H,-1.2096759339,1.1954827922,2.4033017405\H,-3.4350217721,2.2289458
734,-0.0132422828\H,-3.8119060103,-0.2610678478,-1.667115058\H,-3.7935
949349,-0.226619287,1.6957477104\H,-0.7539282734,-1.6996861527,-1.6564
342944\H,-0.7382835954,-1.666878288,1.6811411567\H,-0.3979687211,2.875
2781107,-0.0361764375\H,-2.948429765,-2.3441715617,0.0329014766\H,1.24
96558699,0.2279846734,-2.0644828904\H,1.253438239,0.0678829165,2.04007
26792\H,3.7484426385,0.038223526,-2.1734626249\H,3.7511852385,-0.12437
55375,2.1301747822\H,5.0266167314,-0.1427518373,-0.0259096979\\Version
=ES64L-G09RevD.01\State=1-A\HF=-515.4803254\RMSD=9.177e-09\RMSF=9.566e
-06\Dipole=3.9449808,-1.0214296,-0.0066567\Quadrupole=8.2599331,-7.530
4698,-0.7294633,3.4490459,-0.1048403,-0.3540205\PG=C01 [X(C6H14B9N1)]\
\@

9[10]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C6H14B9N1\PIOTR\09-Nov-2017
\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck
#P freq(noraman, readIso)\\10-CB9-1-Pyridine, C2v\\0,1\B,-1.3003496283
,0.,-2.4434772406\B,1.3003496283,0.,-2.4434772406\B,0.,1.2997737994,-2
.4423057704\B,0.,-1.2997737994,-2.4423057704\B,-0.9223603802,-0.918975
4132,-0.9458252753\B,-0.9223603802,0.9189754132,-0.9458252753\B,0.9223
603802,0.9189754132,-0.9458252753\B,0.9223603802,-0.9189754132,-0.9458
252753\C,0.,0.,-3.3681840991\B,0.,0.,0.1015497929\N,0.,0.,1.6210005453
\C,-1.1980343518,0.,3.6700859508\C,1.1980343518,0.,3.6700859508\C,-1.1
651397868,0.,2.289772501\C,1.1651397868,0.,2.289772501\C,0.,0.,4.37307

99659\H,-2.3758902847,0.,-2.9356264593\H,2.3758902847,0.,-2.9356264593
\H,0.,2.3763597777,-2.9316686344\H,0.,-2.3763597777,-2.9316686344\H,-1
.7052392745,-1.7037877595,-0.5162286125\H,-1.7052392745,1.7037877595,-
0.5162286125\H,1.7052392745,1.7037877595,-0.5162286125\H,1.7052392745,
-1.7037877595,-0.5162286125\H,0.,0.,-4.4445661415\H,-2.1534706222,0.,4
.1776761761\H,2.1534706222,0.,4.1776761761\H,-2.0527335764,0.,1.669818
0312\H,2.0527335764,0.,1.6698180312\H,0.,0.,5.4567823917\\Version=ES64
L-G09RevD.01\State=1-A1\HF=-515.4820162\RMSD=5.383e-09\RMSF=2.188e-06\
Dipole=0.,0.,3.9036003\Quadrupole=-2.5377861,-11.1884041,13.7261903,0.
,0.,0.\PG=C02V [C2(H1C1B1N1C1H1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\@

11[6]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C2H9B9N1(1-)\PIOTR\09-Nov-2
017\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fche
ck #P freq(noraman, readIso)\\6-CN-CB9, Cs\\-1,1\B,-0.7259349846,-0.22
07446317,1.293840216\B,-0.0853873808,0.8807607796,0.\B,-0.7259349846,-
0.2207446317,-1.293840216\B,-1.3693392586,-1.3360578663,0.\B,0.1205459
317,-1.7623835887,0.9154820134\B,1.0351632064,-0.1830991433,0.92141117
45\B,1.0351632064,-0.1830991433,-0.9214111745\B,0.1205459317,-1.762383
5887,-0.9154820134\B,-1.6874750753,0.3255151486,0.\C,1.3899446956,-1.4
370846066,0.\H,2.3245692984,-1.9718149195,0.\H,-1.0579834776,-0.011005
8576,2.4151234568\H,-1.0579834776,-0.0110058576,-2.4151234568\H,-2.268
7568833,-2.1136020614,0.\H,0.1673910182,-2.6690933634,1.6786244223\H,1
.8404508654,0.2446279449,1.6779713999\H,1.8404508654,0.2446279449,-1.6
779713999\H,0.1673910182,-2.6690933634,-1.6786244223\H,-2.7001404024,0
.9359236651,0.\C,0.2064471674,2.4062586928,0.\N,0.4236126071,3.5413726
042,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-360.1835851\RMSD=3.758
e-09\RMSF=9.995e-06\Dipole=0.7995098,-1.3944598,0.\Quadrupole=5.766505
,-10.7982661,5.031761,-4.1237891,0.,0.\PG=CS [SG(C2H3B3N1),X(H6B6)]\\@

