Supplementary Information

1. Material and Methods

1.1. General

Unless otherwise stated, all chemicals were of reagent grade and purchased from *Sigma-Aldrich*. The polymer-supported benzeneboronic acid (2.6-3.2 mmol/g) was acquired from Alfa Aesar. The KHF_2 was purchased from *Fluka Chemie AG*. Catalyst $[Ir(OMe)COD]_2$ was freshly synthesized prior to its use starting from the precursor $[Ir(Cl)COD]_2$ and stored under argon at room temperature to avoid degradation by moisture. Dichlorofluoromethane-*d* for vt-NMR experiments was synthesized according to literature and transferred to the NMR tube via distillation. Acetonitrile and dichloromethane for UV-Vis measurements were of HPLC grade, THF for voltammetric measurements was distilled over CaH_2 prior to its use. Electrolyte tetrabutylammonium hexafluorophosphate ($TBAPF_6$) was purchased from *Fluka Chemie AG* and used as received. Chromatography was performed with Silica gel 60 M, *Macherey-Nagel GmbH & Co*.

1.2. Instruments

Melting Points (m.p.): measured by a Büchi Melting Point B-450/560 apparatus.

Infrared spectra (IR): recorded on a JASCO FT/IR-4100 Fourier Transform Infrared Spectrometer. Compounds were measured as solids or oils (neat). Absorption bands are given in wave numbers (cm^{-1}), and the intensities are characterized as follows: *s* = strong (0–33% transmission), *m* = medium (34–66% transmission), *w* = weak (67–100% transmission).

NMR spectra: were recorded on *Bruker ARX-300/400/500* (300/400/500 MHz). δ in ppm referenced against the corresponding solvent peaks ($CDCl_3$: ^1H 7.26 ppm, ^{13}C 77.0 ppm; CD_2Cl_2: ^1H 5.32 ppm; ^{13}C 54.00 ppm; MeOH-d_4: ^1H 3.31 ppm; ^{13}C , DMSO-d_6): ^1H 3.31 ppm; ^{13}C) or external standards (^{11}B-NMR: BF_3xEt_2O, 0 ppm or ^{19}F-NMR CCl_3F, 0 ppm). ^{13}C and ^{11}B-NMR spectra are proton decoupled. Data are reported as follows: chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet), coupling constant J in Hz, and integration. [Note: For several compounds the ipso ^{13}C signal (attached to the quadrupolar nucleus B) was not observed; all other peaks correlate well with standard shifts for compounds of similar structure and functionality.]

Fluorescence UV/Vis: was recorded on an *Agilent* 84513 instrument. Methanol and dichloromethane were of HPLC grade.

Emission: *Edinburgh Instrument FLS920 fluorimeter* equipped with S900 single photon photomultiplier detection system and Xe 900 xenon arc lamp (450 W).

Cyclic voltammetry: *CHI600C Electrochemical Analyzer, CH Instruments, Inc.* Electrodes: Non-aqueous Ag/Ag$^+$ reference electrode (10 mM AgNO$_3$ in 0.1 M Bu$_4$NPF$_6$ in acetonitrile); platinum wire counter electrode; glassy carbon working electrode. All measurements were performed in THF and with a scan rate of 0.1 V/s. The in THF was distilled over CaH$_2$ prior to its use. All E$_{1/2}$ potentials have been directly obtained from cyclic voltammetric curves as averages of the cathodic and anodic peak potentials. For irreversible peaks, the peak potential is given. The internal standard was the ferrocinium/ferrocene couple standard potential (+0.085 V for THF[1]).

HR-MS/MALDI: were performed by the MS Service of the Institute of Organic Chemistry at the University of Zurich on a Finnigan MAT95 instrument. Regular mass spectra were recorded on a Finnigan Trace DSQ GC-MS. Data are reported as follows: m/z (% relative intensity).

Microwave: reactions were performed in a CEM Discover microwave reactor with appendant active cooling. The data was analyzed via CHemDriver Appl. Software.

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[1] S. I. Bailey, W.-P. Leung, *Electrochimica Acta* **1985**, *30*, 861–863.

