Supplementary Information

Intramolecular C–N bond activation by a transient boryl anion

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Materials and Methods

Synthetic and Characterisation Data for New Compounds

General Considerations

All manipulations were carried out using standard Schlenk line or dry-box techniques under an atmosphere of argon. All glassware and cannulae were dried in a 140 °C oven for a minimum of 12 hours prior to use. All solvents, bar benzene, were collected from an MBraun solvent purification system, stored under argon in Teflon valved ampoules over a mirror of sodium metal or 4 Å molecular sieves, and sparged with argon prior to use. Benzene and C_6D_6 were dried and distilled from molten potassium and stored in Teflon capped ampoule over molecular sieves. NMR samples were prepared under argon in 5 mm Norell Select Series NMR Tube fitted with J. Young Teflon valves. ^{1}H, ^{13}C{^{1}H}, ^{11}B{^{1}H}, and ^{19}F{^{1}H} NMR spectra were recorded on a Bruker Avance 400 MHz spectrometer. ^{1}H and ^{13}C{^{1}H} spectra were referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ = 0 ppm). ^{11}B{^{1}H}, and ^{19}F{^{1}H} were externally referenced to $BF_3{\cdot}OEt_2$ and CF_3CO_2H, respectively. Assignments were confirmed using two-dimensional ^{1}H -^{1}H and ^{13}C -^{1}H NMR correlation experiments. Chemical shifts are quoted in δ (ppm) and coupling constants in Hz. Infrared spectra were obtained using a PerkinElmer Spectrum One with an attenuated total reflectance (ATR) accessory. Samples were suspended in Nujol oil prior to spectroscopic analysis. Elemental analyses were carried out by the Elemental Analysis Service, Science Centre at London Metropolitan University, UK. 4,4'-oxybis(tert-butylbenzene)[S1] and potassium cyclopentadienyl iron dicarbonyl[S2] were prepared by literature methods. All other reagents were purchased from chemical suppliers and used as received.

Synthesis of 4,4'-oxybis(3-bromo-1-tert-butylbenzene): N-bromosuccinimide (11.16 g, 62.68 mmol) was added to a solution of 4,4'-oxybis(tert-butylbenzene) (7.081 g, 25.07 mmol) and ammonium acetate (0.3865 g, 5.015 mmol) in 90 mL of acetonitrile portion-wise over 15 minutes. No efforts were made to exclude air or moisture. This yielded a transparent dark red solution that was stirred for a further 16 hours at room temperature. Volatiles were removed *in vacuo* to give a pale-yellow powder, which was redissolved in dichloromethane (*ca.* 50 mL) and washed with water (2 x 100 mL). The dichloromethane layer was dried with magnesium sulphate and solvent removed *in vacuo* to give a yellow oil that solidified overnight to give 4,4'-oxybis(3-bromo-1-tert-butylbenzene) as a pale-yellow solid. Yield: 9.98 g (90%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 1.04 (s, 18H, ^{t}Bu-CH_3), 6.63 (d, $^{3}J_{HH}$ = 8.6, 2H, *ortho*-C*H*), 6.88 (dd, $^{3}J_{HH}$ = 8.6, $^{4}J_{HH}$ = 2.3, 2H, ^{t}BuCC*H*CH), 7.67 (d, $^{4}J_{HH}$ = 2.3, 2H, BrCC*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 31.0 (C(*C*H_3)), 33.9 (*C*(CH_3)), 114.1 (*C*O), 119.1 (*ortho*-*C*H), 125.6 (^{t}BuC*C*HCH), 130.8 (BrC*C*H), 148.0 (^{t}Bu*C*), 151.6 (Br*C*); **IR** (ATR, cm^{-1}): 2954(m), 2901(sh), 2864(sh),

1591(w), 1572(w), 1480(s), 1463(sh), 1394(m), 1361(m), 1285(s), 1259(s), 1202(sh), 1112(m), 1040(s), 903(m), 886(m), 862(w), 842(m), 830(m), 814(s), 735(w), 711(m), 667(w), 601(m), 570(sh), 436(sh), 425(w); **Anal. Calc.** for $C_{20}H_{24}Br_2O \cdot CH_3OH$ ($C_{21}H_{28}Br_2O_2$): C 53.41%, H 5.98%, N 0%, found: C 53.54%, H 5.49%, N 0%.

Synthesis of H_2(^{F}NON): To a solution of 4,4'-oxybis(3-bromo-1-tert-butylbenzene) (8.000 g, 18.17 mmol), sodium tert-butoxide (5.239 g, 54.52 mmol), palladium acetate (0.204 g, 0.909 mmol) and tri-tertbutylphosphonium tetrafluoroborate (0.791 g, 2.730 mmol) in toluene (120 mL) was added 2,6-diisopropylaniline (7.0 mL, 37.1 mmol) at room temperature. The reaction mixture was then stirred at 100°C for 16 hours. Once the reaction had allowed to cool, the mixture was quenched with water (200 mL) and extracted into toluene (3 x 50 mL). The organic layer was dried with magnesium sulphate before removing the solvent *in vacuo* to yield a thick dark brown oil. The oil was dissolved in hexane (100 mL) and the solution passed through an alumina plug. This gave a pale-yellow solution, which upon evaporation to dryness gave H_2(^{F}NON) as a fine yellow powder. Yield: 6.43 g (56%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 1.09 (br, 24H, CH(C*H*$_3$)$_2$), 1.14 (s, 18H, C(C*H*$_3$)$_3$), 3.30 (sep, ^{3}JHH = 7.0, 4H, C*H*(CH$_3$)$_2$), 5.91 (s, 2H, N*H*), 6.54 (d, ^{4}JHH = 2.3, 2H, Ar-*H*), 6.67 (dd, ^{3}JHH = 8.3, ^{4}JHH = 2.3, 2H, Ar-*H*), 7.07 (d, ^{3}JHH = 8.3 2H, Ar-*H*), 7.14-7.22 (m, 6H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 23.7, 24.4 (CH(*C*H$_3$)$_2$), 28.7 (*C*H(CH$_3$)$_2$), 31.6 (C(*C*H$_3$)$_3$), 34.6 (*C*(CH$_3$)$_3$), 110.4, 114.6, 118.3, 124.1, 128.0, 135.3, 139.3, 141.9, 147.6, 147.9 (Ar*C*); **IR** (ATR, cm^{-1}): 3411(m), 3066(w), 2960(s), 2867(sh), 1603(m), 1586(sh), 1507(s), 1461(m), 1445(sh), 1398(m), 1361(m), 1328(m), 1300(m), 1253(sh), 1241(s), 1199(s), 1182(sh), 1125(m), 1102(sh), 1056(w), 952(w), 934(w), 865(m), 848(sh), 820(m), 801(s), 758(m), 729(w), 700(w), 678(w), 636(m), 585(w), 505(w), 453(w); **MS** (ESI, +ve ion, m/z): Found: 633.4778. Calcd for $C_{44}H_{61}N_2O$ [M+H]+: 633.4784.

Synthesis of K_2(^{F}NON) (1): A mixture of (^{F}NON)H_2 (2.00 g, 3.16 mmol) and KH (0.380 g, 9.61 mmol) in toluene (20 mL) is heated to 100°C, and left to stir for 5 days. After allowing to cool to room temperature, the reaction solution was filtered and solvent removed from the fiterate *in vacuo* to give **1** as a pale brown powder. Yield: 2.05 g (92%). **^{1}H NMR** (400.1 MHz, C_6D_6, 80 °C): δ_H = 1.15 (br, 24H, Dipp-CH(C*H*$_3$)$_2$), 1.19 (s, 18H, ^{t}Bu-C(C*H*$_3$)$_3$), 3.24 (sep, $^3J_{HH}$ = 6.9, 4H, Dipp-C*H*(CH$_3$)$_2$), 6.09 (s, 2H, Ar-*H*), 6.12 (d, $^3J_{HH}$ = 8.0, 2H, Ar-*H*), 6.93 (d, $^3J_{HH}$ = 8.0, 2H, Ar-*H*), 7.00 (t, $^3J_{HH}$ = 7.6, 2H, Ar-*H*), 7.22 (d, $^3J_{HH}$ = 7.6, 4H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 80 °C): δ_C = 24.7 (Dipp-CH(*C*H$_3$)$_2$), 28.1 (Dipp-*C*H(CH$_3$)$_2$), 32.0 (^{t}Bu-C(*C*H$_3$)$_3$), 34.6 (^{t}Bu-*C*(CH$_3$)$_3$), 103.5, 110.4, 117.8, 120.1, 124.3, 141.7, 142.9, 147.4, 150.5, 153.4 (Ar-*C*); **IR** (ATR, Nujol, cm^{-1}): 3045(sh), 2955(s), 2923(s), 2859(s), 1588(sh), 1571(m), 1555(sh), 1487(s), 1458(m), 1414(s), 1397(s), 1362(w), 1352(w), 1327(m), 1297(m), 1252(m), 1223(sh), 1211(w), 1202(sh), 1177(w), 1156(w), 1119(m), 1099(sh), 1053(sh), 1053(w), 1042(w), 1030(w), 956(m), 930(w), 906(w), 859(m), 850(m), 801(w), 782(s), 757(s), 738(s), 699(m), 671(m), 652(m), 586(w),

569(m), 478(sh), 469(m), 413(m); **Anal. Calc.** a satisfactory elemental analysis could not be obtained for this compound, possibly due to decomposition during shipping.

Synthesis of (^{F}NON)Mg(OEt$_2$) (2-OEt$_2$): To a solution of H_2(^{F}NON) (3.24 g, 5.12 mmol) in diethyl ether (30 mL) was added *n*-butyl-*sec*-butylmagnesium (8.04 mL, 5.63 mmol of a 0.7 M hexane solution), giving a clear pale beige coloured solution. This was left to stir at room temperature, open to a slow flow of argon, for 16 hours. Solvent was removed *in vacuo*, then the residue dissolved in hexane to form a pale orange solution. The solution was concentrated *in vacuo* and left to stand at room temperature overnight, yielding **2-OEt$_2$** as large blocky colourless crystals. Yield: 2.07 g (56%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.63 (t, $^{3}J_{HH}$ = 7.1, 6H, O(CH_2CH_3)$_2$), 1.03 (d, $^{3}J_{HH}$ = 6.9, 12H, Dipp-CH(CH_3)$_2$), 1.20 (m, 12H, Dipp-CH(CH_3)$_2$), 1.21 (s, 18H, ^{t}Bu-C(CH_3)$_3$), 3.05 (q, $^{3}J_{HH}$ = 7.1, 4H, O(CH_2CH_3)$_2$), 3.39 (sep, $^{3}J_{HH}$ = 6.9, 4H, Dipp-C*H*(CH_3)$_2$), 6.43-6.46 (m, 4H, Ar-*H*), 7.15-7.19 (m, 2H, Ar-*H*), 7.23-7.25 (m, 4H, Ar-*H*), 7.40 (d, $^{3}J_{HH}$ = 8.6, 2H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 13.4 (O(CH_2CH_3)$_2$), 24.5, 25.0 (Dipp-CH(CH_3)$_2$), 28.2 (Dipp-*C*H(CH_3)$_2$), 31.7 (^{t}Bu-C(CH_3)$_3$), 34.6 (^{t}Bu-*C*(CH_3)$_3$), 67.6 (O(CH_2CH_3)$_2$), 108.4, 113.0, 118.2, 123.8, 123.9, 142.9, 145.5, 146.8, 148.8, 149.8 (AR-*C*); **IR** (ATR, Nujol, cm^{-1}): 3414(w), 3056(w), 2960(s), 2825(sh), 2065(m), 1600(m), 1587(sh), 1508(w), 1432(s), 1405(s), 1381(sh), 1359(m), 1322(s), 1297(s), 1255(m), 1192(m), 1158(s), 1106(m), 1088(m), 1038(m), 950(m), 933(sh), 900(m), 865(w), 856(w), 838(w), 799(s), 782(sh), 755(m), 736(w), 684(w), 651(m), 605(w), 556(w), 520(m), 489(w), 449(m), 425(m), 417(m); **Anal. Calc.** for $C_{48}H_{68}MgN_2O_2$: C 79.04%, H 9.40%, N 3.84%, found: C 78.82%, H 9.46%, N 3.89%.

Synthesis of (^{F}NON)Mg(THF)$_2$ (2-THF): To a solution of H_2(^{F}NON) (2.50 g, 3.94 mmol) in THF (30 mL) was added di-*n*-butyl-magnesium (3.9 mL, 3.94 mmol of a 1.0 M hexane solution), giving a clear pale beige coloured solution. The reaction was left to stir at room temperature, open to a slow flow of argon, for 16 hours. Solvent was removed *in vacuo*, and the residue dissolved in a large amount of hexane (*ca.* 100 mL) to form a pale orange solution. The solution was concentrated *in vacuo* and left overnight, yielding **2-THF** as large colourless needles. Yield: 1.54 g (49%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.96 (br, 8H, O(CH_2CH_2)$_2$), 1.15 (d, $^{3}J_{HH}$ = 7.0, 12H, Dipp-CH(CH_3)$_2$), 1.27 (m, 12H, Dipp-CH(CH_3)$_2$), 1.29 (s, 18H, ^{t}Bu-C(CH_3)$_3$), 3.30 (br, 8H, O(CH_2CH_2)$_2$), 3.60 (sep, $^{3}J_{HH}$ = 7.0, 4H, Dipp-C*H*(CH_3)$_2$), 6.26 (d, $^{4}J_{HH}$ = 2.5, 2H, Ar-*H*), 6.44 (dd, $^{3}J_{HH}$ = 8.4, $^{4}J_{HH}$ = 2.5, 2H, Ar-*H*), 7.20-7.29 (m, 6H, Ar-*H*), 7.71 (d, $^{3}J_{HH}$ = 8.4, 2H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 24.5 (Dipp-CH(CH_3)$_2$), 24.8 (O(CH_2CH_2)$_2$), 26.0 (Dipp-CH(CH_3)$_2$), 28.0 (Dipp-*C*H(CH_3)$_2$), 31.9 (^{t}Bu-C(CH_3)$_3$), 34.6 (^{t}Bu-*C*(CH_3)$_3$), 70.3 (O(CH_2CH_2)$_2$), 106.4, 112.4, 115.3, 123.8, 124.0, 141.9, 146.3, 146.6, 149.6, 150.6 (AR-*C*); **IR** (ATR, Nujol, cm^{-1}): 3052(w), 2957(s), 2925(sh), 2866(m), 1600(m), 1585(w), 1489(s), 1462(m), 1433(m), 1405(m), 1380(w), 1360(w), 1339(m), 1324(sh), 1297(s), 1274(w), 1254(m), 1193(s), 1170(s), 1119(s), 1084(w), 1019(s), 961(sh), 953(s), 935(w), 893(s), 862(s), 795(s), 774(m), 760(m), 726(w), 688(w), 676(w),

657(s), 624(w), 581(w), 555(w), 534(w), 522(m), 496(w), 484(w), 453(m), 434(m), 410(w); **Anal. Calc.** for $C_{52}H_{72}MgN_2O_3 \cdot C_4H_8O$ ($C_{56}H_{80}MgN_2O_4$): C 77.35%, H 9.27%, N 3.22%, found: C 77.54%, H 9.55%, N 3.50%.

Synthesis of (^{F}NON)BF (3-F), Route A: To a solution of **2-OEt$_2$** (3.07 g, 4.21 mmol) in toluene (30 mL) was added $BF_3 \cdot OEt_2$ (0.572 mL, 4.62 mmol) dropwise at –80 °C. The reaction was allowed to warm to room temperature, slowly giving a dark green coloured solution. This was stirred for an additional 16 hours at room temperature to yield a cloudy light green solution. The solution was filtered, and the volatiles removed *in vacuo*. The remaining green solid was then dissolved in toluene (20 mL), filtered, and then volatiles removed *in vacuo* again. The yellow residue was then washed with hexane, yielding **3-F** as a white powder. Yield: 1.41 g (51%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.81 (d, $^3J_{HH}$ = 6.8, 6H, Dipp-CH(C*H*$_3$)$_2$), 1.02 (s, 18H, ^{t}Bu-C(C*H*$_3$)$_3$), 1.26 (d, $^3J_{HH}$ = 6.8, 6H, Dipp-CH(C*H*$_3$)$_2$), 1.30 (d, $^3J_{HH}$ = 6.7, 12H, Dipp-CH(C*H*$_3$)$_2$), 3.57 (sep, $^3J_{HH}$ = 6.8, 2H, Dipp-C*H*(CH$_3$)$_2$), 3.76 (sep, $^3J_{HH}$ = 6.8, 2H, Dipp-C*H*(CH$_3$)$_2$), 6.70 (d, $^4J_{HH}$ = 2.4, 2H, Ar-*H*), 6.82 (dd, $^3J_{HH}$ = 8.4, $^4J_{HH}$ = 2.3, 2H, Ar-*H*), 7.11 (dd, $^3J_{HH}$ = 6.8, $^4J_{HH}$ = 2.5, 2H, Ar-*H*), 7.16-7.22 (m, 4H, Ar-*H*), 7.37 (d, $^3J_{HH}$ = 8.4, 2H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 23.9, 24.6, 25.3, 25.4 (Dipp-CH(*C*H$_3$)$_2$), 28.2, 28.7 (Dipp-*C*H(CH$_3$)$_2$), 31.4 (^{t}Bu-C(*C*H$_3$)$_3$), 34.5 (tBu-*C*(CH$_3$)$_3$), 120.4, 122.0, 122.0, 122.4, 123.9, 125.5, 140.0, 141.3, 147.2, 147.5, 148.3, 149.2 (Ar-*C*); **^{11}B{^{1}H} NMR** (128.4 MHz, C_6D_6, 25 °C): δ_B = 21.7; **^{19}F{^{1}H} NMR** (376.5 MHz, C6D6, 25 °C): δ_F = -99.7, -99.8; **IR** (ATR, nujol, cm^{-1}): 3060(w), 3025(w), 2961(s), 2926(m), 2867(m), 1607(sh), 1587(w), 1500(s), 1463(m), 1445(w), 1410(s), 1392(sh), 1372(s), 1357(m), 1338(sh), 1318(s), 1277(m), 1268(m), 1254(sh), 1245(sh), 1226(w), 1191(s), 1126(m), 1101(m), 1057(m), 1044(sh), 934(m), 885(m), 855(w), 839(s), 821(s), 807(s), 795(w), 765(s), 749(s), 729(m), 684(sh), 673(sh), 665(s), 633(m), 612(w), 599(w), 581(m), 562(m), 549(w), 527(w), 510(w), 490(m), 469(w), 442(w); **Anal. Calc.** for $C_{44}H_{58}BFN_2O$: C 79.98%, H 8.85%, N 4.24%, found: C 78.98%, H 8.84%, N 4.22%.

Synthesis of (^{F}NON)BF (3-F), Route B: To a solution of **2-THF** (7.50 g, 9.38 mmol) in toluene (50 mL) was added $BF_3 \cdot OEt_2$ (1.27 mL, 10.3 mmol) dropwise at –80 °C. The reaction was allowed to warm to room temperature, slowly giving a dark green coloured solution. This was stirred for an additional 16 hours at room temperature to yield a cloudy light green solution. The solution was filtered, and the volatiles removed *in vacuo*. The remaining green solid was then dissolved in toluene (40 mL), filtered, and then volatiles removed *in vacuo*. The yellow residue was then washed with hexane, yielding **3-F** as a white powder. Yield: 2.48 g (40%).

Synthesis of (^{F}NON)BBr (3-Br): To a Schlenk flask loaded with **3-F** (1.3722 g, 2.0767 mmol) was added a solution of 1.0 M BBr_3 in DCM (21.0 mL, 20.8 mmol) giving a deep dark brown solution, which was stirred at room temperature for 2.5 hours. Volatiles were removed *in vacuo* and the brown residue was dissolved in benzene, resulting in a light brown solution with precipitate crashing out. The mixture

was filtered, volatiles from the filtrate were removed *in vacuo* and the remaining brown solid was washed with hexane, yielding **3-Br** as a pale beige powder. Yield: 0.9226 g (62%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.59 (d, $^{3}J_{HH}$ = 6.7, 6H, Dipp-CH(C*H*$_3$)$_2$), 0.91 (s, 18H, ^{t}Bu-C(C*H*$_3$)$_3$), 1.41 (d, $^{3}J_{HH}$ = 6.9, 6H, Dipp-CH(C*H*$_3$)$_2$), 1.48 (d, $^{3}J_{HH}$ = 6.7, 6H, Dipp-CH(C*H*$_3$)$_2$), 1.49 (d, $^{3}J_{HH}$ = 6.9, 6H, Dipp-CH(C*H*$_3$)$_2$), 3.73 (sep, $^{3}J_{HH}$ = 6.7, 2H, Dipp-C*H*(CH$_3$)$_2$), 3.87 (sep, $^{3}J_{HH}$ = 6.9, 2H, Dipp-C*H*(CH$_3$)$_2$), 6.71 (d, $^{4}J_{HH}$ = 2.3, 2H, Ar-*H*), 6.77 (dd, $^{3}J_{HH}$ = 8.4, $^{4}J_{HH}$ = 2.3, 2H, Ar-*H*), 7.05-7.09 (m, 2H, Ar-*H*), 7.17-7.19 (m, 4H, Ar-*H*), 7.30 (d, $^{3}J_{HH}$ = 8.4, 2H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 23.7, 24.3, 25.7, 25.7 (Dipp-CH(*C*H$_3$)$_2$), 28.3, 29.0 (Dipp-*C*H(CH$_3$)$_2$), 31.2 (^{t}Bu-C(*C*H$_3$)$_3$), 34.4 (^{t}Bu-*C*(CH$_3$)$_3$), 121.4, 122.2, 123.9, 125.5, 126.0, 140.9, 146.1, 146.2, 148.2, 148.4, 150.9 (Ar-*C*); **^{11}B{^{1}H} NMR** (128.4 MHz, C_6D_6, 25 °C): δ_B = 28.2; **IR** (ATR, nujol, cm^{-1}): 3057(w), 2960(s), 2926(m), 2867(m), 1606(sh), 1586(w), 1507(sh), 1496(m), 1464(m), 1441(sh), 1404(m), 1378(m), 1362(sh), 1349(s), 1317(w), 1301(w), 1239(sh), 1267(s), 1255(sh), 1242(sh), 1215(w), 1205(w), 1183(s), 1136(m), 1122(m), 1113(m), 1075(m), 1054(w), 1042(w), 929(m), 889(w), 876(w), 842(m), 815(m), 803(s), 791(sh), 761(m), 738(w), 726(m), 675(sh), 657(s), 626(w), 596(w), 582(w), 565(m), 533(w), 511(w), 501(sh), 488(w), 474(m), 465(sh); **Anal. Calc.** for $C_{44}H_{58}BBrN_2O$: C 73.23%, H 8.10%, N 3.88%, found: C 73.29%, H 8.29%, N 3.75%.