11[10]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C2H9B9N1(1-)\PIOTR\06-Nov-2
017\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fche
ck #P freq(noraman, readIso)\\1-CB9-10-CN, C4v\\-1,1\B,-1.2954404916,0
.,-0.0788612681\B,0.,1.2954404916,-0.0788612681\B,1.2954404916,0.,-0.0
788612681\B,0.,-1.2954404916,-0.0788612681\B,-0.9165538537,-0.91655385
37,1.4206474635\B,-0.9165538537,0.9165538537,1.4206474635\B,0.91655385
37,0.9165538537,1.4206474635\B,0.9165538537,-0.9165538537,1.4206474635
\C,0.,0.,2.354003734\B,0.,0.,-1.1638377876\C,0.,0.,-2.7036217667\N,0.,
0.,-3.859246341\H,0.,0.,3.4307852366\H,-2.413914443,0.,-0.4787671159\H
,0.,2.413914443,-0.4787671159\H,2.413914443,0.,-0.4787671159\H,0.,-2.4
13914443,-0.4787671159\H,-1.6774887244,-1.6774887244,1.9192231135\H,-1
.6774887244,1.6774887244,1.9192231135\H,1.6774887244,1.6774887244,1.91
92231135\H,1.6774887244,-1.6774887244,1.9192231135\\Version=ES64L-G09R
evD.01\State=1-A1\HF=-360.1856208\RMSD=4.783e-09\RMSF=3.036e-06\Dipole
=0.,0.,1.9441842\Quadrupole=5.2579705,5.2579705,-10.515941,0.,0.,0.\PG
=C04V [C4(H1C1B1C1N1),2SGV(H2B2),2SGD(H2B2)]\\@

19[6]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C1H9B9\PIOTR\09-Nov-2017\0\
\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck #P
freq(noraman, readIso)\\6-ylide-CB9, Cs\\0,1\B,-0.7899308687,0.1053149
723,1.3370390285\B,-0.5879512446,1.1669021047,0.\B,-0.7899308687,0.105
3149723,-1.3370390285\B,-0.9187526592,-1.1109844157,0.\B,0.6390044359,
-0.9253999484,0.9286210128\B,0.8443068869,0.8918435899,0.9309246648\B,
0.8443068869,0.8918435899,-0.9309246648\B,0.6390044359,-0.9253999484,-
0.9286210128\B,-1.9214799451,0.2807038916,0.\C,1.6646912291,-0.1140514
219,0.\H,2.7336348972,-0.2418863298,0.\H,-1.1794493345,0.1439800019,2.

4493448586\H,-1.1794493345,0.1439800019,-2.4493448586\H,-1.4996898966,
-2.1419039168,0.\H,1.0522149906,-1.7240172432,1.6929489086\H,1.3485233
625,1.6480939691,1.6821314515\H,1.3485233625,1.6480939691,-1.682131451
5\H,1.0522149906,-1.7240172432,-1.6929489086\H,-3.091815529,0.39438656
51,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-267.1826806\RMSD=5.945e
-09\RMSF=1.128e-05\Dipole=0.6168566,0.561506,0.\Quadrupole=0.9327385,0
.9392856,-1.8720241,-1.1953517,0.,0.\PG=CS [SG(C1H3B3),X(H6B6)]\\@

19[1O]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C1H9B9\PIOTR\06-Nov-2017\0\
\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck #P
freq(noraman, readIso)\\1-CB9-10-ylide, C4v\\0,1\B,-1.3530280872,0.,-0
.5279852463\B,0.,1.3530280872,-0.5279852463\B,1.3530280872,0.,-0.52798
52463\B,0.,-1.3530280872,-0.5279852463\B,-0.9274715788,-0.9274715788,0
.9643679731\B,-0.9274715788,0.9274715788,0.9643679731\B,0.9274715788,0
.9274715788,0.9643679731\B,0.9274715788,-0.9274715788,0.9643679731\C,0
.,0.,1.8649425456\B,0.,0.,-1.4202404407\H,0.,0.,2.9418870336\H,-2.4550
276693,0.,-0.956500601\H,0.,2.4550276693,-0.956500601\H,2.4550276693,0
.,-0.956500601\H,0.,-2.4550276693,-0.956500601\H,-1.683102483,-1.68310
2483,1.4661588363\H,-1.683102483,1.683102483,1.4661588363\H,1.68310248
3,1.683102483,1.4661588363\H,1.683102483,-1.683102483,1.4661588363\\Ve
rsion=ES64L-G09RevD.01\State=1-A1\HF=-267.1618233\RMSD=2.209e-09\RMSF=
3.430e-06\Dipole=0.,0.,-0.2297859\Quadrupole=-2.8883388,-2.8883388,5.7
766775,0.,0.,0.\PG=C04V [C4(B1C1H1),2SGV(H2B2),2SGD(H2B2)]\\@