2. Syntheses and Characterization

2.1. 1,3,5,7,9-Pentakis(4,4,5,5-tetramethyl-1,2,3-dioxaborolyl)corannulene (3) – [1,3,5,7,9-corannulene pentaboronic acid, 2,3-dimethylbutane-2,3-diol pentaester]
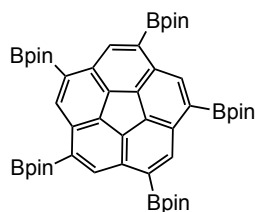
A flame-dried microwave tube, equipped with magnetic stir bar, was evacuated and charged with [Ir(OMe)COD]$_2$ (160 mg, 0.24 mmol), 4,4'-dimethyl-2,2'-bipyridine (88 mg, 0.48 mmol), B$_2$pin$_2$ (1.68 g, 6.6 mmol), NaOMe (7.1 mg, 0.13 mmol) and cyclohexane (dry, 1.6 ml). After preheating the suspension to 40 °C for 10 min, corannulene **1** (300 mg, 1.2 mmol) was added and the mixture was degassed with argon. The tube was sealed firmly and irradiated in the microwave with 300 W at 80 °C for 4 h. The mixture was allowed to cool to ambient temperature and diluted with CH$_2$Cl$_2$ and water. The aqueous layer was extracted three times with CH$_2$Cl$_2$ and the combined organic layers were dried over MgSO$_4$, filtered and concentrated under reduced pressure. To the crude brown solid MeOH (7 ml) was added and the resulting precipitate was filtered and recrytallized from CH$_2$Cl$_2$/MeOH to afford the desired product as colorless solid (655 mg, 0.74 mmol) in 62 % yield. The spectroscopic data were in [2]

M.p.: decomposition above 140 °C. IR (neat, cm^{-1}): 2977w, 2937w, 1738m, 1450m, 1369s, 1297m, 1268m, 1216m, 1142s, 1108w, 986m, 856m, 727w. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 8.97 (s, 5H), 1.46 (s, 60H). ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 138.74, 136.81, 133.09, 83.64, 25.03. ^{11}B-NMR (128.5 MHz, CDCl$_3$): δ = 22.54. MS (MALDI), m/z: 879.5 [M]$^+$. UV (DCM, nm): λ$_{max}$ 274, 31.

[2] M. N. Eliseeva, L. T. Scott, *J. A. Chem. Soc.* **2012**, *134*, 15169-15172.

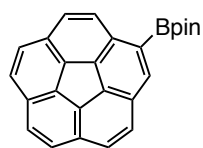## 2.2. 2-corannulyl-4,4,5,5-tetramethyl-1,2,3-dioxaborolane (4)

Bpin

A flame-dried microwave tube (3 ml), equipped with magnetic stir bar, was evacuated and charged with [Ir(OMe)COD]$_2$[3] (33 mg, 0.075 mmol), 4,4'-dimethyl-2,2-bipyridine (18 mg, 0.12 mmol), B$_2$pin$_2$ (334 mg, 1.3 mmol), sodium methoxide (1.3 mg, 0.024 mmol) and cyclohexane (dry, 0.8 ml). After preheating the suspension to 40 °C for 15 min, corannulene **1** (300 mg, 1.2 mmol) was added and the mixture was degassed with argon. The microwave tube was sealed firmly and the mixture was irradiated in the microwave with 300 W at 80 °C for 35 min. (Attention: use Max. Power[4]). The mixture was allowed to cool to ambient temperature and diluted with CH$_2$Cl$_2$ and water. The aqueous layer was extracted three times with CH$_2$Cl$_2$ and the combined organic layers were dried over MgSO$_4$, filtered and concentrated under reduced pressure. The crude brown solid was purified by column chromatography (9:1 hexane/CH$_2$Cl$_2$, after separation of corannulene the polarity was increased 7:3 hexane/CH$_2$Cl$_2$) to obtain the desired product as slightly yellow powder in 59 % yield (266 mg, 0.71 mmol). Corannulene (72.1 mg, 0.29 mmol, 24 %) could be recovered and 2-(Bpin)corannulene (90.4 mg, 0.18 mmol, 15 %) was obtained as side product.