Synthesis of the C-N activated product (4): To a solution of **3-Br** (0.21 g, 0.29 mmol) in THF (10mL) was added a small strip of lithium ribbon. The reaction was stirring vigorously at room temperature for 16 hours resulting opaque green-brown solution. The reaction mixture was filtered, and volatiles were removed from the fluorescent yellow green filtrate *in vacuo*. The dull yellow residue was dissolved in hexane, yielding a bright yellow solution with a white precipitate. This solution was filtered, the filtrate concentrated *in vacuo* and slowly cooled to –20 °C overnight to give **4** as small colourless crystals. Yield: 0.18 g (86%). **^{1}H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.28 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 0.54 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 0.84 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.12 (s, 9H, ^{t}Bu-C(C*H*$_3$)$_3$), 1.13 (br, 8H, (O(CH$_2$)(C*H*$_2$))$_2$), 1.19 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.29 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.40 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.44 (d, $^{3}J_{HH}$ = 6.9, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.44 (s, 9H, ^{t}Bu-C(C*H*$_3$)$_3$), 1.46 (d, $^{3}J_{HH}$ = 6.9, 6H, Dipp-CH(C*H*$_3$)$_2$), 2.87 (sep, $^{3}J_{HH}$ = 6.9, 1H, Dipp-C*H*(CH$_3$)$_2$), 3.09 (br, 8H, (O(C*H*$_2$)(CH$_2$))$_2$), 3.30 (sep, $^{3}J_{HH}$ = 6.9, 1H, Dipp-C*H*(CH$_3$)$_2$), 3.80 (sep, $^{3}J_{HH}$ = 6.9, 1H, Dipp-C*H*(CH$_3$)$_2$), 4.47 (sep, $^{3}J_{HH}$ = 6.9, 1H, Dipp-C*H*(CH$_3$)$_2$), 6.12 (d, $^{4}J_{HH}$ = 2.4, 1H, Ar-*H*), 6.65 (dd, $^{3}J_{HH}$ = 8.3, $^{4}J_{HH}$ = 2.4, 1H, Ar-*H*), 6.70 (dd, $^{3}J_{HH}$ = 8.2, $^{4}J_{HH}$ = 2.5, 1H, Ar-*H*), 6.89 (dd, $^{3}J_{HH}$ = 7.7, $^{4}J_{HH}$ = 1.1, 1H, Ar-*H*), 7.02-7.06 (m, 1H, Ar-*H*), 7.05 (d, $^{4}J_{HH}$ = 2.5, 1H, Ar-*H*), 7.09-7.14 (m, 2H, Ar-*H*), 7.21-7.25 (m, 1H, Ar-*H*), 7.29 (dd, $^{3}J_{HH}$ = 7.7, $^{4}J_{HH}$ = 1.7, 1H, Ar-*H*), 7.39 (d, $^{3}J_{HH}$ = 8.3, 1H, Ar-*H*), 7.57 (d, $^{3}J_{HH}$ = 8.2, 1H, Ar-*H*); **^{13}C{^{1}H} NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 22.5, 23.0, 23.2, 23.3 (Dipp-CH(*C*H$_3$)$_2$), 25.3 (O(CH$_2$)(*C*H$_2$))$_2$), 25.4, 26.05, 26.3 (Dipp-CH(*C*H$_3$)$_2$), 27.7 (Dipp-*C*H(CH$_3$)$_2$), 27.9 (Dipp-CH(*C*H$_3$)$_2$), 28.3 (Dipp-*C*H(CH$_3$)$_2$), 31.6, 32.1 (^{t}Bu-C(*C*H$_3$)$_3$), 33.7, 34.3 (Dipp-*C*H(CH$_3$)$_2$), 34.5, 34.5, (^{t}Bu-*C*(CH$_3$)$_3$, 67.9 (O(CH$_2$)(*C*H$_2$))$_2$), 114.0, 115.3, 115.4, 120.7, 122.0, 122.7,

123.0, 123.4, 123.5, 123.6, 125.1, 125.3, 127.6, 128.0, 141.4, 144.5, 146.0, 146.7, 146.9, 149.2, 150.5, 151.1, 151.2, 153.2 (Ar-*C*); **$^{11}B\{^1H\}$ NMR** (128.4 MHz, C_6D_6, 25 °C): δ_B = 32.5; **IR** (ATR, nujol, cm^{-1}): 3054(sh), 2959(s), 2925(s), 2863(m), 1588(w), 1569(w), 1501(m), 1485(s), 1426(s), 1378(m), 1357(m), 1321(sh), 1300(m), 1276(m), 1249(m), 1189(s), 1156(s), 1120(m), 1097(w), 1042(s), 1015(s), 942(sh), 914(w), 881(m), 868(w), 828(s), 802(s), 782(sh), 768(w), 755(m), 722(w), 698(w), 673(w), 655(w), 647(w), 628(w), 604(w), 573(w), 553(w), 536(w), 510(w), 468(m), 405(w); **Anal. Calc.** a satisfactory elemental analysis could not be obtained for this compound, possibly due to decomposition during shipping.

Synthesis of [{(^{r}NON)BOCFeCp}$_2$] (5): To a solution of **3-Br** (0.16 g, 0.22 mmol) in THF (15 mL) was added potassium cyclopentadienyliron dicarbonyl (0.058 g, 0.27 mmol), which was then stirred at room temperature for 48 hours. Volatiles were removed from the reaction mixture *in vacuo* yielding a dark brown solid. This residue was extracted into pentane (15 mL), filtered and the remaining clear red brown filtrate was concentrated *in vacuo*. The reaction vessel left to stand for overnight to yield **5** as thin yellow crystals. Yield: 3% (crystalline yield). **^1H NMR** (400.1 MHz, C_6D_6, 25 °C): δ_H = 0.45 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 0.49 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 0.50 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 0.64 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 1.02 (s, 18H, ^{t}Bu-C(CH_3)$_3$), 1.17 (s, 18H, ^{t}Bu-C(CH_3)$_3$), 1.17 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 1.29 (d, $^3J_{HH}$ = 6.7, 6H, Dipp-CH(CH_3)$_2$), 1.39 (d, $^3J_{HH}$ = 6.7, 6H, Dipp-CH(CH_3)$_2$), 1.55 (d, $^3J_{HH}$ = 6.6, 6H, Dipp-CH(CH_3)$_2$), 2.11 (sep, $^3J_{HH}$ = 6.6, 2H, Dipp-C*H*(CH$_3$)$_2$), 3.24 (sep, $^3J_{HH}$ = 6.7, 2H, Dipp-C*H*(CH$_3$)$_2$), 3.56 (sep, $^3J_{HH}$ = 6.6, 2H, Dipp-C*H*(CH$_3$)$_2$), 4.14 (s, 5H, Cp-*H*), 4.96 (sep, $^3J_{HH}$ = 6.6, 2H, Dipp-C*H*(CH$_3$)$_2$), 6.50 (d, $^4J_{HH}$ = 2.4, 2H, Ar-*H*), 6.85 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 2.4, 2H, Ar-*H*), 6.86 (dd, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 2.4, 2H, Ar-*H*), 7.00 (d, $^4J_{HH}$ = 2.4, 2H, Ar-*H*), 7.04 – 7.07 (m, 4H, Ar-*H*), 7.08 – 7.13 (m, 6H, Ar-*H*), 7.20 (d, $^3J_{HH}$ = 8.5, 2H, Ar-*H*), 7.27 (dd, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.8, 2H, Ar-*H*), 7.47 (d, $^3J_{HH}$ = 8.3, 2H, Ar-*H*); **$^{13}C\{^1H\}$ NMR** (100.6 MHz, C_6D_6, 25 °C): δ_C = 23.0, 23.1, 23.5, 23.9, 24.2, 25.8, 26.0 (Dipp-CH(CH_3)$_2$), 28.4, 28.7 (Dipp-C*H*(CH$_3$)$_2$), 29.0 (Dipp-CH(CH_3)$_2$), 30.3 (Dipp-C*H*(CH$_3$)$_2$), 31.2, 31.4 (^{t}Bu-C(CH_3)$_3$), 31.6 (Dipp-C*H*(CH$_3$)$_2$), 34.5, 34.6 (^{t}Bu-C(CH$_3$)$_3$), 84.1 (Cp-*C*), 118.7, 121.0, 121.4, 121.6, 122.4, 122.4, 123.4, 123.6, 126.4, 126.8, 127.0, 127.6, 142.4, 143.9, 146.3, 146.6, 147.3, 147.5, 147.7, 147.8, 148.0, 148.8, 149.0, 150.2 (Ar-*C*), 215.7 (*C*O); **$^{11}B\{^1H\}$ NMR** a clear $^{11}B\{^1H\}$ signal was unable to be distinguished from the baseline; **Anal. Calc.** a satisfactory elemental analysis could not be obtained for this compound, possibly due to decomposition during shipping.

4,4’-oxybis(3-bromo-1-tert-butylbenzene)

NMR Spectra of New Compounds

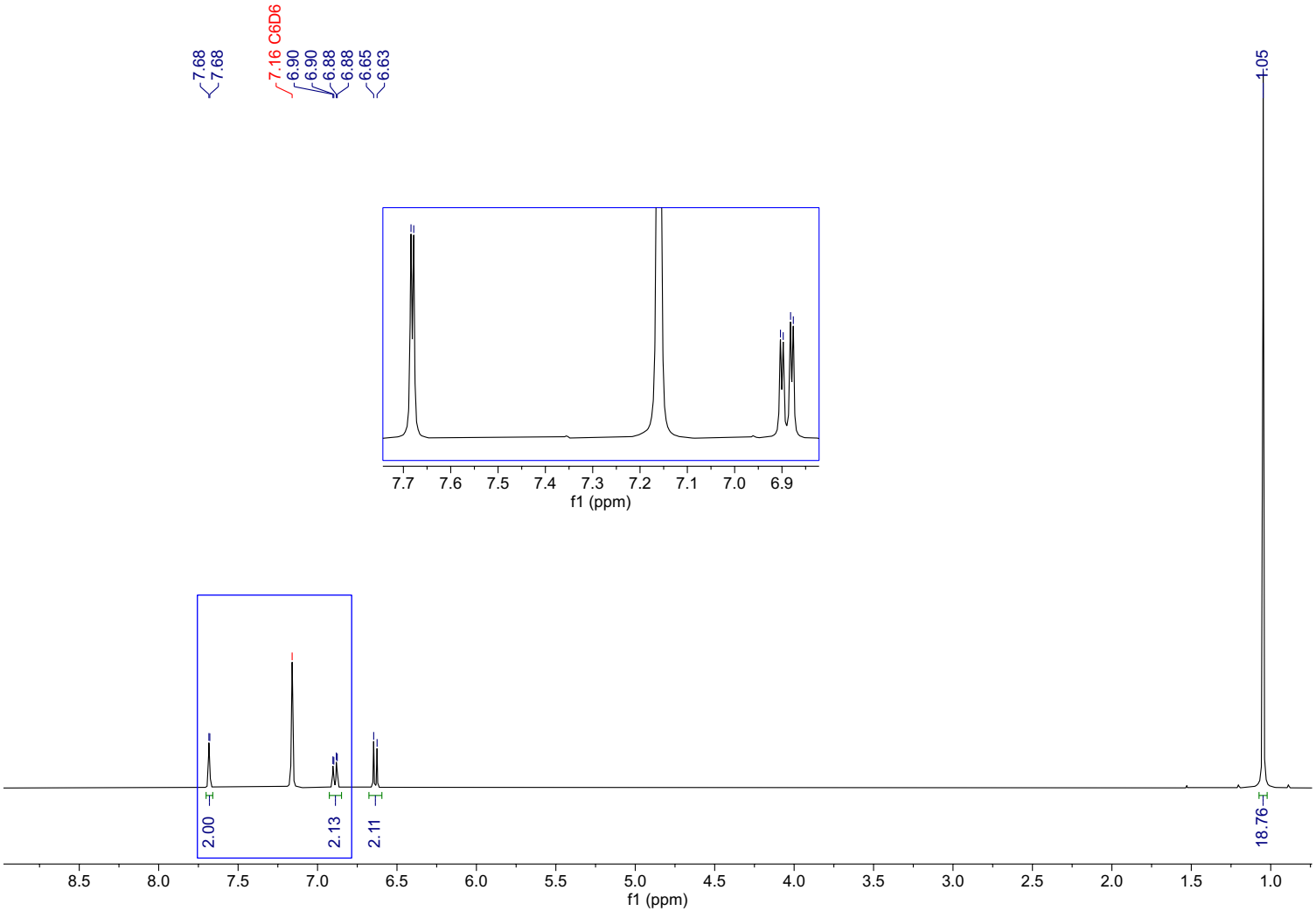


Figure S1: ^{1}H NMR spectrum of 4,4’-oxybis(3-bromo-1-tert-butylbenzene) (400 MHz, C_6D_6, 298K).

4,4’-oxybis(3-bromo-1-tert-butylbenzene)

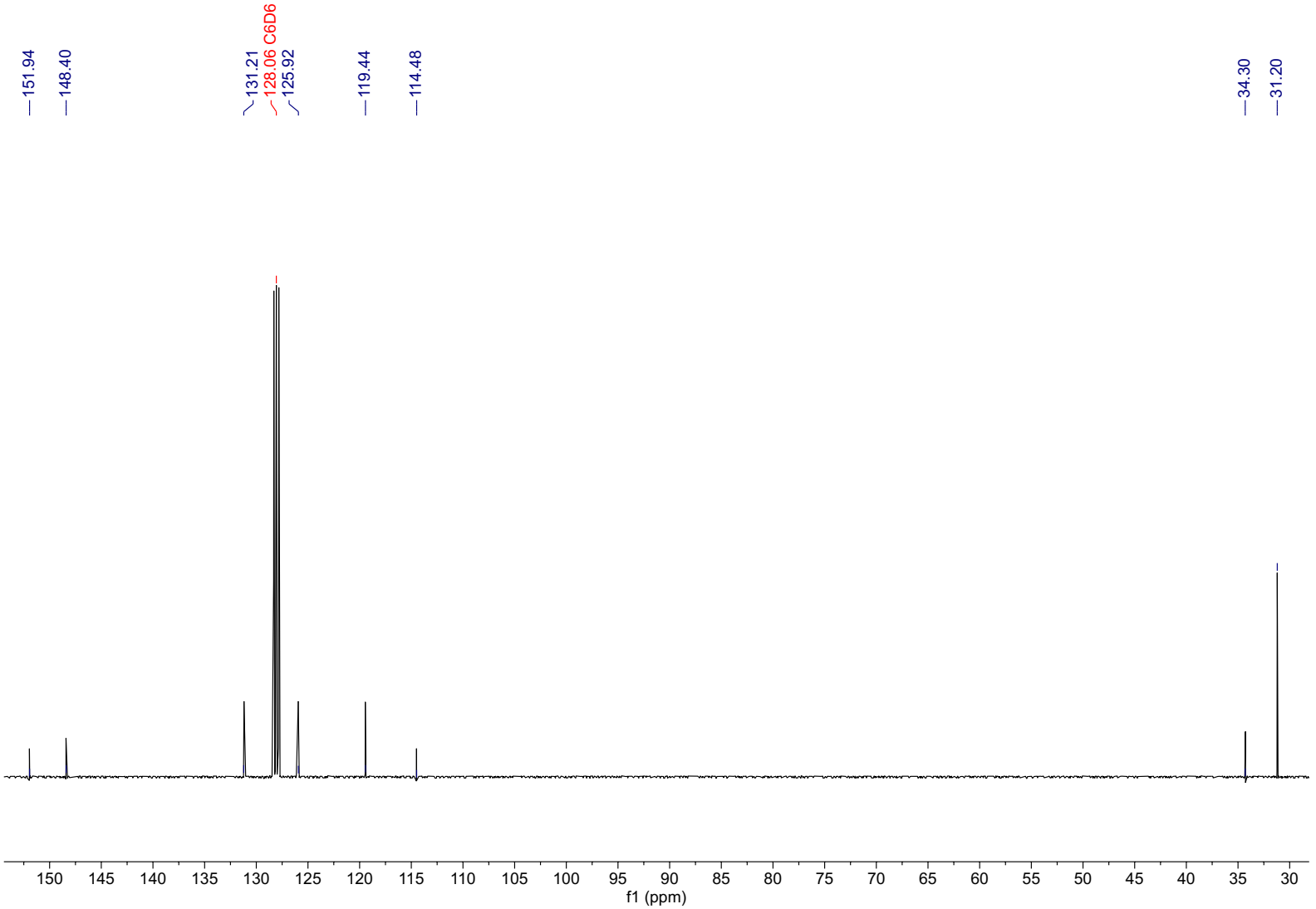


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of 4,4’-oxybis(3-bromo-1-tert-butylbenzene) (101 MHz, C_6D_6, 298K).

$H_2(^FNON)$

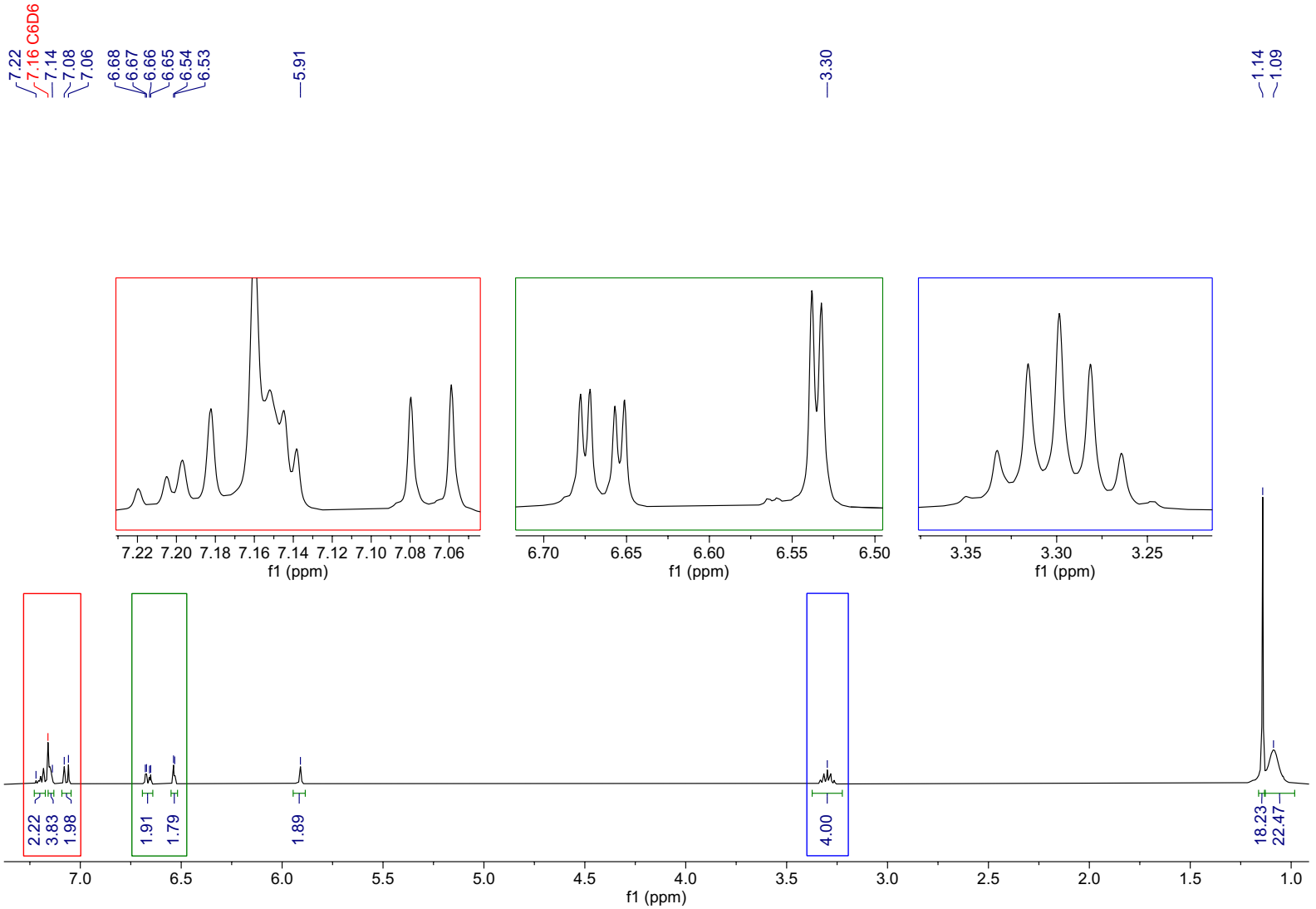


Figure S3: ^{1}H NMR spectrum of $H_2(^FNON)$ (400 MHz, C_6D_6, 298K).