20[1]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C6H16B11N1\PIOTR\10-Nov-201
7\0\\#P M062X/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck
#P freq(noraman, readIso)\\1-CB11-1-Pyridine, Cs, staggered\\0,1\B,2.
6126373131,-0.0491542383,0.\B,2.0428160042,0.8303318751,-1.439265407\B
,2.0428160042,0.8303318751,1.439265407\B,1.1200170592,2.2525403485,-0.
8875280501\B,1.1200170592,2.2525403485,0.8875280501\B,-0.3014060269,1.
6819251606,0.\B,0.2831122221,0.8088455929,-1.435582247\B,0.2831122221,
0.8088455929,1.435582247\B,1.2001706236,-0.6178030946,0.8919305142\B,1
.2001706236,-0.6178030946,-0.8919305142\C,-0.1179742253,-0.017469145,0
.\C,-2.9682166049,-2.0978262867,-1.19436798\C,-2.9682166049,-2.0978262
867,1.19436798\C,-1.8559302951,-1.2827751087,-1.167167365\C,-1.8559302
951,-1.2827751087,1.167167365\B,2.5651718113,1.7267543431,0.\C,-3.5413
939284,-2.5107010631,0.\N,-1.3247872916,-0.8726426934,0.\H,3.60759181,
-0.6896537392,0.\H,2.6290816952,0.8174651136,-2.4670465289\H,2.6290816
952,0.8174651136,2.4670465289\H,1.0522190958,3.2451276848,-1.527934887
3\H,1.0522190958,3.2451276848,1.5279348873\H,-3.3661211811,-2.40225367
71,-2.1531172708\H,-3.3661211811,-2.4022536771,2.1531172708\H,-1.40701
65051,2.1045778384,0.\H,-0.4316102973,0.736042398,-2.3758953129\H,-0.4
316102973,0.736042398,2.3758953129\H,1.0330026197,-1.650602458,1.44991
21667\H,1.0330026197,-1.650602458,-1.4499121667\H,-1.3558533972,-0.936
1036494,-2.0585691673\H,-1.3558533972,-0.9361036494,2.0585691673\H,-4.
4152683565,-3.1513880761,0.\H,3.5570733025,2.3717721331,0.\\Version=ES
64L-G09RevD.01\State=1-A'\HF=-566.3980834\RMSD=5.238e-09\RMSF=1.732e-0
6\Dipole=-4.6363937,-3.2256855,0.\Quadrupole=2.6646621,-2.9231416,0.25
84796,8.2696483,0.,0.\PG=CS [SG(C2H4B3N1),X(C4H12B8)]\\@

20[12]a

1\1\GINC-LOCALHOST\FOpt\RM062X\6-31G(2d,p)\C6H16B11N1\PIOTR\23-Aug-201
6\0\\#P M062x/6-31G(2d,p) FOpt(tight) geom(noangle, nodistance) fcheck
#P freq(noraman, readIso)\\12-Pyr-CB11, Cs\\0,1\B,2.6436973047,-0.020
1173249,0.\B,2.0696426624,0.8526582396,-1.4354300232\B,2.0696426624,0.
8526582396,1.4354300232\B,1.136304933,2.2608958056,-0.8863422739\B,1.1

36304933,2.2608958056,0.8863422739\B,-0.2804247559,1.6871045407,0.\B,0
.3071402991,0.8114800481,-1.443472828\B,0.3071402991,0.8114800481,1.44
3472828\B,1.2407723923,-0.6084785764,0.8948170916\B,1.2407723923,-0.60
84785764,-0.8948170916\B,-0.1677044432,-0.0670888937,0.\C,-3.098139791
4,-2.1685001344,-1.1962347934\C,-3.0981397914,-2.1685001344,1.19623479
34\C,-1.9793700497,-1.3595102557,-1.162555942\C,-1.9793700497,-1.35951
02557,1.162555942\C,2.4527619791,1.6650077878,0.\C,-3.6702129096,-2.57
95451204,0.\N,-1.4383379841,-0.9604716058,0.\H,3.7272889235,-0.4890638
463,0.\H,2.7744452342,0.9549111782,-2.3770124748\H,2.7744452342,0.9549
111782,2.3770124748\H,1.2336098544,3.2830665157,-1.4695201456\H,1.2336
098544,3.2830665157,1.4695201456\H,-3.5050787051,-2.4678932315,-2.1529
306055\H,-3.5050787051,-2.4678932315,2.1529306055\H,-1.3176268269,2.26
03242722,0.\H,-0.3174931759,0.798080119,-2.4531112673\H,-0.3174931759,
0.798080119,2.4531112673\H,1.2406910493,-1.6230258283,1.509905117\H,1.
2406910493,-1.6230258283,-1.509905117\H,-1.4800264307,-1.0051289829,-2
.0545575649\H,-1.4800264307,-1.0051289829,2.0545575649\H,-4.5481807247
,-3.214976388,0.\H,3.3537458742,2.2617147986,0.\\Version=ES64L-G09RevD
.01\State=1-A'\HF=-566.4685932\RMSD=2.849e-09\RMSF=8.380e-07\Dipole=-3
.0385051,-2.1364038,0.\Quadrupole=7.194252,-3.088281,-4.105971,13.5995
138,0.,0.\PG=CS [SG(C2H4B3N1),X(C4H12B8)]\\@

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