M.p.: 157 °C. IR (neat cm^{-1}): 3028w, 2977m, 2927w, 1476m, 1459m, 1444m, 1416m, 1379s, 1344s, 1300s, 1274m, 1143s, 1084m, 1038w, 972m, 898w, 853m, 832s, 663m, 553m. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 8.49 (s, 1H), 8.46 (d, 1H, J = 5 Hz), 7.84-7.78 (m, 7H), 1.45 (s, 12H). ^{13}C-NMR (125.8 MHz, 300 K, DMSO-d_6): δ = 137.46, 136.98, 136.05, 135.94, 135.46, 135.45, 134.27, 131.49, 130.78, 130.72, 129.71, 128.94, 127.55, 127.14, 127.09, 127.08, 127.00, 126.94, 126.93, 126.85, 83.95, 25.04. ^{11}B-NMR (128.5 MHz, CDCl$_3$): δ = 22.59. MS (EI) m/z: 376.1 [M]$^+$. HR-MS (EI) m/z: found 376.1628; calc (C$_{26}$H$_{21}$BO$_2$) 376.1635. UV (DCM, nm): λ$_{max}$ 257, 29.

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[3] The yield is strongly depending on the quality of the catalyst. Using freshly synthesized catalyst is highly recommended. The catalyst should be stored under argon at room temperature.

[4] Max. Power is a method for the microwave that regulates the temperature by actively cooling the reaction vessel by a nitrogen flow. This makes it possible to have both, high irradiation and the desired temperature, at the same time.

2.3. Bis(1,5-cyclooctadiene)di-μ-methoxydiiridium(I)
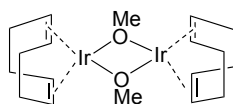
To a suspension of [Ir(Cl)COD]$_2$ (250 mg, 0.37 mmol) in degased methanol (25 ml) potassium hydroxide (42 mg, 0.75 mmol) was added. The reaction mixture was stirred at room temperature for 2 h. During that time the color changed from deep red to a bright yellow. The mixture was poured into degassed water (50 ml). The yellow precipitate was filtered, washed with additional degassed water and dried *under vacuo* to afford the pure product (210 mg, 0.26 mmol) in 85 % yield.

The spectroscopic data were in good accordance to literature.[5]

^{1}H-NMR (500 MHz, CDCl$_3$): δ = 3.55-3.54 (d, 8H, J = 5 Hz), 3.25 (s, 6H), 2.25-2.21 (m, 8H), 1.38-1.36 (d, 8H, J = 10 Hz). ^{13}C-NMR: δ = (125 MHz, CDCl$_3$): 56.36 (s, OMe), 31.40 (s, CH$_2$).

2.4. Dichlorofluoromethane-*d*
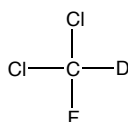
A 100-ml round bottom flask, equipped with stir bar and connected to an all glas distillation apparatus, carefully sealed with teflon band and evacuated. The collecting round bottom flask was cooled with dry ice/acetone bath. The reaction was performed under argon and was vented via an adapted mercury bubbler. The flask was charged with antimony trifluoride (50 g, 0.28 mmol) of a freshly opened bottle and chloroform-*d* (100 g, 0.84 mol) as well as antimony pentachloride (3 ml, 0.023 mmol) were added. Attention: The addition of latter is a highly exothermic reaction. The mixture was heated gently to 30 °C so that the distillation proceeded slowly until only a viscous slurry remains in the reaction flask. The desired product was afforded as colorless liquid in 76 % yield.

The spectroscopic data were in good accordance to literature.[6]

^{1}H-NMR (500 MHz, 193 K, neat): δ = 7.47 (d, J_{H-F} = 50 Hz). ^{13}C-NMR (500 MHz, 193 K, neat): δ = 104.2 (dt, J_{C-F} = 292 Hz, J_{C-D} = 34 Hz).