$H_2(^FNON)$

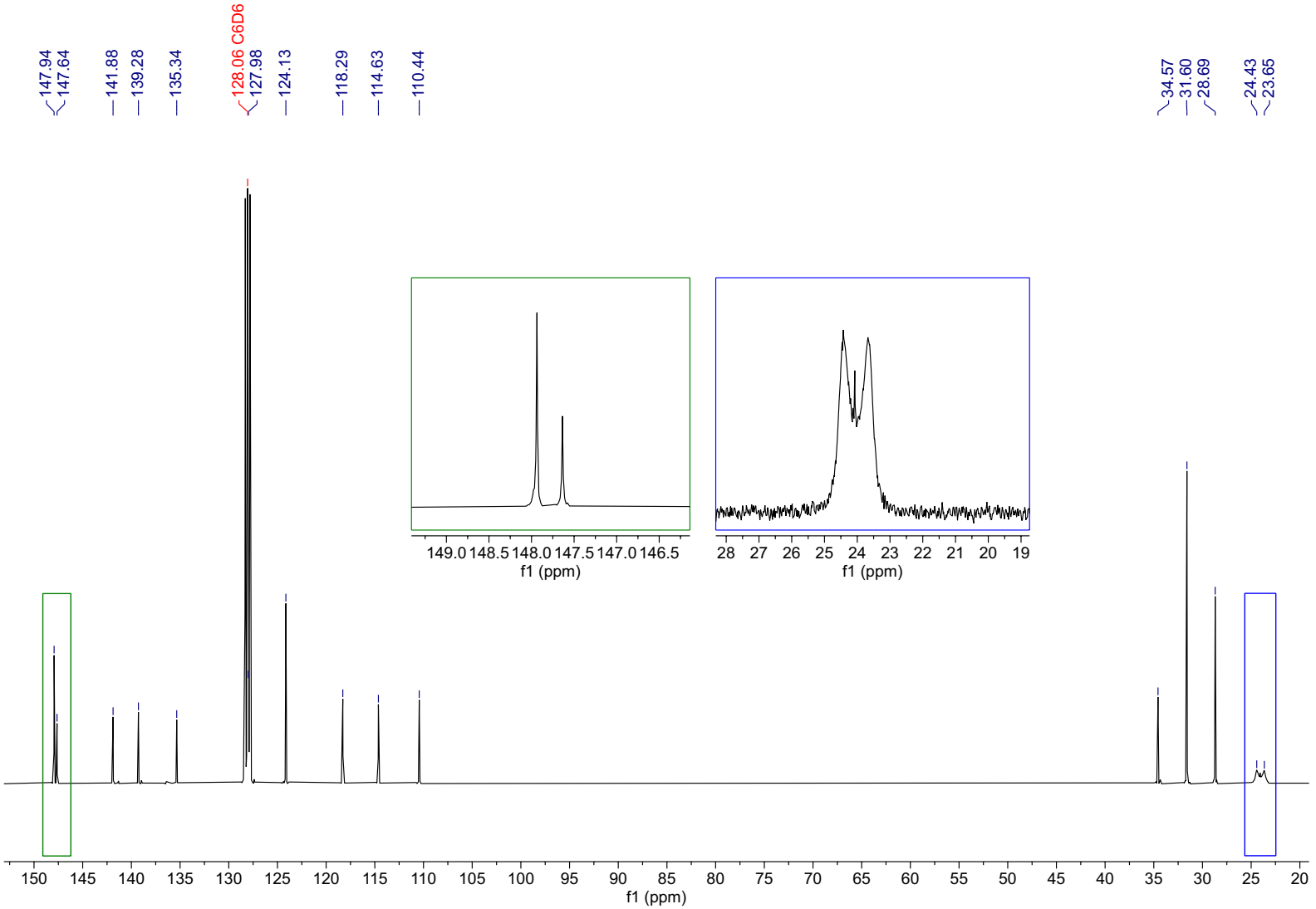


Figure S4: $^{13}C\{^1H\}$ NMR spectrum of $H_2(^FNON)$ (101 MHz, C_6D_6, 298K).

$K_2(^{F}NON)$ (1)

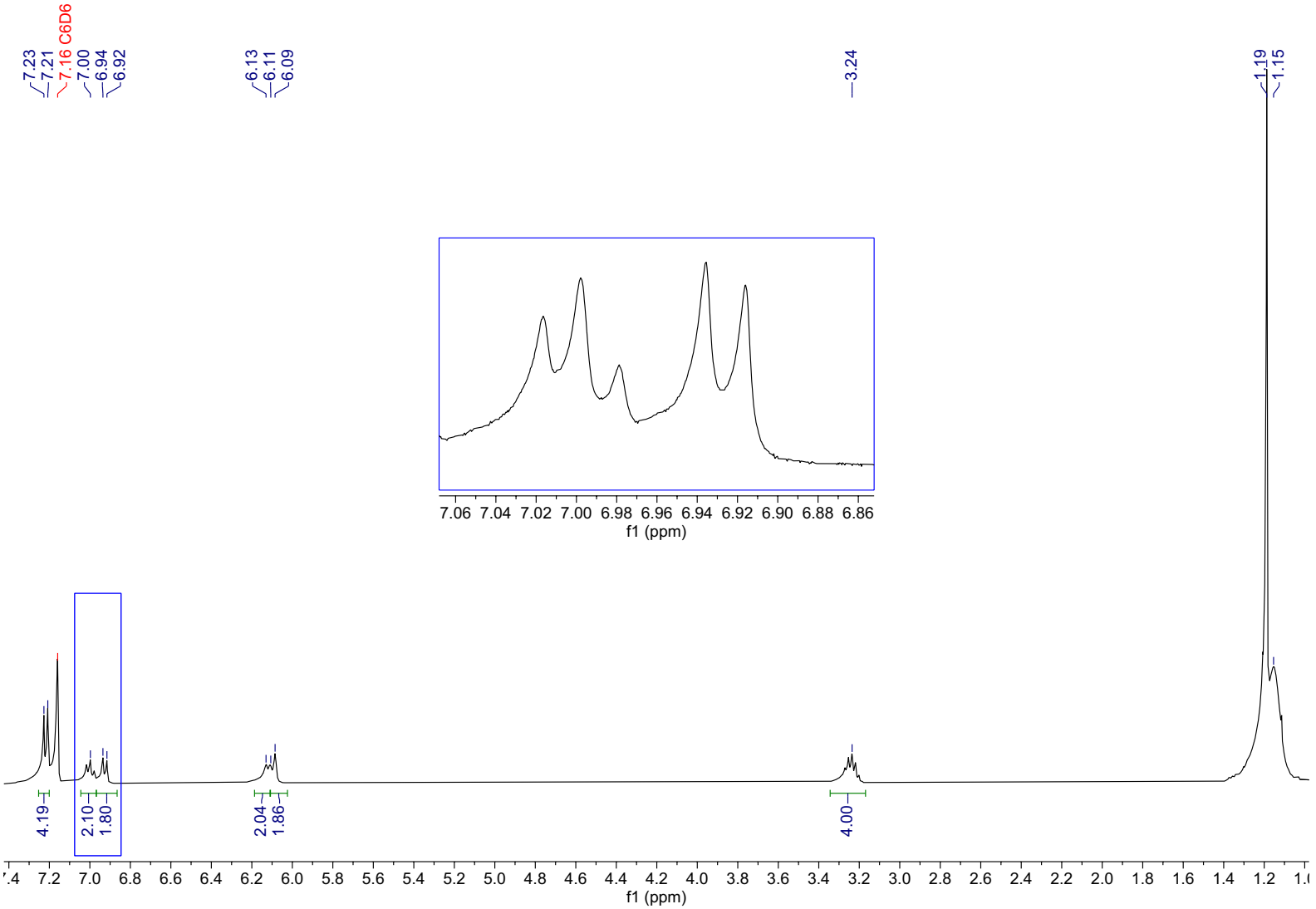


Figure S5: ^{1}H NMR spectrum of $K_2(^{F}NON)$ (**1**) (400 MHz, C_6D_6, 353K).

$K_2(^{F}NON)$ (1)

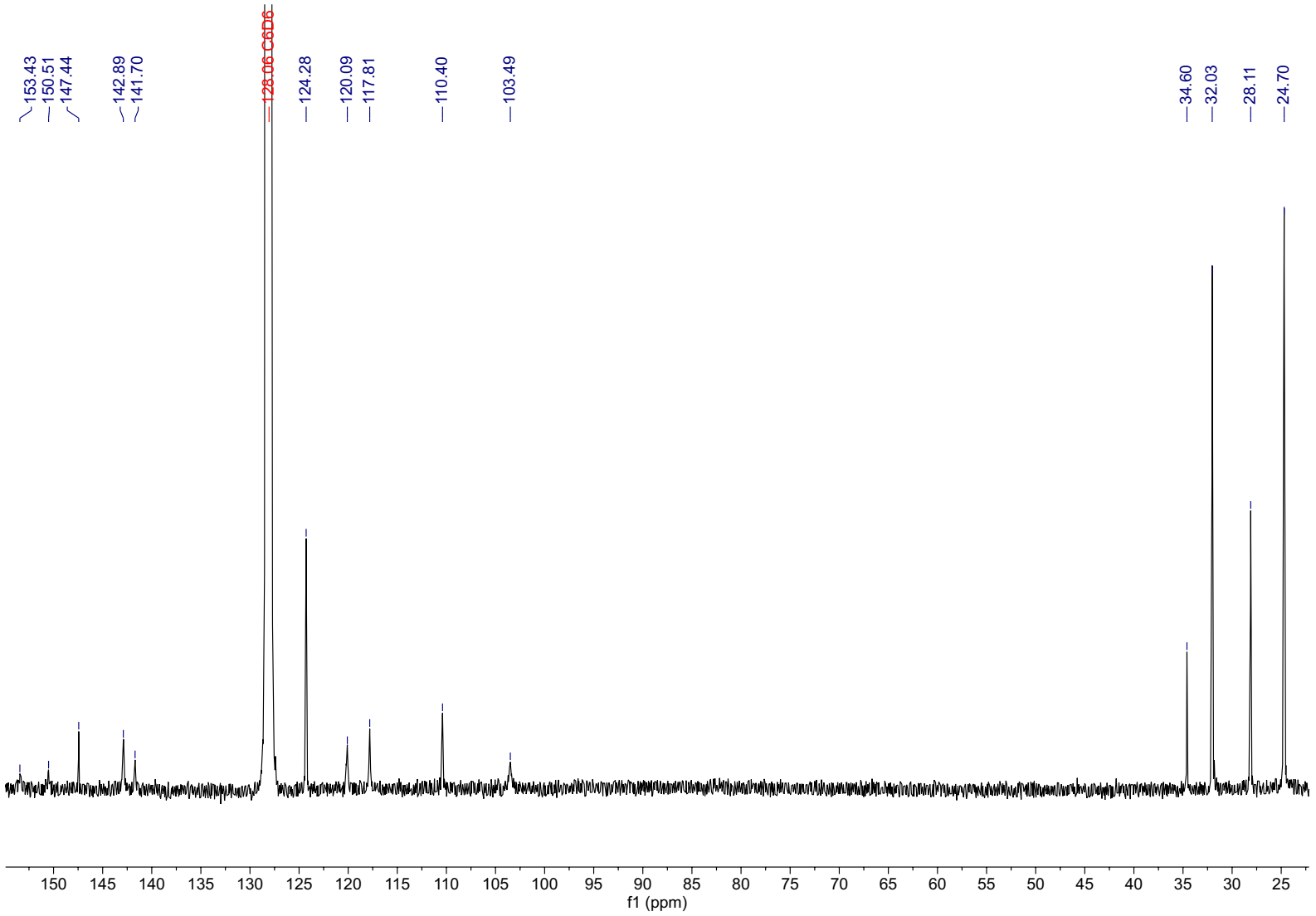


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of $K_2(^{F}NON)$ (**1**) (101 MHz, C_6D_6, 353K).

(^{F}NON)Mg(OEt$_2$) (2-OEt$_2$)

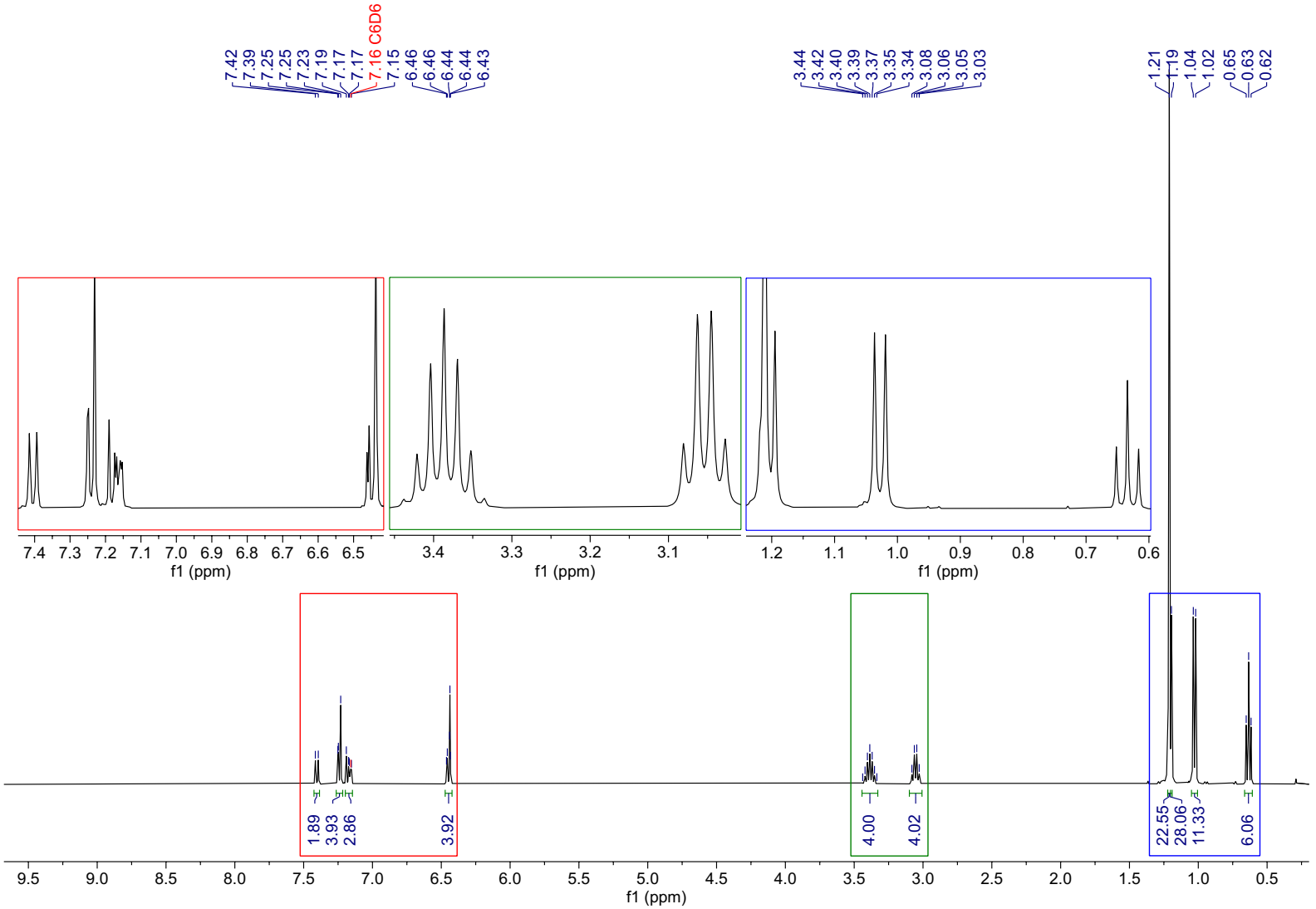


Figure S7: ^{1}H NMR spectrum of (^{F}NON)Mg(OEt$_2$) (**2-OEt$_2$**) (400 MHz, C_6D_6, 298K).

(^{F}NON)Mg(OEt$_2$) (2-OEt$_2$)

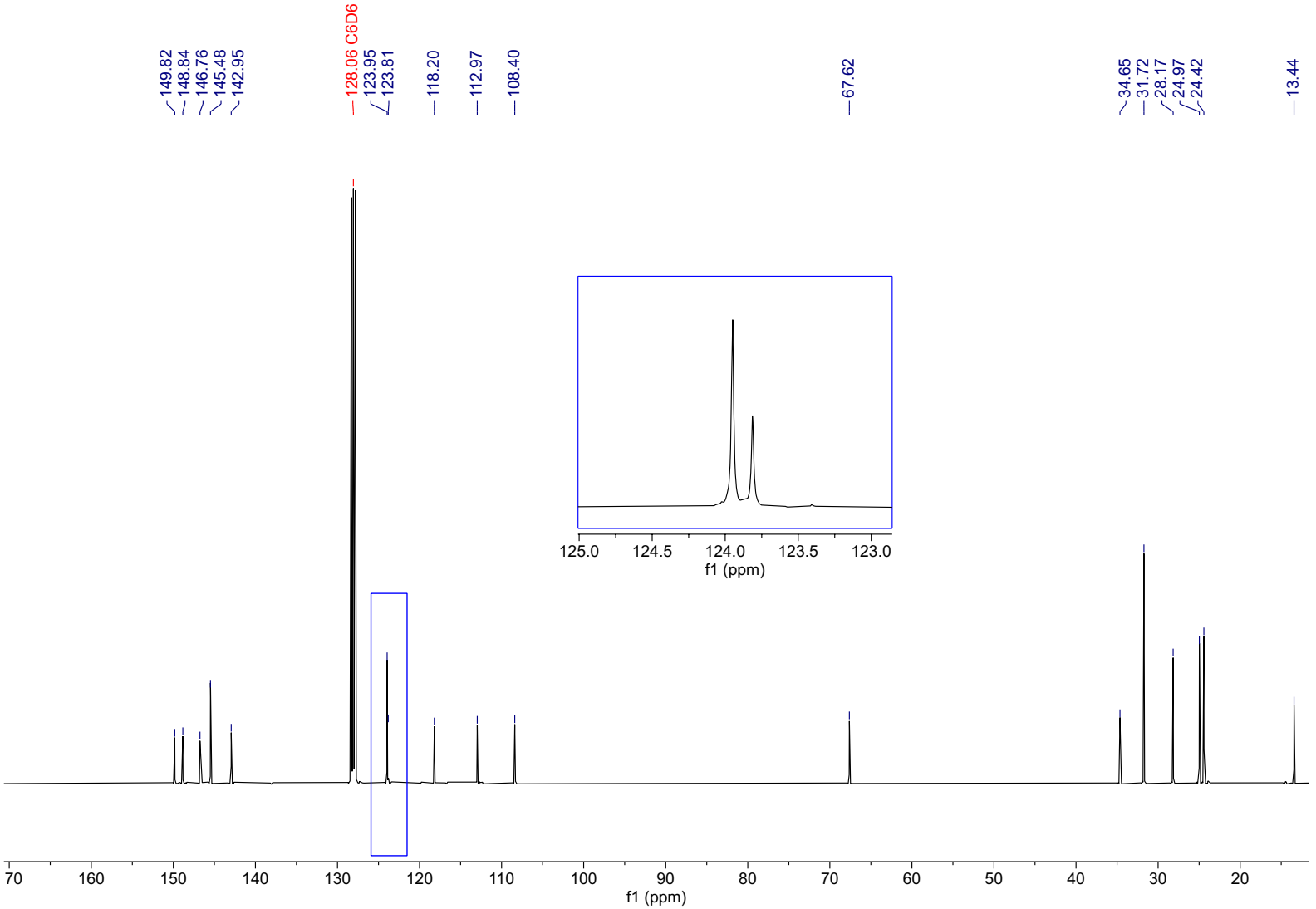


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of (^{F}NON)Mg(OEt$_2$) (**2-OEt$_2$**) (101 MHz, C_6D_6, 298K).

(^{F}NON)Mg(THF)$_2$ (2-THF)

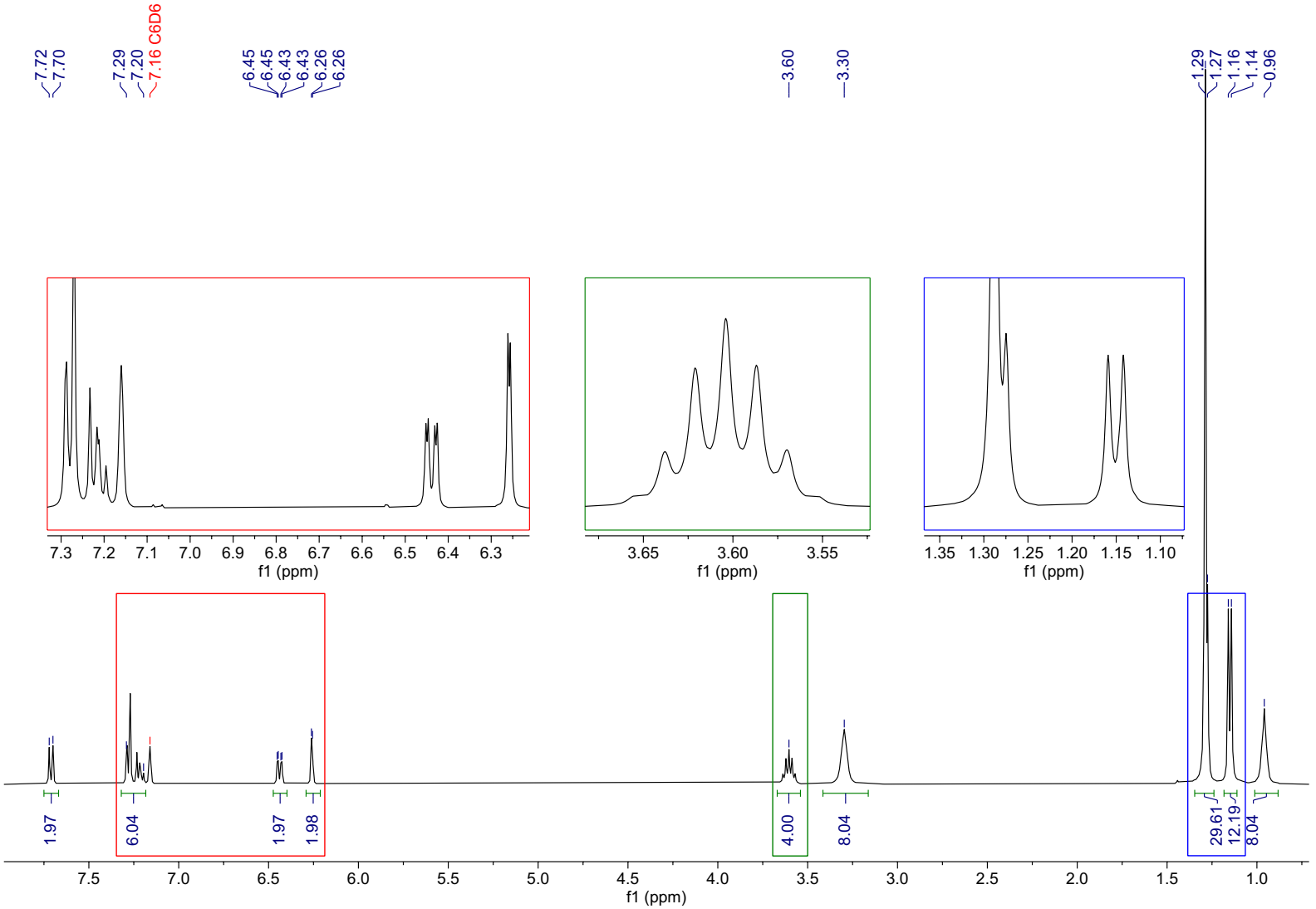


Figure S9: ^{1}H NMR spectrum of (^{F}NON)Mg(THF)$_2$ (**2-THF**) (400 MHz, C_6D_6, 298K).

(^{F}NON)Mg(THF)$_2$ (2-THF)

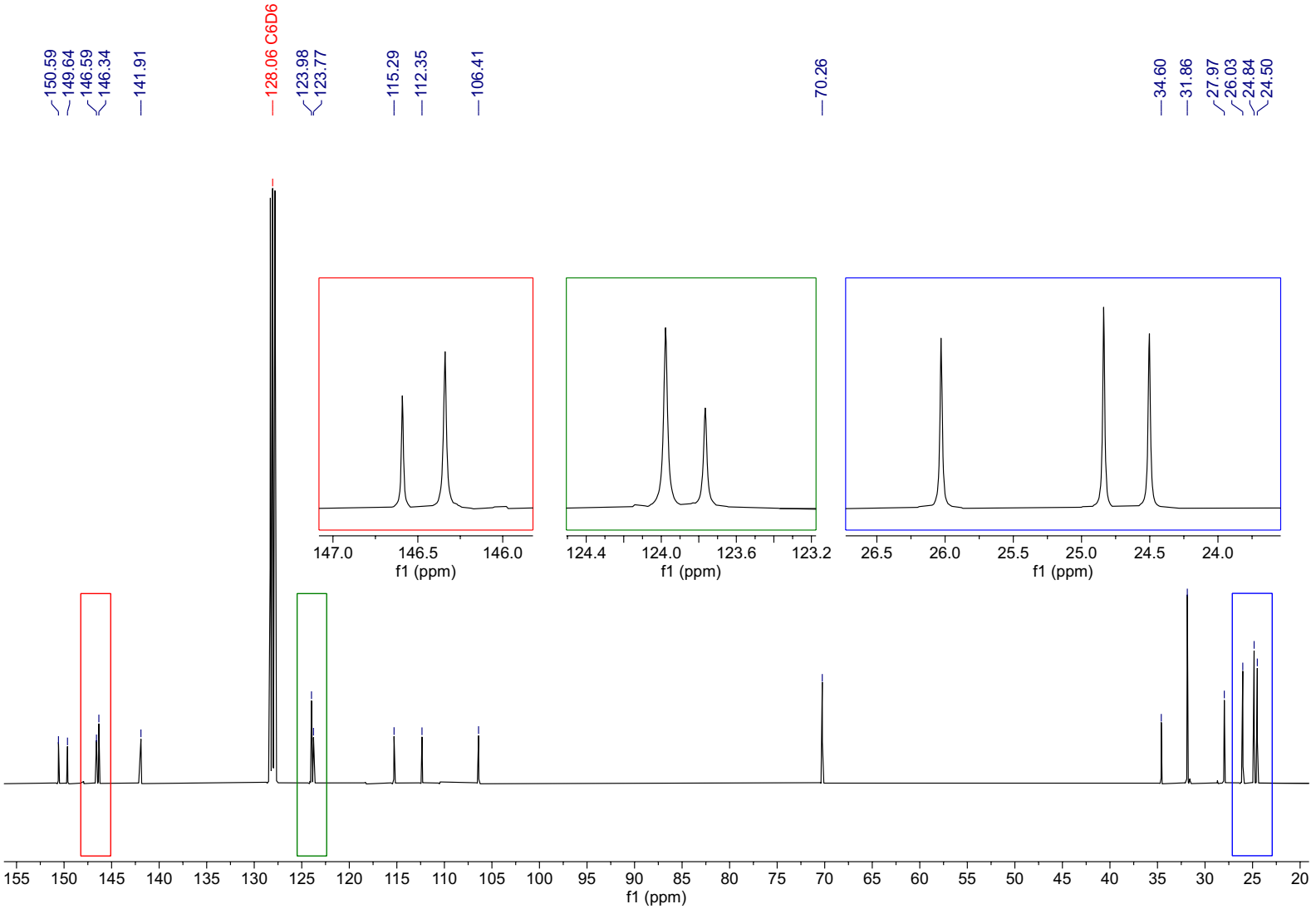


Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of (^{F}NON)Mg(THF)$_2$ (**2-THF**) (101 MHz, C_6D_6, 298K).

(^{F}NON)BF (3-F)

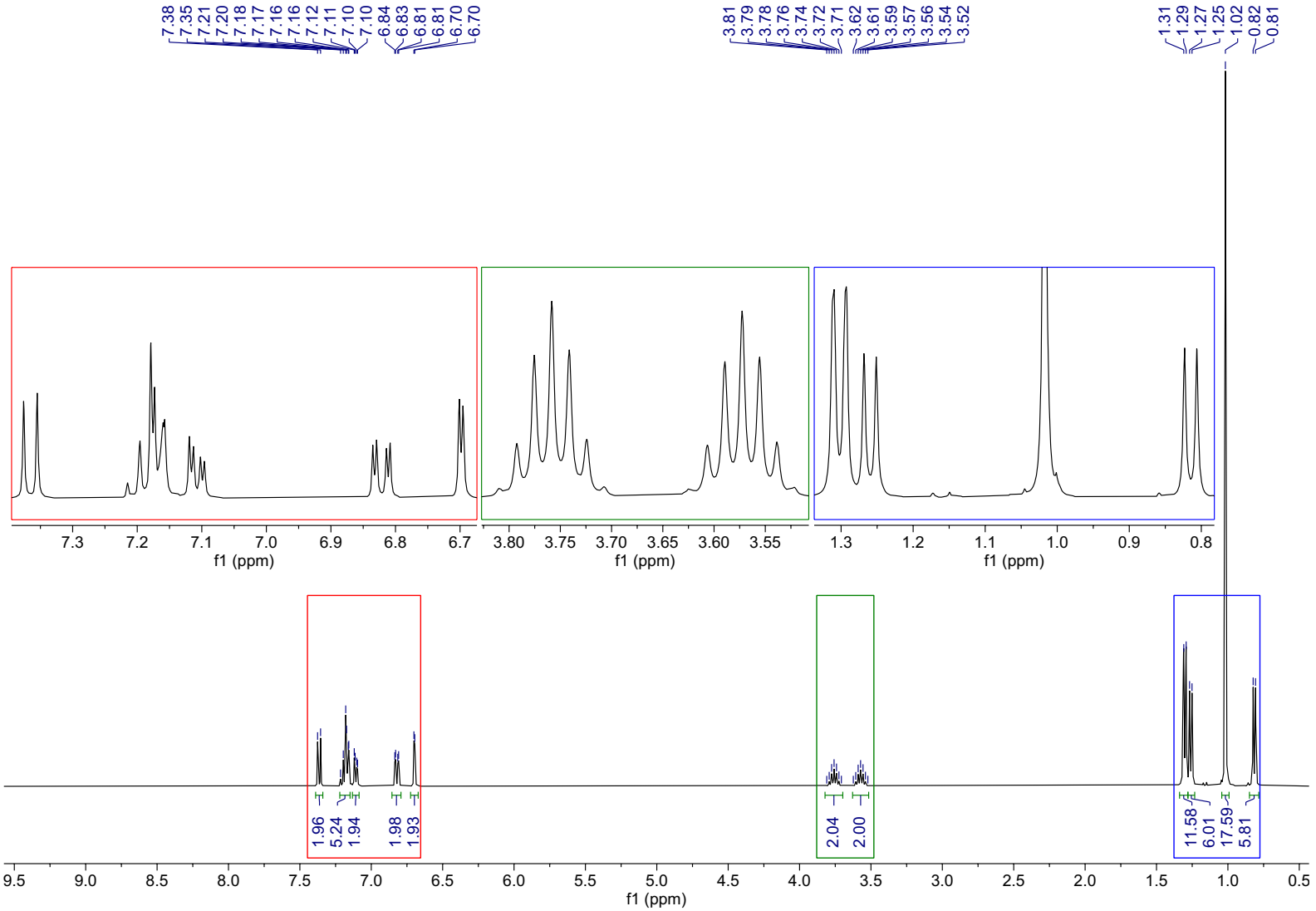


Figure S11: ^{1}H NMR spectrum of (^{F}NON)BF (**3-F**) (400 MHz, C_6D_6, 298K).

(^{F}NON)BF (3-F)

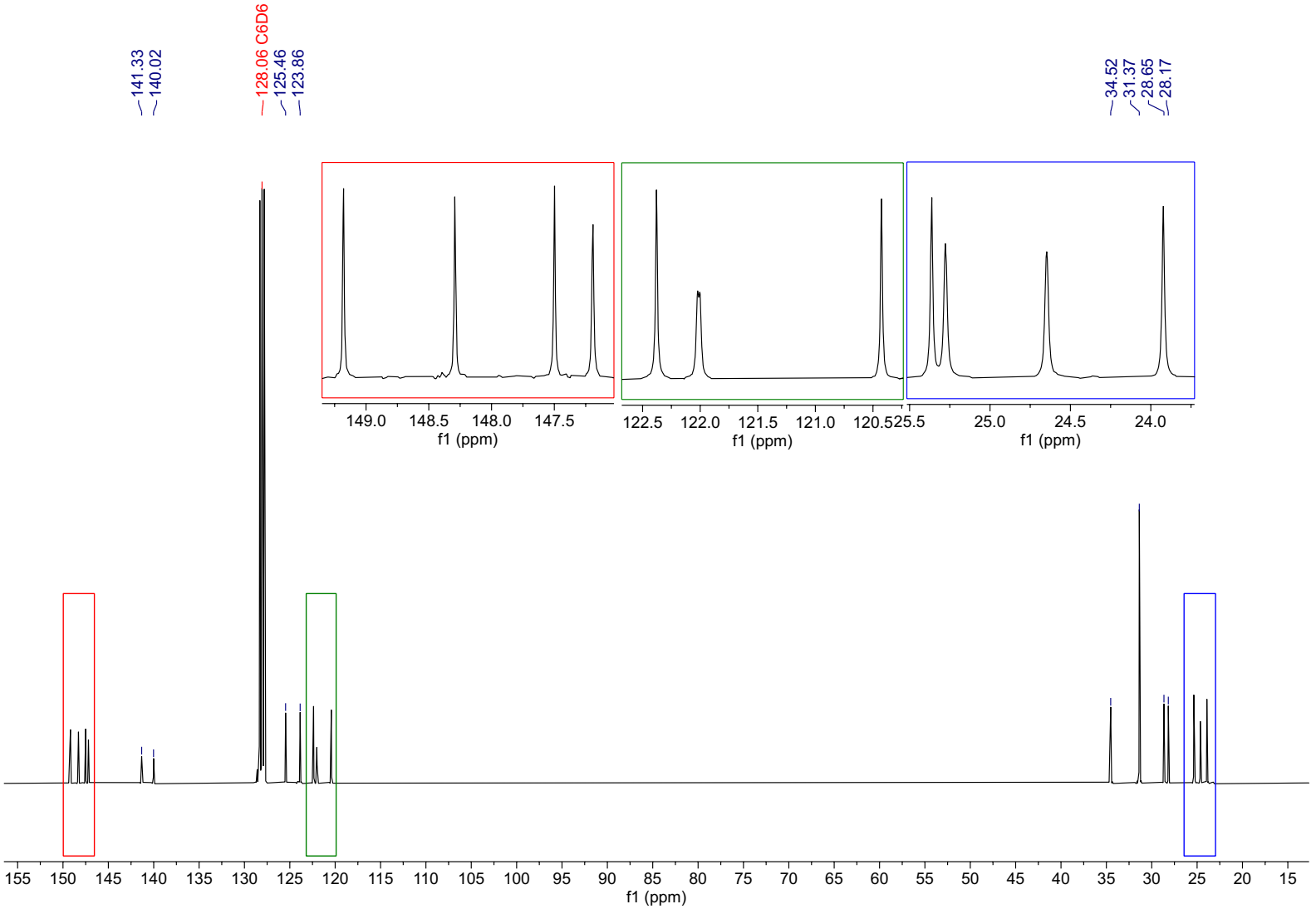


Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum of (^{F}NON)BF (**3-F**) (101 MHz, C_6D_6, 298K).

(^{F}NON)BF (3-F)

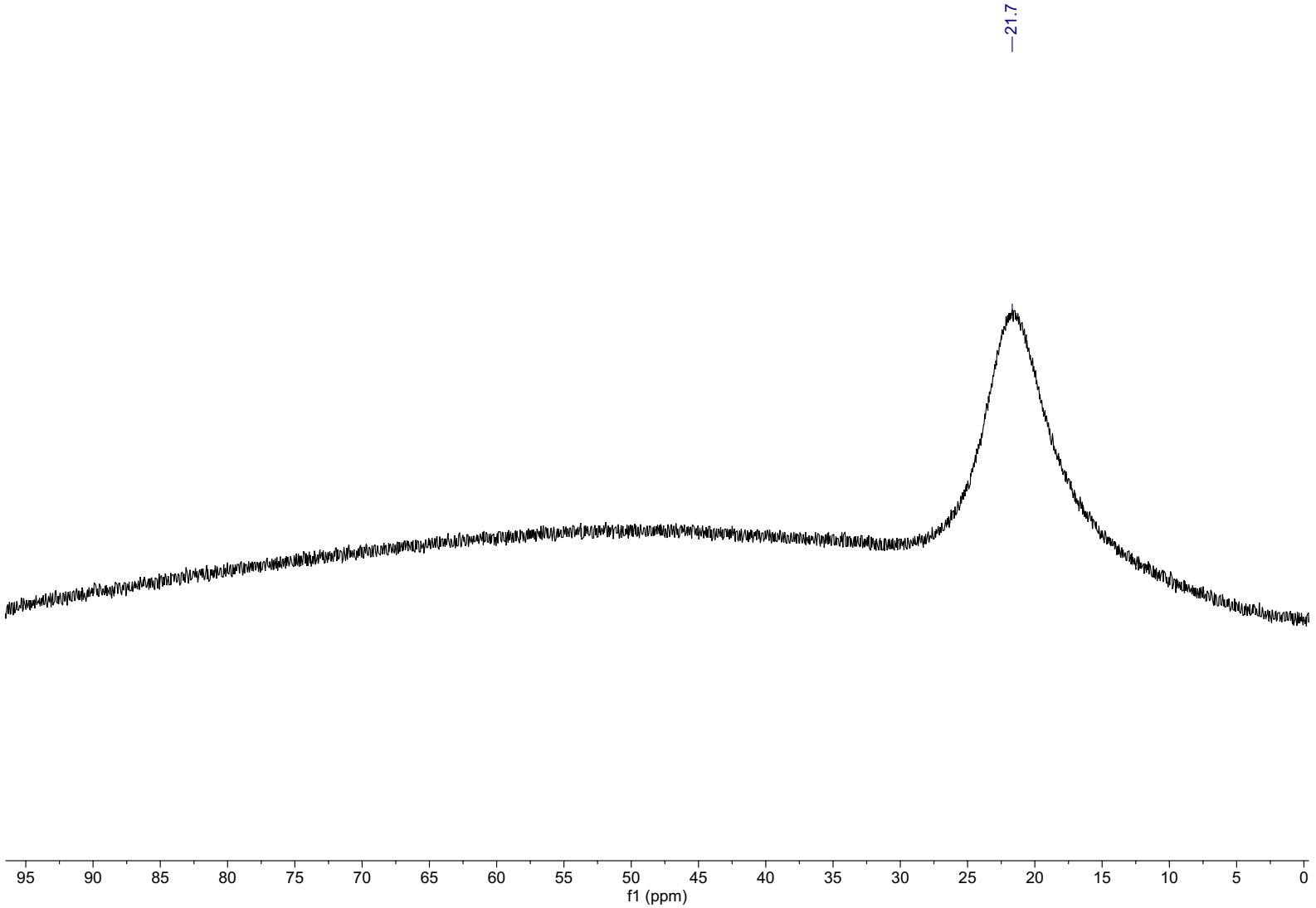


Figure S13: $^{11}B\{^{1}H\}$ NMR spectrum of (^{F}NON)BF (**3-F**) (128 MHz, C_6D_6, 298K).

(^{F}NON)BF (3-F)

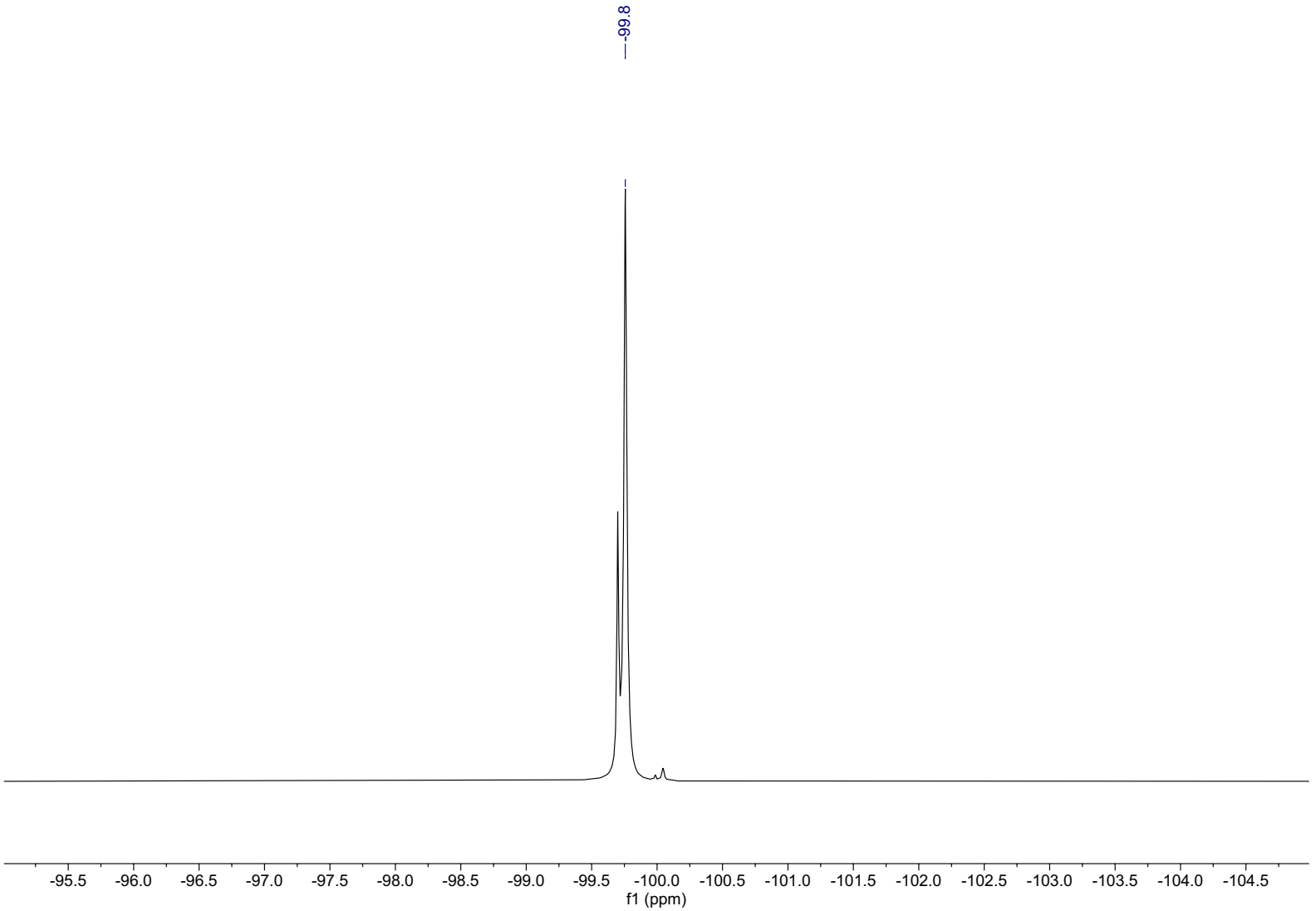


Figure S14: $^{19}F\{^{1}H\}$ NMR spectrum of (^{F}NON)BF (**3-F**) (376 MHz, C_6D_6, 298K).

(^{F}NON)BBr (3-Br)

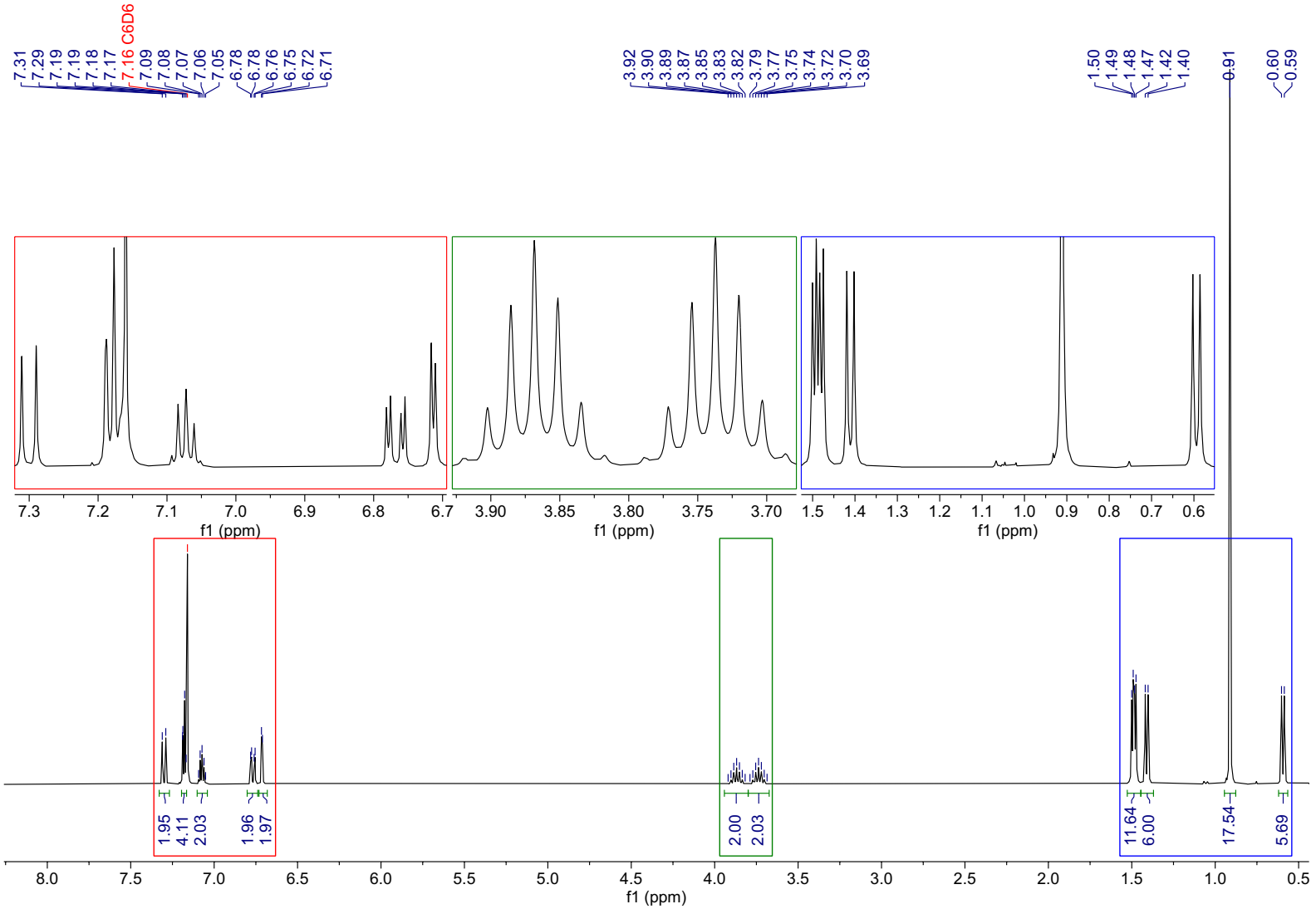


Figure S15: ^{1}H NMR spectrum of (^{F}NON)BBr (**3-Br**) (400 MHz, C_6D_6, 298K).

(^{F}NON)BBr (3-Br)

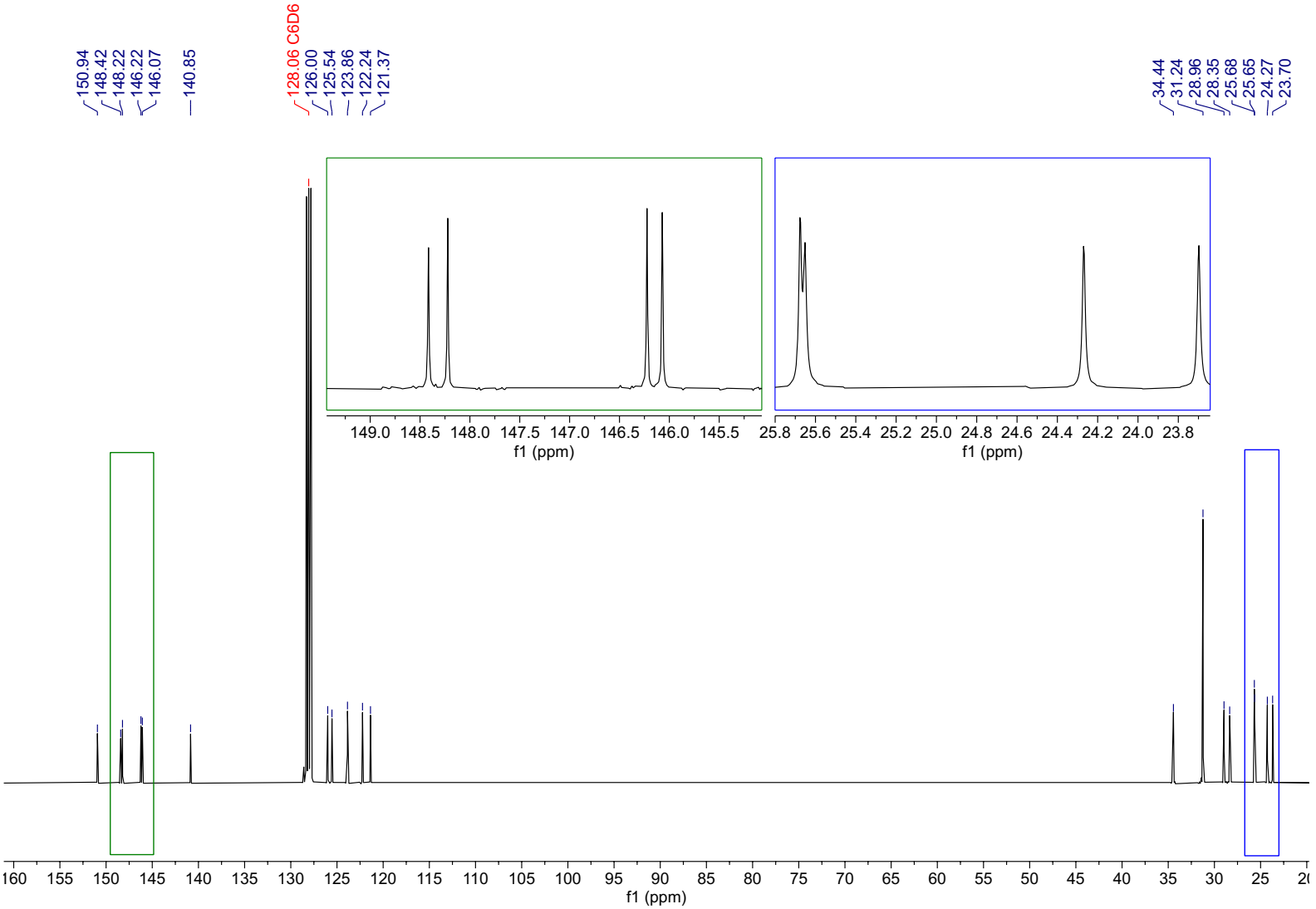


Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of (^{F}NON)BBr (**3-Br**) (101 MHz, C_6D_6, 298K).

(^{F}NON)BBr (3-Br)

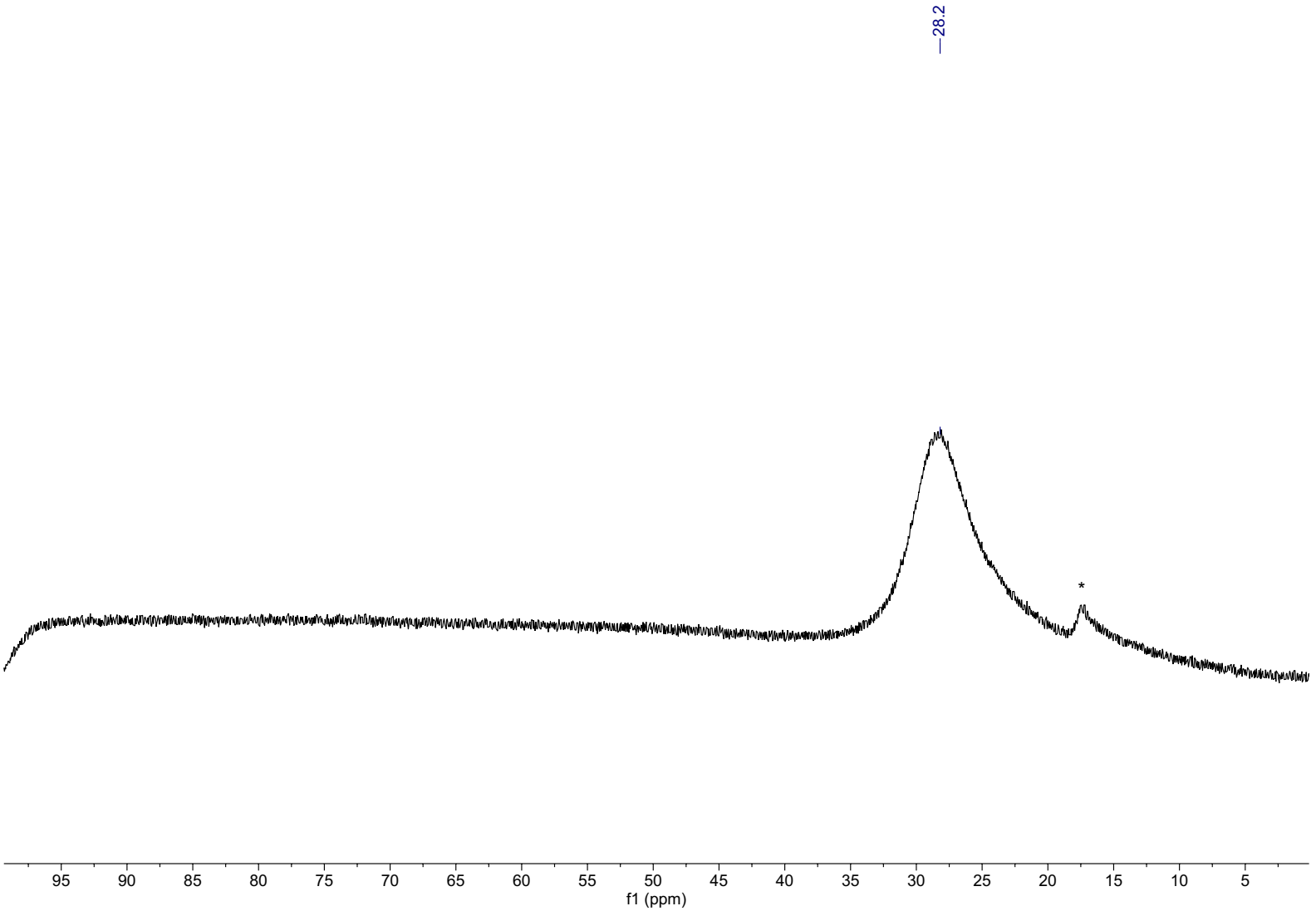


Figure S17: $^{11}B\{^{1}H\}$ NMR spectrum of (^{F}NON)BBr (**3-Br**) (128 MHz, C_6D_6, 298K). * = Unknown boron containing impurity.

C-N activated product (4)

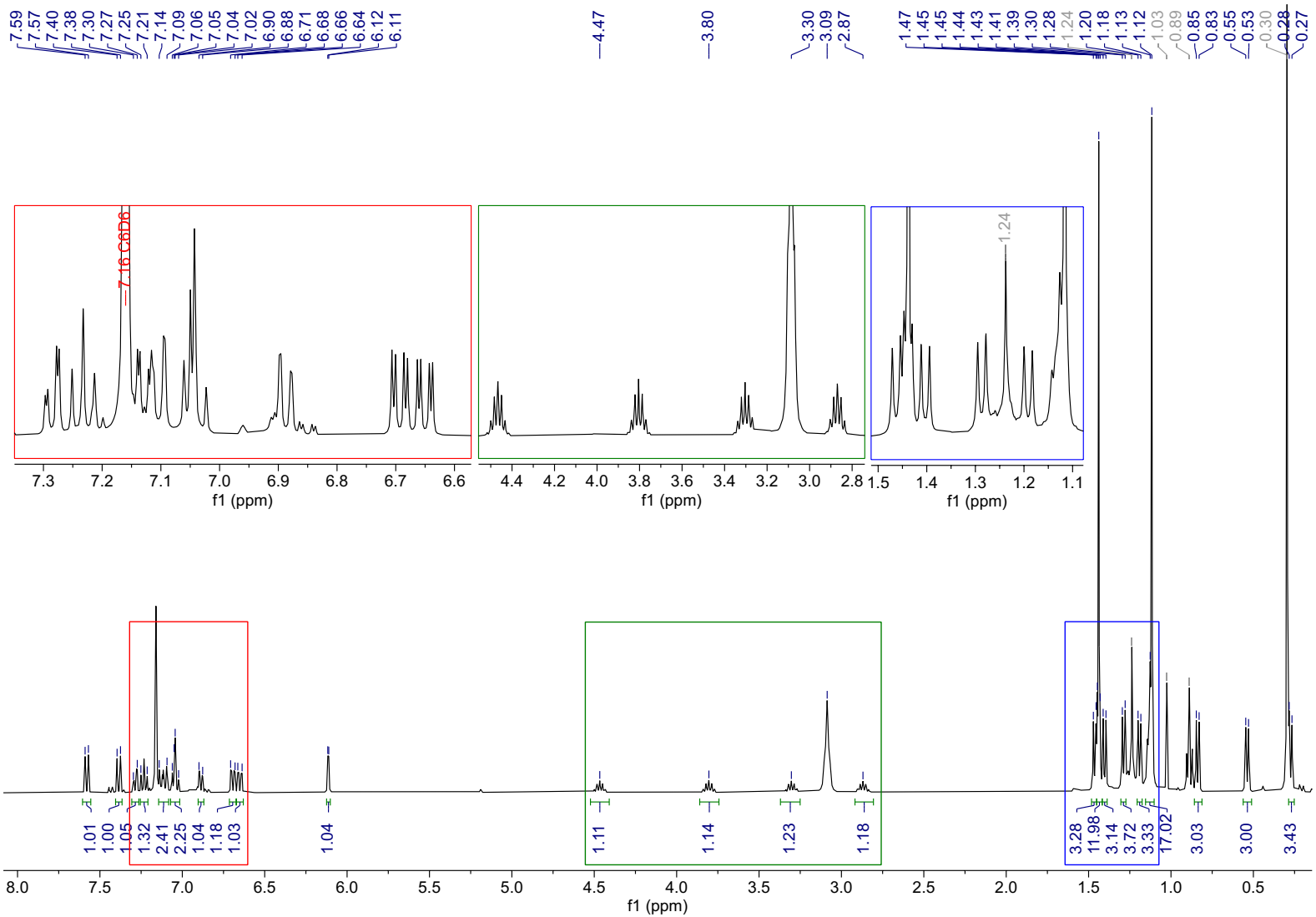


Figure S18: ^{1}H NMR spectrum of **4** (400 MHz, C_6D_6, 298K).

C-N activated product (4)

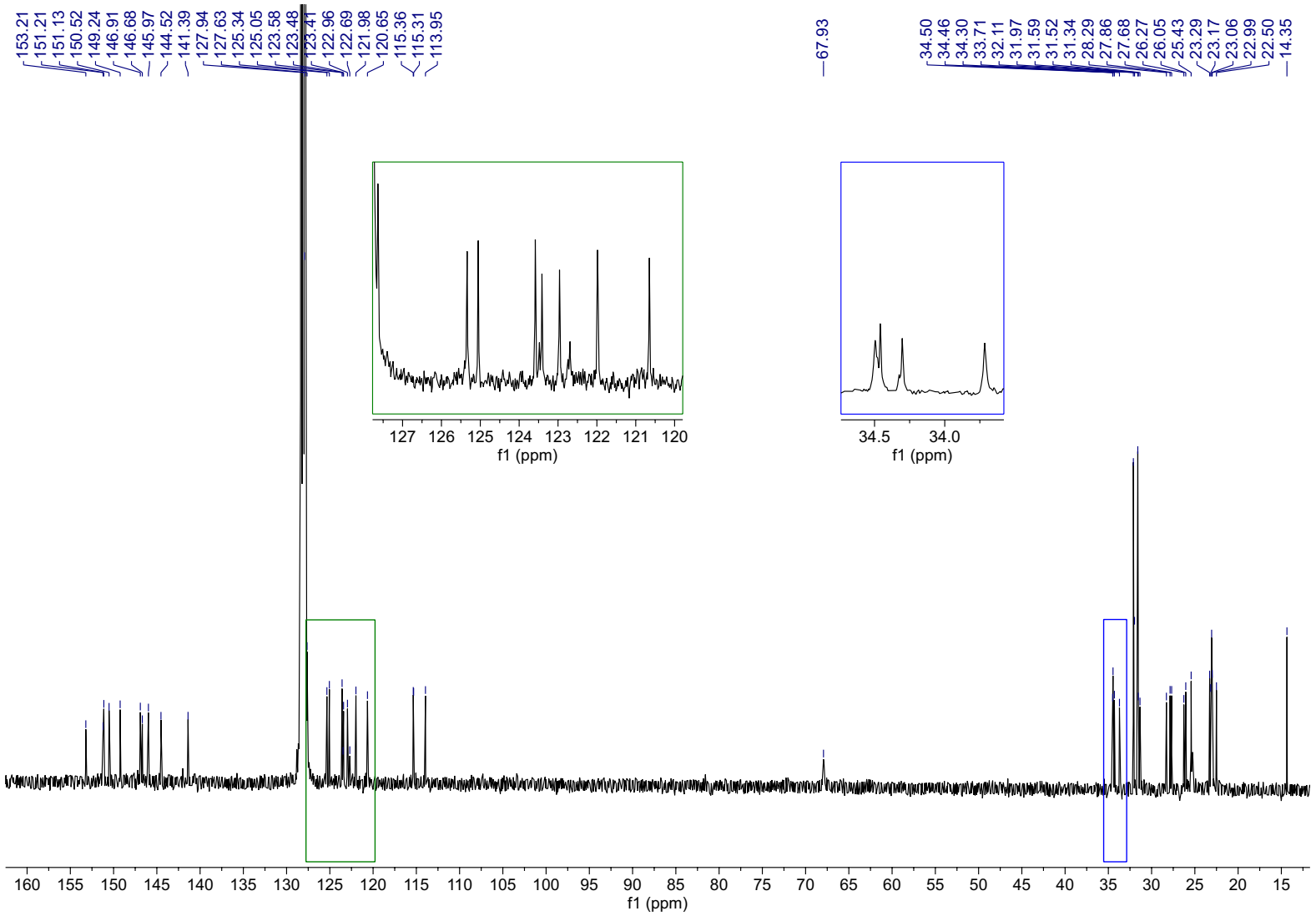


Figure S19: $^{13}C\{^{1}H\}$ NMR spectrum of **4** (101 MHz, C_6D_6, 298K).

C-N activated product (4)

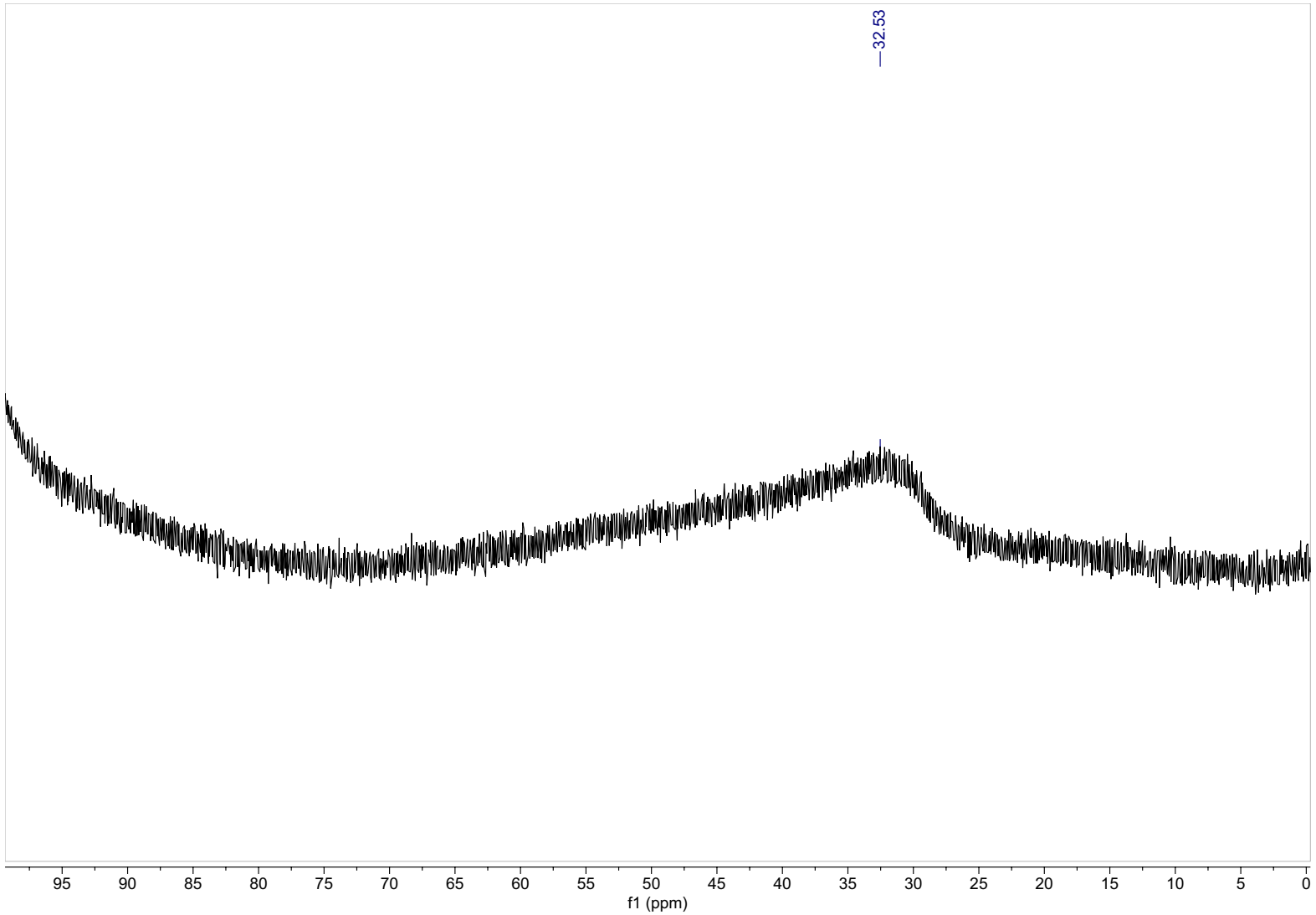


Figure S20: $^{11}B\{^{1}H\}$ NMR spectrum of **4** (128 MHz, C_6D_6, 298K).

[{(ᶠNON)BOCFeCp}$_2$] (5)

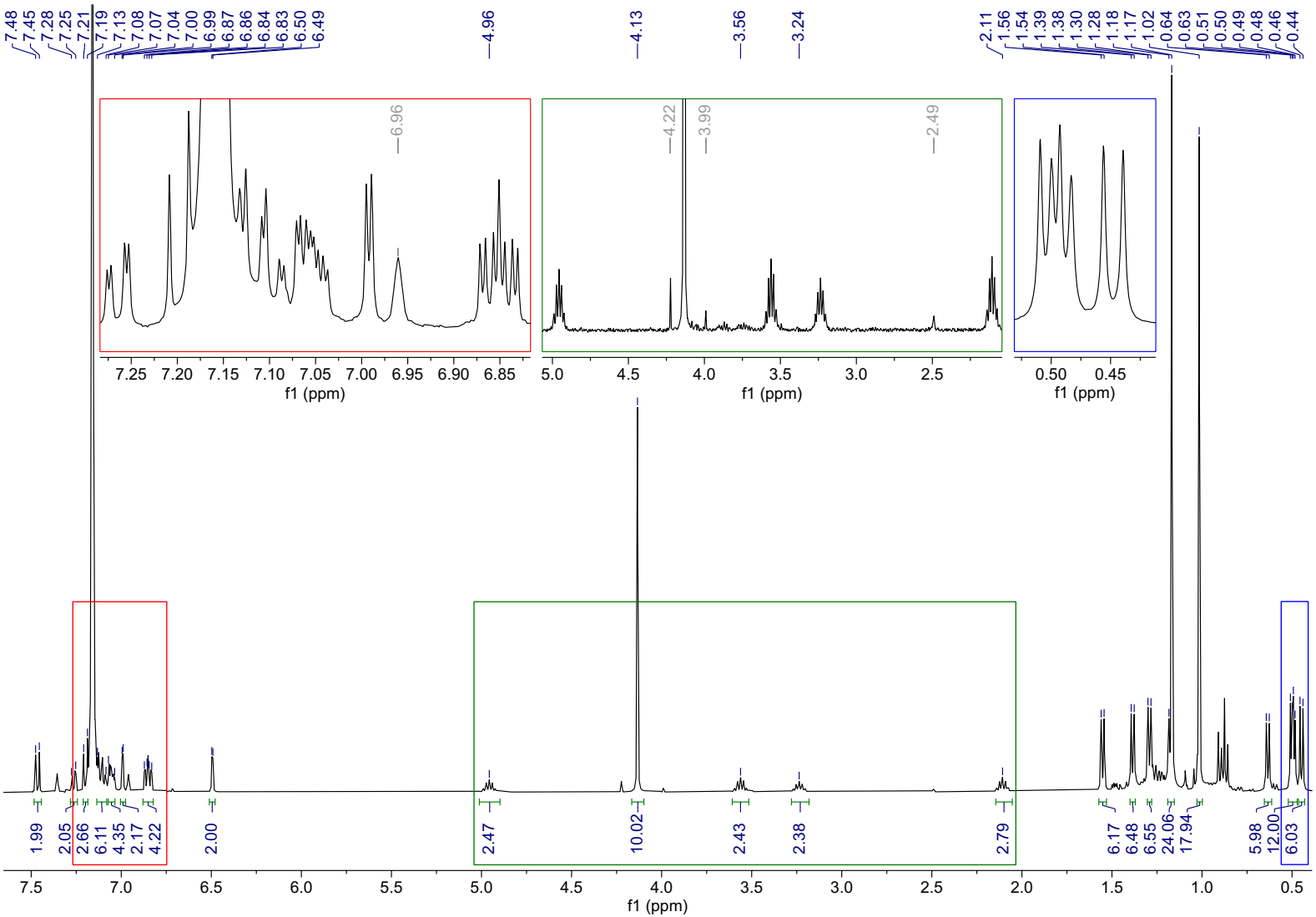


Figure S21: ^{1}H NMR spectrum of **5** (400 MHz, C_6D_6, 298K).

[{(ᶠNON)BOCFeCp}$_2$] (5)

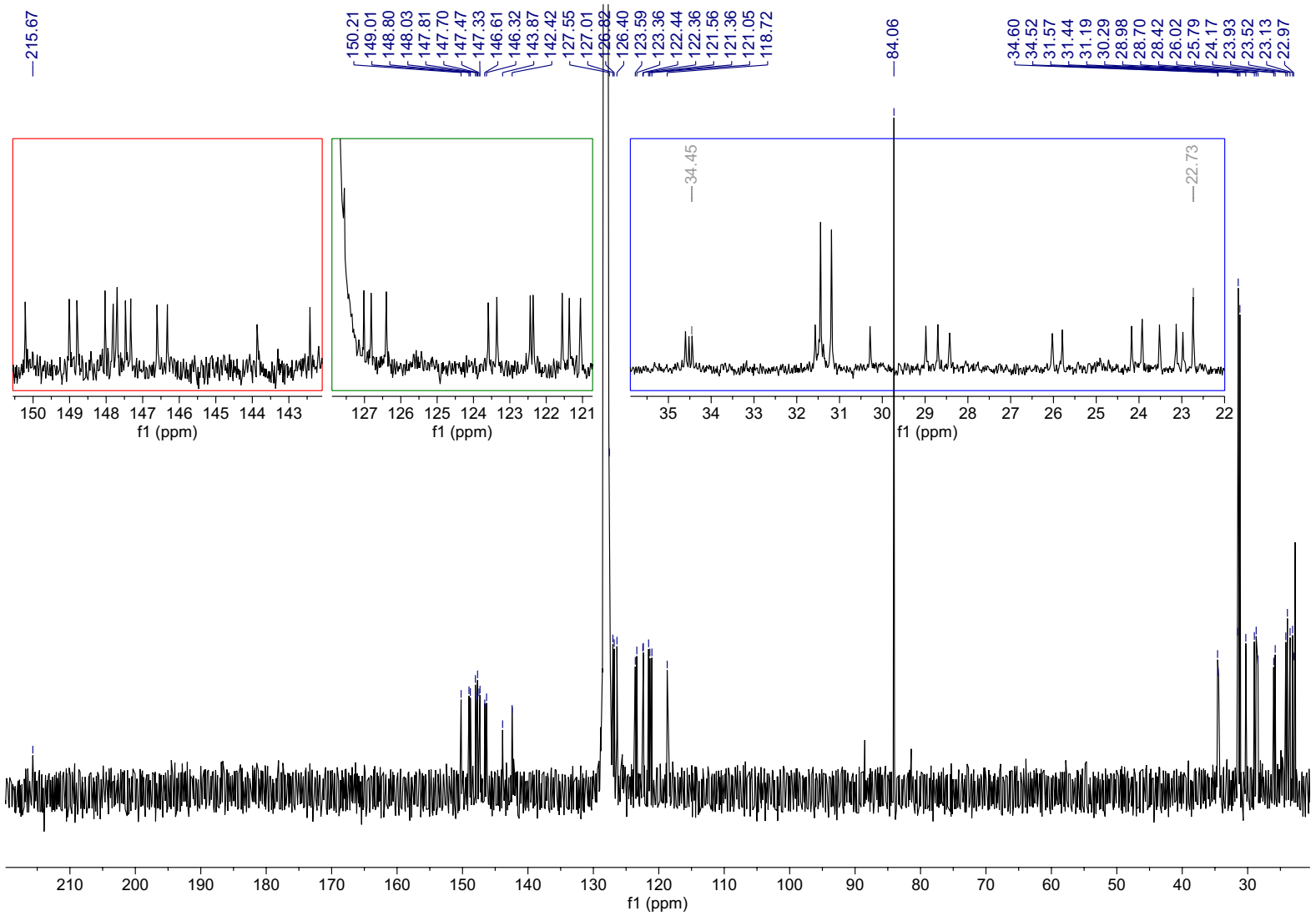


Figure S22: $^{13}C\{^1H\}$ NMR spectrum of **5** (101 MHz, C_6D_6, 298K).

X-ray crystallographic studies

Single-crystal X-ray diffraction data were collected using either a Rigaku Supernova dual-source diffractometer or a Rigaku Xcaliber single-source (Mo) diffractometer. Crystals were selected under Paratone-N oil, mounted on Micromount loops and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device.[S3] Data were collected at 150 K using mirror monochromated Cu K_α (λ = 1.5418 Å) or Mo K_α (λ = 0.71073 Å) radiation. Data collected were processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[S4] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite.[S4] Structures were subsequently solved using SHELXT-2018 and refined on F^2 using the SHELXL 2018 package and the graphical interface Olex2.[S5-S7]

Finalised CIFs for all X-ray diffraction structures (2301629-2301637) have been deposited at the Cambridge Crystallographic Data Centre. These can be obtained free-of-charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Table S1: Crystallographic and refinement parameters for the structures of compounds 4,4'-oxybis(3-bromo-1-tert-butylbenzene), $H_2(^FNON)$, **1** and **2-OEt$_2$**.

	4,4'-oxybis(3-bromo-1-tert-butylbenzene)	**$H_2(^FNON)$**	**$1{\cdot}2C_6H_6$**	**2-OEt$_2$**
Formula	$C_{20}H_{24}Br_2O$	$C_{44}H_{60}N_2O$	$C_{56}H_{70}K_2N_2O$	$C_{48}H_{68}MgN_2O_2$
M	440.21	632.94	865.34	729.35
Cell Setting	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space Group	*Cc*	*C*2/*c*	$P2_1/c$	*P*-1
a/Å	8.75690(10)	70.8297(10)	18.2232(2)	10.7933(6)
b/Å	16.9749(2)	10.40514(14)	9.80740(10)	10.9169(6)
c/Å	12.7839(2)	44.9198(6)	28.2050(6)	19.6634(10)
α/°	90	90	90	99.184(5)
β/°	91.5310(10)	105.4574(14)	99.342(2)	93.750(4)
γ/°	90	90	90	100.054(5)
V/Å^3	1899.62(4)	31908.1(8)	4974.00(13)	2241.7(2)
Z	4	32	4	2
Unique/I > 2σI	2821/2791	31872/23219	9738/8403	7881/4855
R_{int}	0.0183	0.1069	0.0209	0.1072
Parameters	214	1910	552	525
R_1 (all data/ I > 2σI)	0.0214/0.0212	0.0983/0.0686	0.0557/0.0480	0.1249/0.0769
wR_2 (all data/ I > 2σI)	0.0557/0.0555	0.2086/0.1782	0.1385/0.1309	0.2229/0.1889
GooF	1.076	1.055	1.042	0.991
Residual max/min	0.434/-0.370	0.583/-0.427	0.813/-0.553	0.368/-0.525
T/K	150	150	150	150
Radiation, λ (Å)	Cu Kα, (1.54184)	Cu Kα, (1.54184)	Cu Kα, (1.54184)	Mo Kα, (0.71073)
CCDC deposition number	2301629	2301630	2301631	2301632

Table S2: Crystallographic and refinement parameters for the structures of compounds **2-THF**, **3-F**, **3-Br**, **4** and **5.**

	2-THF	**3-F**	**3-Br·C_6H_6**	**4·0.5C_6H_{14}**	**5·3C_6H_6**
Formula	$C_{52}H_{74}MgN_2O_3$	$C_{44}H_{58}BFN_2O$	$C_{50}H_{64}BBrN_2O$	$C_{55}H_{81}BLiN_2O_3$	$C_{118}H_{144}B_2Fe_2N_4O_4$
M	799.44	660.73	799.75	835.96	1815.68
Cell Setting	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic
Space Group	*P2₁/n*	*P*-1	*P*-1	*P2₁/n*	*P*-1
a/Å	15.18110(10)	11.5584(9)	11.0832(8)	11.7476(2)	11.85390(10)
b/Å	11.81750(10)	12.1098(15)	12.2624(9)	17.0185(3)	12.9432(2)
c/Å	27.6540(2)	15.8128(18)	19.3619(17)	26.4191(7)	18.7438(2)
α/°	90	89.601(9)	74.717(7)	90	106.5440(10)
β/°	103.4550(10)	88.022(8)	74.915(7)	97.504(2)	99.3330(10)
γ/°	90	61.747(10)	64.183(7)	90	105.4520(10)
V/Å^3	4825.03(7)	1948.4(4)	2252.7(3)	5236.64(19)	2567.41(6)
Z	4	2	2	4	2
Unique/I > 2σI	10166/8994	7485/6556	9202/7573	10266/7576	10683/9809
R_{int}	0.0405	0.0165	0.0566	0.0255	0.0416
Parameters	568	487	542	677	600
R_1 (all data/ I > 2σI)	0.0437/0.0389	0.0484/0.0420	0.0785/0.0614	0.0870/0.0649	0.0421/0.0384
wR_2 (all data/ I > 2σI)	0.1077/0.1039	0.1047/0.0990	0.1437/0.1358	0.1855/0.1682	0.0972/0.0955
GooF	1.054	1.029	1.055	1.026	1.071
Residual max/min	0.220/-0.255	0.232/-0.377	0.712/-0.678	0.482/-0.414	0.221/-0.369
T/K	150	150	150	150	150
Radiation, λ (Å)	Cu Kα, (1.54184)	Cu Kα, (1.54184)	Cu Kα, (1.54184)	Cu Kα, (1.54184)	Cu Kα, (1.54184)
CCDC deposition number	2301633	2301634	2301635	2301636	2301637

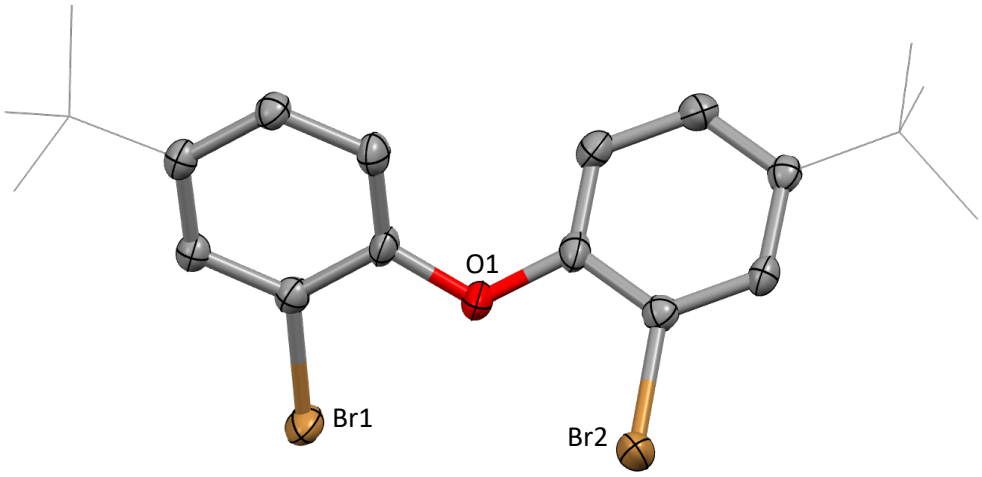


Figure S23: Molecular structure of 4,4'-oxybis(3-bromo-1-tert-butylbenzene) as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

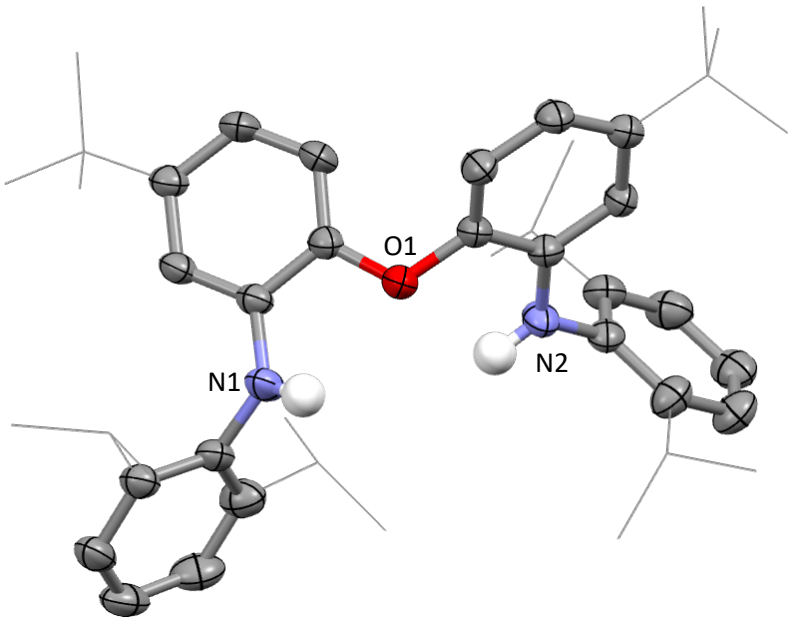


Figure S24: Molecular structure of H_2(^{F}NON) as determined by X-ray crystallography. Non-coordinating solvent molecules and most hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

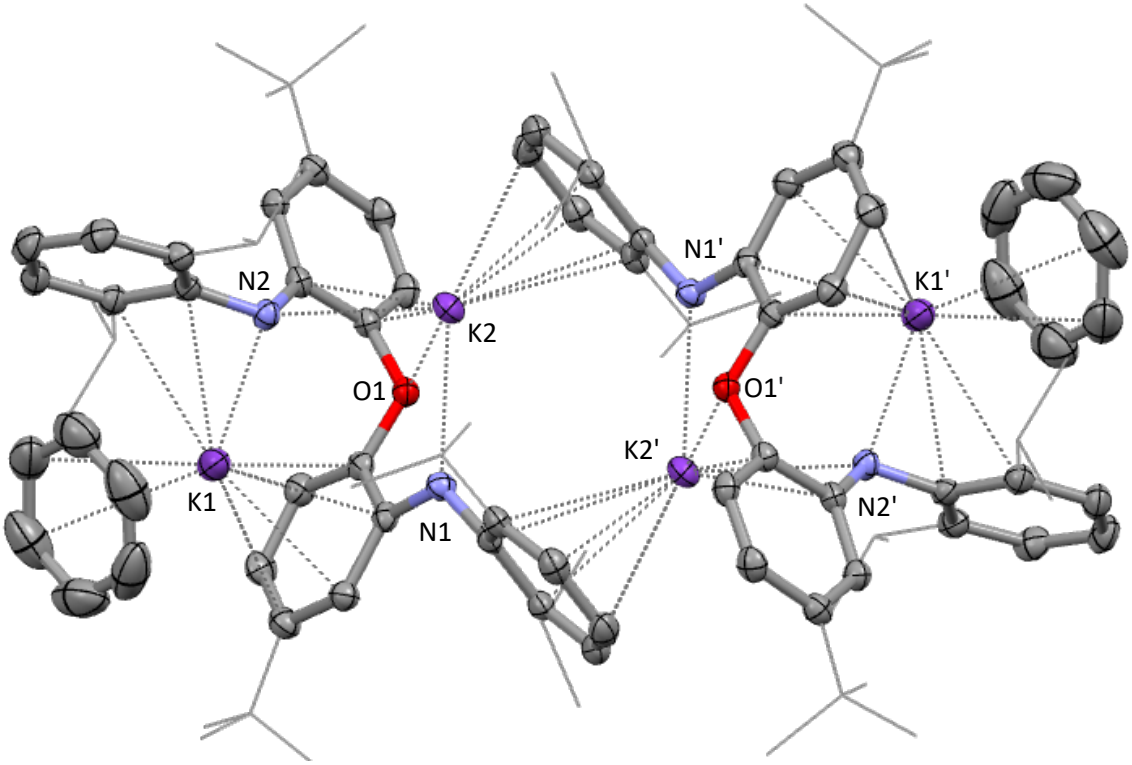


Figure S25: Molecular structure of **1** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

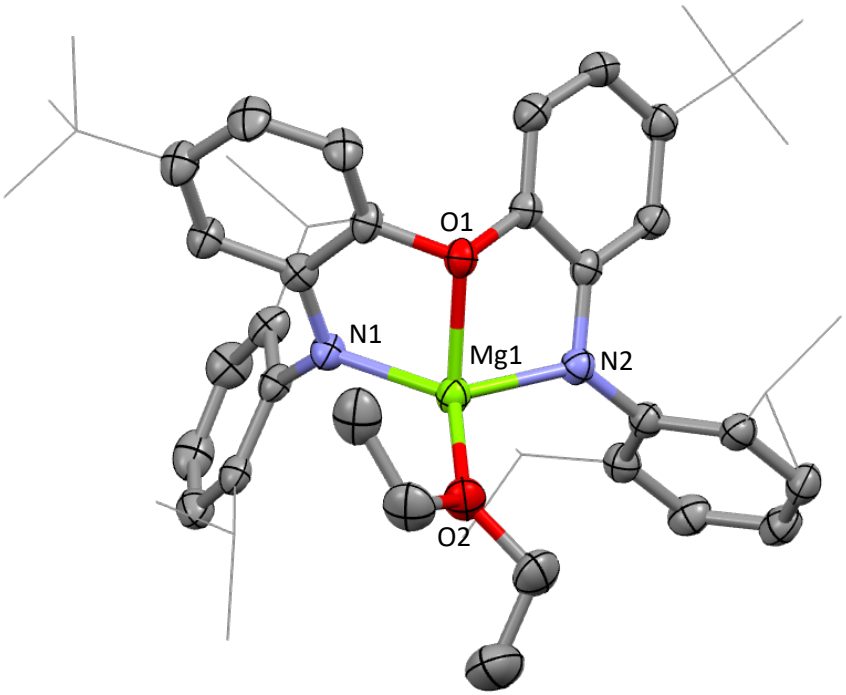


Figure S26: Molecular structure of **2-OEt$_2$** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

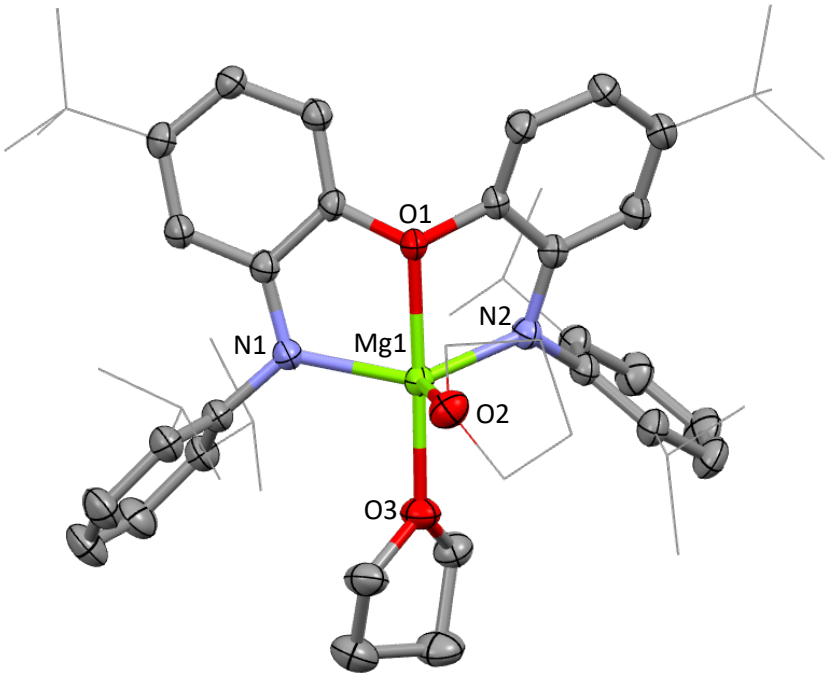


Figure S27: Molecular structure of **2-THF** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl, *iso*-propyl groups and one coordinated THF molecule have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

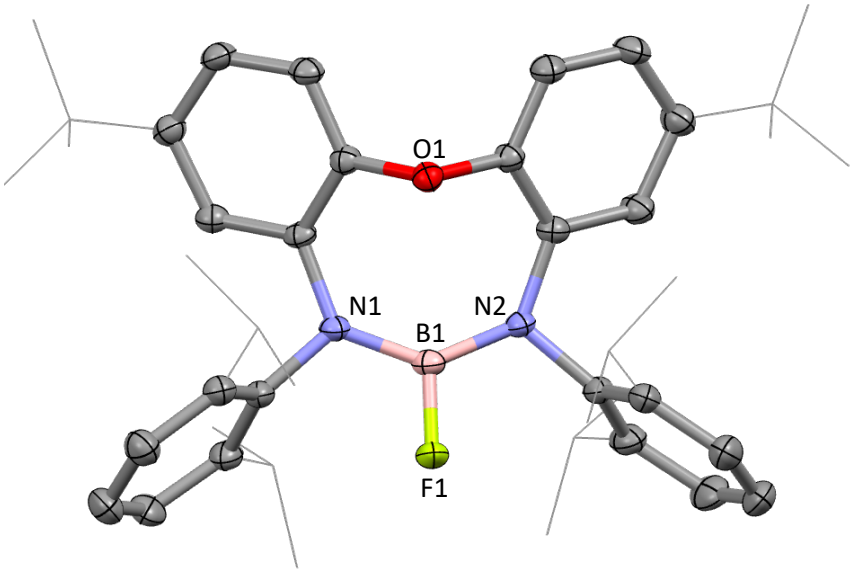


Figure S28: Molecular structure of **3-BF** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

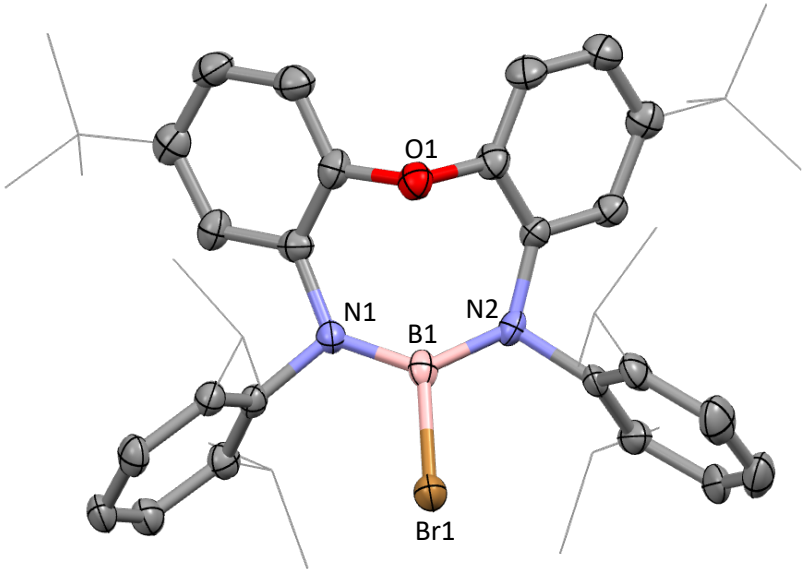


Figure S29: Molecular structure of **3-Br** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

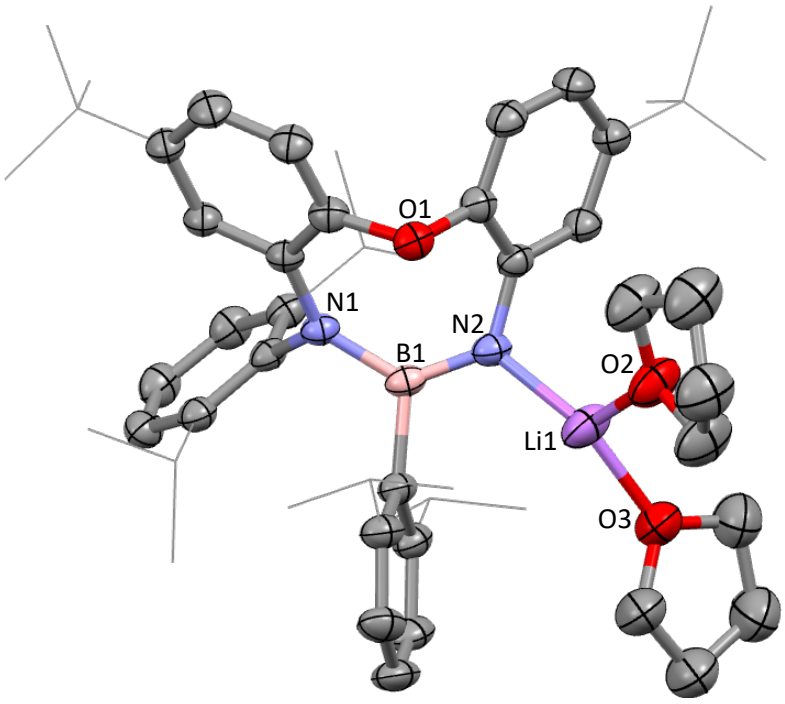


Figure S30: Molecular structure of **4** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

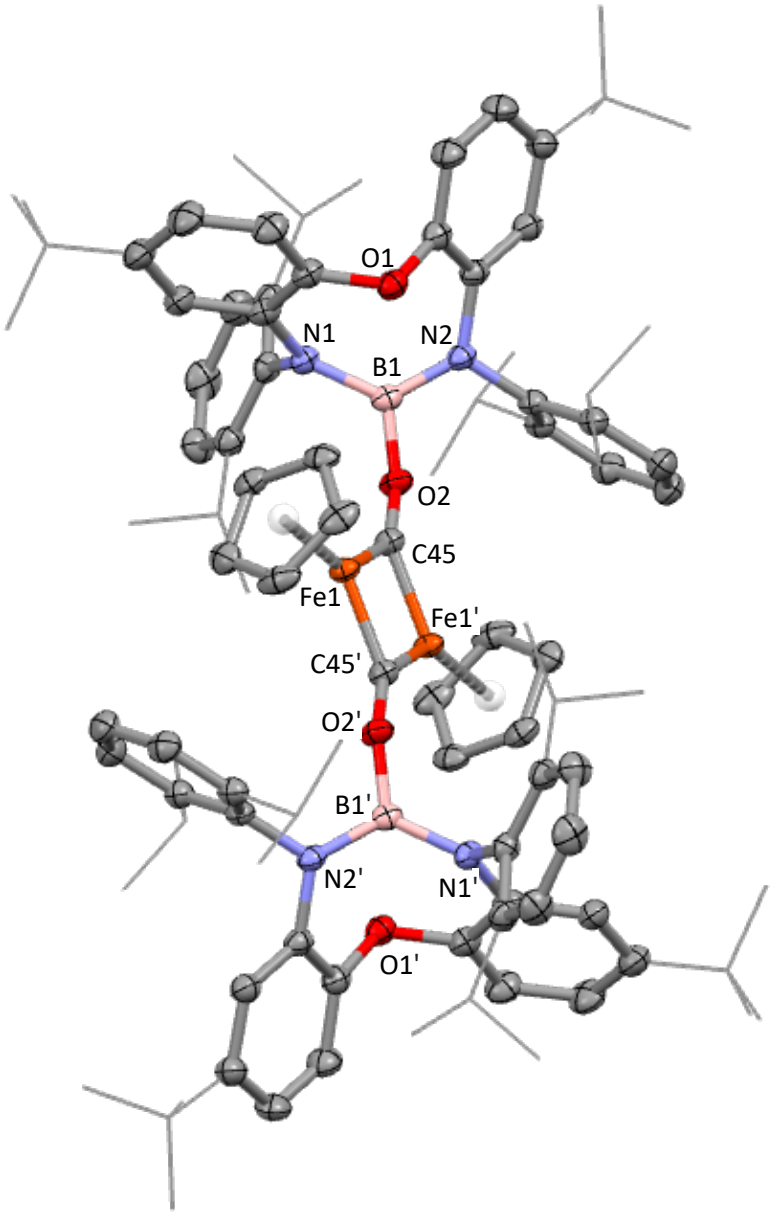


Figure S31: Molecular structure of **5** as determined by X-ray crystallography. Non-coordinating solvent molecules and hydrogen atoms have been removed, and *tert*-butyl and *iso*-propyl groups have been displayed in wireframe for clarity. Displacement ellipsoids set at the 50% probability level.

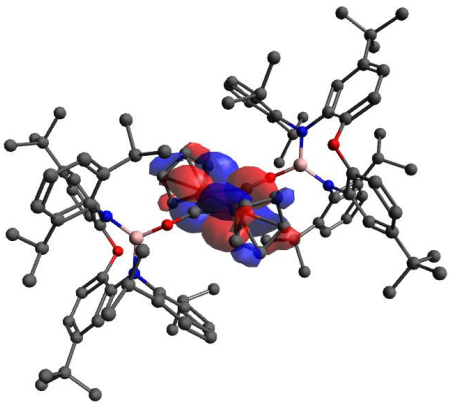
Computational details

Density functional theory (DFT) calculations for geometry optimisation were performed using the Gaussian 16 program[S8] using the PBE0 hybrid density functional approximation[S9] with Grimme's D3 dispersion correction with Becke-Johnson dampening[S10] and the def2-SVP basis set[S11] and the ultrafine integration grid. The structures were confirmed as minima on the potential energy surface *via* analytical frequency calculations, yielding no negative eigenvalues, except for the insertion transition state which was verified as a saddle point on the potential energy surface with a single negative eigenvalue. The corresponding imaginary stretching frequency was verified as the reaction coordinate *via* the intrinsic reaction coordinate method. Thermochemical properties were calculated using the hessian matrix from these analytical frequency calculations with the "freqchk" utility program accompanying Gaussian 16/C.01, with a pressure of 1.0 atmospheres, unscaled stretching frequencies, and a temperature of 193.65 K, that of a dry-ice/acetone bath.

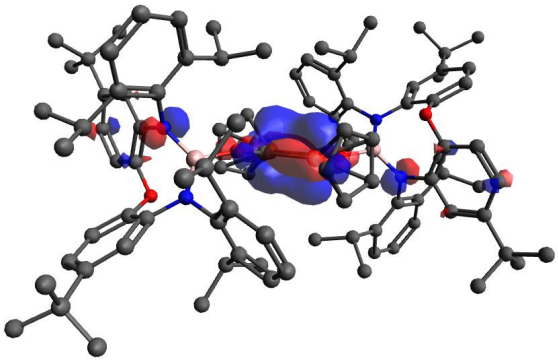
Single point calculations were performed in the ORCA 5.0.4 program[S12] using Libint[S13] and with functional data from libXC.[S14] The functional was chosen per recent reviews,[S15] specifically for main-group reaction barrier heights, to be the nonempirical double-hybrid DSD-PBEP86-D3BJ[S16] with RIJCOSX resolution of the identity approximation[S17] with a CPCM solvent correction (tetrahydrofuran)[S18] and with Grimme's D3 dispersion correction with Becke-Johnson dampening,[S10] frozen-core approximation for the MP2-part of the double-hybrid, using the def2-QZVPP basis set for orbitals,[S19] the def2/J basis set for coulomb auxiliary basis,[S20] and the def2-QZVPP/C for correlation auxiliary basis.[S21] Final energies were obtained by adding the free energy correction from the thermochemical properties calculated (*vide supra*) to the electronic energies from the just described method.

For the C–N bond activation mechanism, the starting point for the boryl anion (**B'**) optimisation was taken from the solid-state structure of the corresponding fluoride complex by removing errant solvent molecules and the fluoride, then optimising the geometry for the singlet monoanion. The starting point for the inserted product was taken from the correspondingly lithiated solid-state structure, again removing errant solvent molecules and the lithium with coordinated THF molecules. For computational efficiency, the *tert*-butyl moieties were truncated to methyl groups in each case. The transition state geometry was found by scanning along a decreasing B-C distance and optimising to a saddle point from the highest energy point along the scan coordinate.

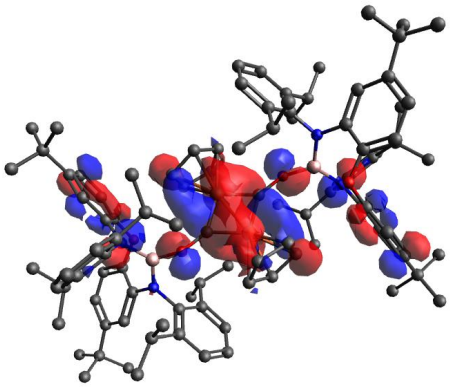
Complex **5** was probed using Gaussian 16/C.01 at the PBE0-D3BJ/def2-TZVP//PVE0-D3BJ/def2-SVP level of theory and the ultrafine integration grid, it was verified as a minimum on the potential energy surface *via* analytical frequency calculations, yielding no negative eigenvalues, no thermodynamic entropic properties were investigated for this complex, and no *in silico* truncation of the molecule was performed.



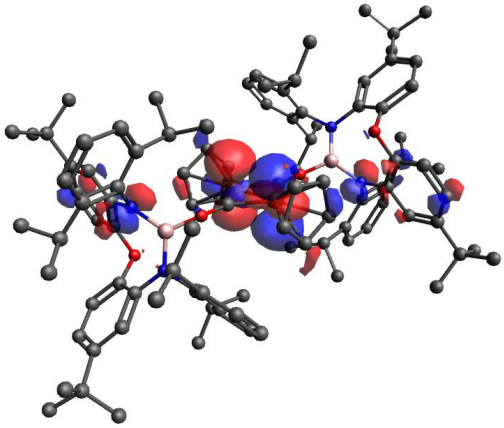
HOMO



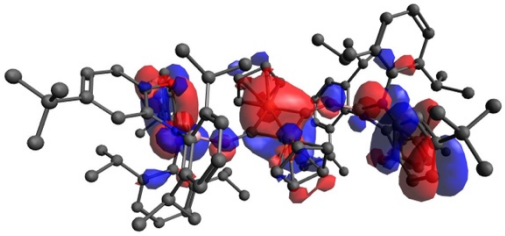
HOMO-1



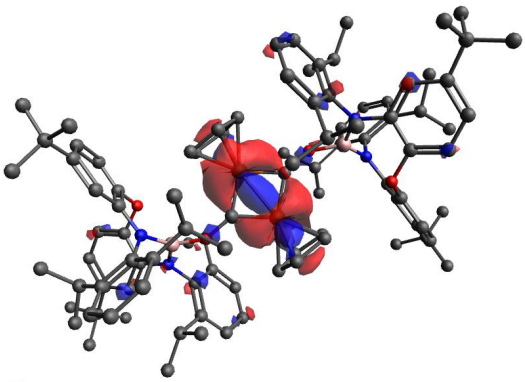
HOMO-2



HOMO-4



HOMO-6



HOMO-21

Figure S32: Selected molecular orbitals of the model complex **5**. Isosurface value = 0.04.

Cartesian Coordinates and Computed Energies (Hartrees):

Boryl (B')

Nuclear Repulsion : 5343.27008906
Electronic Energy : -7022.48469083
One Electron Energy: -12953.34533385
Two Electron Energy: 5930.86064302
Max COSX asymmetry : 0.00000412
CPCM Dielectric : -0.06706212
Virial components:
Potential Energy : -3353.13600135
Kinetic Energy : 1673.92139957
Virial Ratio : 2.00316216
DFT components:
N(Alpha) : 150.999676552321 electrons
N(Beta) : 150.999676552321 electrons
N(Total) : 301.999353104642 electrons
E(X) : -71.441785922516
E(C) : -4.749610458321
E(XC) : -76.191396380837
CPCM Solvation Model Properties:
Surface-charge : 0.94331007
Charge-correction : -0.00462592
Dispersion: -0.073377861374
RI-MP2 CORRELATION ENERGY: -3.879305853
Total single point energy: -1683.167285486163
Thermal correction: 0.677739
Total free energy: -1682.506822

O	-0.113400	-2.498100	0.757300
N	1.265900	-0.083700	0.242700
N	-1.283700	-0.103900	0.079200
C	1.474200	-1.236200	-0.533300
C	-2.056000	-1.232700	0.155500
C	0.700300	-2.395000	-0.344800
C	-1.470500	-2.456000	0.548000
C	-3.447700	-1.202700	-0.035700
H	-3.901500	-0.254800	-0.333200
C	2.414400	-1.237600	-1.574900
H	3.032700	-0.344900	-1.702300

C	2.568300	-2.320600	-2.441300
C	0.836300	-3.477500	-1.207000
H	0.216900	-4.359600	-1.027800
C	-4.239000	-2.336900	0.173400
C	-2.245700	-3.582600	0.757200
H	-1.746500	-4.502700	1.070600
C	1.755500	-3.444700	-2.253100
H	1.849600	-4.304600	-2.922000
C	-3.632700	-3.529500	0.577200
H	-4.239900	-4.422500	0.747100
B	-0.046200	0.500900	0.400000
C	-1.747600	1.258000	-0.067400
C	-3.385100	3.539600	-0.599600
C	-2.591700	1.835800	0.966400
C	-1.900600	1.777800	-1.416700
C	-2.668000	2.914900	-1.626000
C	-3.339400	2.963900	0.679700
H	-2.728100	3.329600	-2.637400
H	-3.926700	3.419800	1.483700
H	-3.994300	4.424500	-0.796500
C	2.416000	0.622000	0.691000
C	4.702400	1.939900	1.622800
C	2.761700	1.881700	0.153600
C	3.210800	0.026500	1.696200
C	4.355500	0.696300	2.137800
C	3.901900	2.524400	0.646700
H	4.976200	0.240000	2.914000
H	4.172500	3.504500	0.245000
H	5.594800	2.457600	1.985300
C	-2.496100	1.281300	2.372400
H	-2.257800	0.209000	2.287000
C	-1.327200	1.946800	3.104000
H	-1.555100	3.006900	3.304200
H	-0.425100	1.893900	2.465200
H	-1.102300	1.450600	4.063600
C	-3.790000	1.376200	3.170600
H	-4.076100	2.422600	3.367800
H	-3.678700	0.881200	4.149700
H	-4.622600	0.896000	2.632300
C	-1.155000	1.102100	-2.551300
H	-0.239700	0.663400	-2.112600

C	-0.705500	2.062200	-3.649600
H	-0.164900	2.924900	-3.232700
H	-1.561400	2.451800	-4.224900
H	-0.040800	1.549600	-4.364200
C	-1.936800	-0.062500	-3.164600
H	-2.871500	0.303400	-3.622100
H	-2.207200	-0.810200	-2.407200
H	-1.345700	-0.571200	-3.946000
C	1.945300	2.547100	-0.935300
H	1.233800	1.794100	-1.301400
C	2.810200	2.987500	-2.115500
H	3.505200	3.798600	-1.842600
H	2.174500	3.362700	-2.932700
H	3.411000	2.152500	-2.510400
C	1.110600	3.697700	-0.376100
H	1.751300	4.470200	0.082100
H	0.412500	3.305700	0.379000
H	0.511000	4.169900	-1.170100
C	2.825700	-1.303200	2.315700
H	1.805400	-1.534500	1.979700
C	2.778700	-1.230700	3.841100
H	2.111000	-0.422300	4.175300
H	3.774000	-1.050600	4.279900
H	2.401300	-2.178600	4.257400
C	3.741800	-2.429800	1.836700
H	4.784500	-2.255000	2.152200
H	3.727600	-2.510000	0.739600
H	3.419500	-3.398700	2.251400
C	3.552500	-2.253200	-3.575200
H	3.826900	-3.257400	-3.931500
H	4.474900	-1.732400	-3.276600
H	3.132600	-1.702000	-4.433800
C	-5.725700	-2.251900	-0.033000
H	-6.172900	-1.478000	0.611700
H	-6.220100	-3.208500	0.191800
H	-5.969500	-1.979900	-1.072900

Boryl Insertion Transition State

Nuclear Repulsion : 5343.27008906
Electronic Energy : -7022.48469083

One Electron Energy: -12953.34533385
Two Electron Energy: 5930.86064302
Max COSX asymmetry : 0.00000412
CPCM Dielectric : -0.06706212
Virial components:
Potential Energy : -3353.13600135
Kinetic Energy : 1673.92139957
Virial Ratio : 2.00316216
DFT components:
N(Alpha) : 150.999676552321 electrons
N(Beta) : 150.999676552321 electrons
N(Total) : 301.999353104642 electrons
E(X) : -71.441785922516
E(C) : -4.749610458321
E(XC) : -76.191396380837
DFET-embed. en. : 0.000000000000
CPCM Solvation Model Properties:
Surface-charge : 0.94331007
Charge-correction : -0.00462592
Dispersion: -0.073377861
RI-MP2 CORRELATION ENERGY: -3.879305853
Total single point energy: -1683.167285
Thermal correction: 0.676889
Total free energy: -1682.490396

O	-0.014800	2.413900	-1.023400
N	1.309400	0.073300	-0.436600
N	-1.206700	-0.016700	-0.385300
C	1.358000	1.147300	0.464000
C	-1.977000	1.098000	-0.600800
C	0.592800	2.295200	0.202300
C	-1.386600	2.320000	-1.012500
C	-3.388900	1.094500	-0.508800
H	-3.880200	0.181300	-0.166200
C	2.101300	1.106900	1.650500
H	2.727600	0.230800	1.836000
C	2.035300	2.129300	2.600300
C	0.508200	3.317000	1.139500
H	-0.115000	4.184200	0.908800
C	-4.168100	2.200500	-0.852000
C	-2.149600	3.417100	-1.366800

H	-1.622400	4.322000	-1.679700
C	1.214600	3.232300	2.339000
H	1.136900	4.038600	3.073800
C	-3.546700	3.368300	-1.308400
H	-4.143100	4.237700	-1.596100
B	0.103800	-0.532200	-0.980900
C	-1.841200	-1.160000	0.187900
C	-3.065500	-3.375000	1.385100
C	-2.426200	-2.159900	-0.625000
C	-1.898200	-1.254700	1.598200
C	-2.514200	-2.373500	2.173400
C	-3.021200	-3.258900	-0.005300
H	-2.560200	-2.457200	3.263000
H	-3.466900	-4.041500	-0.626300
H	-3.539500	-4.244200	1.849900
C	2.546900	-0.576300	-0.708600
C	5.015800	-1.787800	-1.212500
C	2.859200	-1.805700	-0.087000
C	3.473100	0.052600	-1.565500
C	4.702400	-0.569400	-1.804300
C	4.095000	-2.396900	-0.363900
H	5.423900	-0.091600	-2.473600
H	4.343000	-3.355800	0.100000
H	5.979100	-2.265700	-1.412200
C	-2.455500	-2.035800	-2.134100
H	-1.866500	-1.138700	-2.380100
C	-1.736700	-3.202000	-2.803700
H	-2.197200	-4.174200	-2.558700
H	-0.685600	-3.198600	-2.477400
H	-1.755300	-3.087900	-3.900200
C	-3.882200	-1.867900	-2.657100
H	-4.506400	-2.751500	-2.440800
H	-3.874200	-1.726200	-3.750600
H	-4.370800	-0.989400	-2.209200
C	-1.333200	-0.156700	2.478000
H	-0.693000	0.462600	1.835000
C	-0.462700	-0.685100	3.614700
H	0.345900	-1.325100	3.233300
H	-1.043200	-1.271400	4.346400
H	-0.000100	0.155100	4.156800
C	-2.442400	0.750400	3.013400

H	-3.130000	0.190400	3.670500
H	-3.030800	1.180100	2.189600
H	-2.014700	1.583700	3.594800
C	1.887200	-2.489200	0.854400
H	1.088800	-1.761900	1.065400
C	2.534200	-2.883300	2.180500
H	3.311100	-3.654400	2.049100
H	1.776100	-3.298100	2.864100
H	3.003800	-2.020100	2.678800
C	1.211500	-3.679800	0.178100
H	1.944600	-4.459700	-0.090400
H	0.703900	-3.318000	-0.729600
H	0.452400	-4.124300	0.842600
C	3.136800	1.369400	-2.235600
H	2.072300	1.563700	-2.044000
C	3.306100	1.295800	-3.751500
H	2.704400	0.473900	-4.167700
H	4.356600	1.132100	-4.044800
H	2.973500	2.235300	-4.222000
C	3.937800	2.521800	-1.629900
H	5.020800	2.384700	-1.791000
H	3.762800	2.593200	-0.545700
H	3.646000	3.482800	-2.084300
C	2.805000	2.014600	3.886100
H	2.768300	2.950300	4.463300
H	3.862900	1.769900	3.701100
H	2.396400	1.212500	4.523600
C	-5.664200	2.126000	-0.712300
H	-6.059200	1.177100	-1.108600
H	-6.159700	2.949900	-1.247500
H	-5.971300	2.184400	0.346000

C–N activated product (4')

Nuclear Repulsion : 5359.31835964
Electronic Energy : -7038.65048425
One Electron Energy: -12987.07658931
Two Electron Energy: 5948.42610506
Max COSX asymmetry : 0.00000687
CPCM Dielectric : -0.07023797
Virial components:

Potential Energy : -3353.37876793
Kinetic Energy : 1674.04664332
Virial Ratio : 2.00315731
DFT components:
N(Alpha) : 150.999861457579 electrons
N(Beta) : 150.999861457579 electrons
N(Total) : 301.999722915158 electrons
E(X) : -71.455465462264
E(C) : -4.749879190027
E(XC) : -76.205344652291
CPCM Solvation Model Properties:
Surface-charge : 0.94422670
Charge-correction : -0.00470210
Dispersion: -0.075817978
RI-MP2 CORRELATION ENERGY: -3.869564091
Total single point energy: -1683.277507
Thermal correction: 0.68302
Total free energy: -1682.594487

O	-2.190300	1.346700	-1.053200
N	0.282100	0.636600	0.231500
N	-1.553100	-1.148500	0.013600
C	-0.597300	1.612200	0.740900
C	-2.812100	-0.828800	-0.275200
C	-1.831100	1.915400	0.138900
C	-3.179400	0.387600	-0.924700
C	-3.907100	-1.702300	-0.020900
H	-3.683600	-2.633800	0.506100
C	-0.227300	2.361300	1.867700
H	0.748700	2.154600	2.310800
C	-1.039800	3.347000	2.427300
C	-2.664000	2.882000	0.699800
H	-3.617800	3.077900	0.205100
C	-5.209700	-1.445900	-0.449100
C	-4.458000	0.651100	-1.379500
H	-4.642100	1.597300	-1.896800
C	-2.281200	3.594000	1.830900
H	-2.945600	4.357700	2.245700
C	-5.487200	-0.271700	-1.162100
H	-6.498400	-0.069100	-1.525600
B	-0.243200	-0.743800	-0.053600

C	0.819500	-1.935600	-0.311300
C	2.491300	-4.177300	-0.774400
C	1.628900	-2.015500	-1.464600
C	0.853000	-3.024600	0.601400
C	1.686300	-4.120200	0.358900
C	2.453700	-3.127600	-1.682800
H	1.705600	-4.951100	1.070200
H	3.068700	-3.177100	-2.585700
H	3.139700	-5.040500	-0.950900
C	1.606500	1.122800	0.025200
C	4.169400	2.233000	-0.383100
C	2.709500	0.671400	0.786800
C	1.809500	2.139400	-0.951800
C	3.083700	2.679600	-1.127100
C	3.972300	1.232700	0.557400
H	3.228700	3.463400	-1.875200
H	4.820200	0.880700	1.150600
H	5.163400	2.661000	-0.537800
C	1.561300	-0.948000	-2.540200
H	1.028700	-0.089000	-2.108200
C	2.944200	-0.471100	-2.975800
H	3.517500	-1.277700	-3.461300
H	3.523500	-0.108600	-2.113700
H	2.869500	0.354300	-3.700600
C	0.723700	-1.434600	-3.723100
H	1.188200	-2.310900	-4.205500
H	0.616900	-0.643900	-4.484700
H	-0.283100	-1.725600	-3.388000
C	-0.043600	-3.071200	1.830200
H	-0.492600	-2.073600	1.942800
C	0.689500	-3.416900	3.124600
H	1.492700	-2.697800	3.343400
H	1.141000	-4.422300	3.095300
H	-0.013400	-3.401700	3.973600
C	-1.203100	-4.034000	1.579800
H	-0.841200	-5.068200	1.449100
H	-1.735000	-3.723600	0.670400
H	-1.915300	-4.024100	2.422100
C	2.592200	-0.362900	1.888700
H	1.576200	-0.775000	1.840800
C	2.775400	0.263900	3.272400

H	3.776400	0.713400	3.379800
H	2.664500	-0.500600	4.058700
H	2.032600	1.051200	3.467000
C	3.585300	-1.505700	1.682500
H	4.624200	-1.159700	1.811700
H	3.486900	-1.939900	0.678500
H	3.414100	-2.310200	2.413200
C	0.672800	2.682800	-1.800300
H	-0.182700	2.005100	-1.685900
C	0.995300	2.717300	-3.293500
H	1.259300	1.720800	-3.672900
H	1.827400	3.401200	-3.528400
H	0.114600	3.066900	-3.855100
C	0.251500	4.075400	-1.322400
H	1.059700	4.806900	-1.494500
H	0.010100	4.081900	-0.250500
H	-0.640500	4.417600	-1.870900
C	-0.603900	4.087400	3.660500
H	-1.090000	5.072100	3.732200
H	0.485500	4.243500	3.671700
H	-0.861500	3.527600	4.576100
C	-6.311400	-2.421800	-0.131900
H	-5.955700	-3.462800	-0.181400
H	-7.156400	-2.318100	-0.830300
H	-6.707200	-2.264700	0.887000

[{(^{F}NON)BOCFeCp}$_2$] (5)

Nuclear Repulsion: 29665.1690049664
Electronic Energy: -6,979.56962812296
Dispersion Energy: -0.4192138237
Virial Ratio: 2.0041
CPCM Solvation Model Properties:
Total single point energy: -6979.9888
Thermal correction: 1.903133
Total free energy: -6,978.085667

Fe	-0.26920	0.81090	-0.79200
O	-2.53580	-0.20330	0.73560
O	-4.67280	0.30300	-2.13110
N	-4.51300	-1.31610	0.05550

N	-4.57410	1.21660	0.44260
C	-5.64280	-1.39620	-0.77140
C	-6.62910	-2.36560	-0.59220
H	-6.50900	-3.05900	0.24130
C	-3.96250	-2.56560	0.48710
C	-6.37460	1.39870	2.10200
C	-1.58060	2.33990	-1.30380
H	-2.45210	2.65680	-0.73770
C	-4.20550	-2.99540	1.80600
C	-5.73320	-0.53640	-1.87630
C	-1.28960	-0.08520	0.34410
C	-0.26300	2.85020	-1.15310
H	0.05790	3.60060	-0.43390
C	-5.01090	1.57950	1.76280
C	-0.21980	1.25600	-2.80870
H	0.13030	0.57260	-3.57850
C	-4.89630	1.64720	-1.91380
C	-4.11270	2.15750	2.68470
C	-7.39970	0.89690	1.10450
H	-6.85280	0.48450	0.24840
C	-4.86100	2.10480	-0.58720
C	-3.67950	-4.22860	2.20400
H	-3.84230	-4.57730	3.22640
C	-7.72430	-2.47930	-1.45540
C	-2.95550	-5.01750	1.31660
H	-2.55040	-5.97750	1.64500
C	-4.99530	-2.14420	2.77940
H	-5.50470	-1.37000	2.18750
C	-6.83120	-0.60270	-2.72070
H	-6.89190	0.08600	-3.56540
C	-3.24630	-3.35560	-0.42970
C	-2.66430	2.44780	2.35170
H	-2.45250	2.02390	1.36440
C	-4.58760	2.50100	3.95600
H	-3.89750	2.94370	4.67820
C	-1.55400	1.34480	-2.32370
H	-2.39670	0.74300	-2.65790
C	-5.12700	3.46160	-0.36760
H	-5.13240	3.81650	0.66370
C	-5.11420	2.51300	-2.96890
H	-5.09790	2.11430	-3.98520

C	-6.79770	1.75860	3.38340
H	-7.84650	1.62080	3.65650
C	-1.58060	-2.94940	-2.28030
H	-0.97230	-2.31260	-1.62040
H	-1.47300	-2.57480	-3.31000
H	-1.16810	-3.97130	-2.26250
C	0.57640	2.19340	-2.09230
H	1.64570	2.35430	-2.20150
C	-3.04630	-2.91490	-1.86470
H	-3.36720	-1.86660	-1.93560
C	-2.74920	-4.58530	0.01060
H	-2.18770	-5.21520	-0.68380
C	-8.71940	-3.62440	-1.25210
C	-6.07190	-2.93490	3.51740
H	-6.74250	-3.45790	2.81780
H	-6.68450	-2.25750	4.13180
H	-5.64010	-3.68970	4.19310
C	-7.82190	-1.56130	-2.50770
H	-8.66340	-1.60030	-3.19910
C	-3.92600	-3.73510	-2.81020
H	-3.63940	-4.79930	-2.79490
H	-3.82220	-3.37270	-3.84490
H	-4.98780	-3.66620	-2.53030
C	-5.38520	4.35380	-1.41680
C	-5.35640	3.86570	-2.72670
H	-5.53090	4.52740	-3.57390
C	-1.72550	1.77650	3.34920
H	-1.78820	2.24200	4.34600
H	-0.68780	1.84870	3.00230
H	-1.96700	0.71140	3.45700
C	-5.68860	5.81800	-1.08810
C	-5.91350	2.29820	4.31120
H	-6.26390	2.57210	5.30940
C	-7.97230	-4.95140	-1.45910
H	-7.54190	-5.00510	-2.47100
H	-8.65820	-5.80410	-1.33130
H	-7.14800	-5.06990	-0.73990
C	-2.38980	3.94870	2.26600
H	-3.00320	4.42760	1.48990
H	-1.33310	4.12350	2.01120
H	-2.59380	4.45600	3.22280

B	-3.85220	-0.07710	0.32490
C	-4.06970	-1.41950	3.75520
H	-3.53850	-2.13400	4.40490
H	-4.63990	-0.72540	4.39180
H	-3.31560	-0.83180	3.21490
C	-8.26200	2.04870	0.58240
H	-8.85180	2.50230	1.39570
H	-8.96420	1.68200	-0.18280
H	-7.64720	2.83680	0.12670
C	-8.27760	-0.21910	1.66200
H	-7.67930	-1.06330	2.03160
H	-8.93930	-0.60090	0.87140
H	-8.91680	0.13070	2.48820
C	-9.29810	-3.58190	0.16820
H	-8.51280	-3.63610	0.93640
H	-9.97860	-4.43310	0.32730
H	-9.86710	-2.65550	0.33660
C	-4.50780	6.42750	-0.31990
H	-4.34330	5.92280	0.64300
H	-4.69630	7.49190	-0.10720
H	-3.57730	6.35190	-0.90330
C	-9.87970	-3.55820	-2.24540
H	-10.44600	-2.61910	-2.14830
H	-10.57720	-4.38860	-2.05820
H	-9.53360	-3.64630	-3.28640
C	-6.95350	5.88390	-0.21960
H	-7.81720	5.45510	-0.75080
H	-7.19170	6.92900	0.03490
H	-6.83080	5.32870	0.72230
C	-5.92300	6.65100	-2.34860
H	-5.03790	6.65880	-3.00280
H	-6.13950	7.69360	-2.06980
H	-6.77930	6.27860	-2.93110
Fe	0.26920	-0.81120	0.79170
O	2.53570	0.20300	-0.73590
O	4.67260	-0.30290	2.13110
N	4.51280	1.31600	-0.05560
N	4.57420	-1.21660	-0.44250
C	5.64250	1.39630	0.77140
C	6.62870	2.36580	0.59220
H	6.50870	3.05910	-0.24140

C	3.96230	2.56550	-0.48740
C	6.37490	-1.39870	-2.10170
C	1.58070	-2.34010	1.30370
H	2.45230	-2.65690	0.73770
C	4.20540	2.99520	-1.80630
C	5.73290	0.53660	1.87640
C	1.28950	0.08490	-0.34440
C	0.26310	-2.85050	1.15270
H	-0.05760	-3.60090	0.43340
C	5.01110	-1.57960	-1.76260
C	0.21950	-1.25650	2.80840
H	-0.13080	-0.57310	3.57820
C	4.89630	-1.64700	1.91390
C	4.11310	-2.15770	-2.68450
C	7.39980	-0.89690	-1.10410
H	6.85290	-0.48450	-0.24810
C	4.86110	-2.10470	0.58740
C	3.67960	4.22830	-2.20450
H	3.84240	4.57680	-3.22690
C	7.72380	2.47970	1.45540
C	2.95540	5.01730	-1.31730
H	2.55040	5.97740	-1.64580
C	4.99550	2.14390	-2.77950
H	5.50470	1.36960	-2.18730
C	6.83080	0.60310	2.72080
H	6.89160	-0.08550	3.56560
C	3.24600	3.35570	0.42930
C	2.66470	-2.44810	-2.35160
H	2.45280	-2.02420	-1.36430
C	4.58810	-2.50130	-3.95580
H	3.89810	-2.94400	-4.67800
C	1.55380	-1.34500	2.32360
H	2.39640	-0.74320	2.65790
C	5.12730	-3.46160	0.36790
H	5.13270	-3.81650	-0.66340
C	5.11420	-2.51280	2.96910
H	5.09780	-2.11400	3.98540
C	6.79810	-1.75870	-3.38310
H	7.84690	-1.62080	-3.65610
C	1.58030	2.95000	2.28000
H	0.97180	2.31330	1.62030

H	1.47260	2.57570	3.30980
H	1.16800	3.97200	2.26200
C	-0.57650	-2.19390	2.09180
H	-1.64580	-2.35490	2.20080
C	3.04600	2.91520	1.86430
H	3.36670	1.86680	1.93540
C	2.74910	4.58530	-0.01130
H	2.18750	5.21530	0.68310
C	8.71880	3.62480	1.25210
C	6.07230	2.93450	-3.51710
H	6.74280	3.45740	-2.81740
H	6.68510	2.25700	-4.13130
H	5.64070	3.68930	-4.19300
C	7.82140	1.56180	2.50780
H	8.66290	1.60100	3.19930
C	3.92580	3.73540	2.80970
H	3.63950	4.79960	2.79420
H	3.82200	3.37310	3.84440
H	4.98760	3.66620	2.52980
C	5.38540	-4.35360	1.41720
C	5.35650	-3.86540	2.72700
H	5.53100	-4.52700	3.57430
C	1.72590	-1.77680	-3.34910
H	1.78890	-2.24200	-4.34600
H	0.68810	-1.84940	-3.00240
H	1.96710	-0.71160	-3.45660
C	5.68900	-5.81780	1.08860
C	5.91400	-2.29830	-4.31090
H	6.26440	-2.57230	-5.30900
C	7.97170	4.95180	1.45900
H	7.54120	5.00560	2.47080
H	8.65750	5.80460	1.33110
H	7.14750	5.07030	0.73970
C	2.39030	-3.94900	-2.26600
H	3.00380	-4.42790	-1.49000
H	1.33360	-4.12390	-2.01110
H	2.59420	-4.45620	-3.22280
B	3.85210	0.07700	-0.32500
C	4.07010	1.41920	-3.75550
H	3.53910	2.13370	-4.40530
H	4.64050	0.72510	-4.39200

H	3.31590	0.83150	-3.21540
C	8.26220	-2.04860	-0.58200
H	8.85210	-2.50220	-1.39520
H	8.96420	-1.68190	0.18330
H	7.64740	-2.83680	-0.12640
C	8.27770	0.21920	-1.66160
H	7.67930	1.06340	-2.03130
H	8.93930	0.60110	-0.87090
H	8.91700	-0.13050	-2.48770
C	9.29750	3.58230	-0.16820
H	8.51220	3.63630	-0.93640
H	9.97800	4.43350	-0.32740
H	9.86660	2.65580	-0.33650
C	4.50810	-6.42760	0.32060
H	4.34350	-5.92290	-0.64230
H	4.69670	-7.49190	0.10800
H	3.57770	-6.35200	0.90410
C	9.87910	3.55880	2.24540
H	10.44560	2.61980	2.14830
H	10.57650	4.38930	2.05810
H	9.53300	3.64690	3.28640
C	6.95370	-5.88370	0.22000
H	7.81740	-5.45480	0.75100
H	7.19200	-6.92890	-0.03450
H	6.83090	-5.32870	-0.72200
C	5.92350	-6.65070	2.34920
H	5.03850	-6.65850	3.00350
H	6.14020	-7.69320	2.07050
H	6.77980	-6.27810	2.93160

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