[5] T. E. Hurst, T. K. Macklin, M. Becker, E. Hartmann, W. Kügel, J.-C. Parisienne-La Salle, A. S. Batsanov, T. B. Marder, V. Snieckus, *Chem. Eur. J.* **2010**, *16*, 8155-8161.
[6] F. A. L. Anet, J. S. Siegel, *J. Org. Chem.* **1988**, *53*, 2629-2630.

2.5. 1,3,5,7,9-*Pentakis*(2-fluorophenyl)corannulene (5) starting from (3)
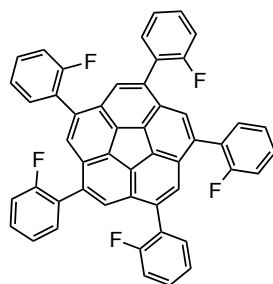
To a flame dried and evacuated microwave tube equipped with magnetic stir bar and septa, **3** (20 mg, 0.023 mmol), 2-bromofluorobenzene (40 mg, 0.23 mmol), Pd(dppf)Cl$_2$ (3.7 mg, 0.005 mmol), Cs$_2$CO$_3$ (89 mg, 0.27 mmol) and MeOH (2 ml) were added. The suspension was degassed with argon for 10 min. The reaction vessel was firmly sealed by a teflon cap and the reaction mixture was heated in a microwave reactor with 300 W at 95 °C for 2 h. After cooling to room temperature the mixture was diluted with dichloromethane and extracted with water three times. The combined organic layers were collected, dried over MgSO$_4$ and concentrated under reduced pressure. The crude mixture was purified by column chromatography with hexane/EtOAc (10:1) as eluent to give the desired compound as a yellow solid (6.8 mg, 0.01 mmol) in 42 % yield.

M.p.: > 400 °C. IR (neat, cm^{-1}): 2987.2*m*, 2970.8*m*, 2901.4*m*, 1576.5*w*, 1492.6*m*, 1450.2*m*, 1435.7*w*, 1394.3*w*, 1318.1*w*, 1263.2*w*, 1245.8*m*, 1209.2*m*, 1102.1*w*, 1065.5*m*, 1056.8*m*, 1037.5*m*, 936.3*w*, 887.1*w*, 826.4*m*, 799.4*w*. ^{1}H-NMR (500 MHz, CD$_2$Cl$_2$): δ = 5.68 (d, *J* = 3 Hz, 5H), 7.52-7.41 (m, 10H), 7.29-7.22 (m, 10H). ^{13}C-NMR (125.8 MHz, CD$_2$Cl$_2$): δ = 136.29, 136.02, 133.06, 130.60, 130.50, 128.05, 125.03, 116.63, 116.34, 100.15. HR-MS (APCI) *m/z*: found 721.1953 [M + H]$^+$; calc (C$_{50}$H$_{25}$BF$_5$) 720.1995. UV (DCM, nm): λ$_{max}$ 280.

2.6. Potassium 1,3,5,7,9-Corannulene pentatrifluoroborate (6)
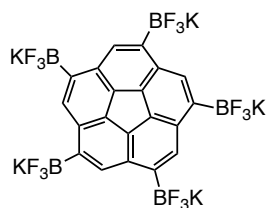
Method A (KHF$_2$)

To a suspension of **3** (100 mg, 0.113 mmol) in MeOH (40 ml) aq. KHF$_2$ (4.5 M, 0.6 ml, 27 mmol) was added. The suspension was stirred over night at room temperature. The precipitate was filtered and washed with additional MeOH to obtain the product as a colorless solid in 98 % (88 mg, 0.112 mmol) yield with 91 % purity.

Method B (KF, L-(+)-tartaric acid)

To as suspension of **1** (20 mg, 0.023 mmol) in MeOH/MeCN (1:1, 2 ml) aq. KF (anhydrous, 10 mM) and a solution of L-(+)-tartaric acid in THF were added. The reaction mixture was stirred over night while the color turned from colorless to red. The solvent was evaporated and the crude brown red solid was redissolved in DMF. The precipitate was filtered and the filtrate was evaporated to give a red solid, which was washed with acetonitrile and methanol to obtain the desired product (17.5 mg, 0.022) in 98 % yield.

M.p.: decomposition above 316 °C. IR (neat, cm^{-1}): 3599m, 1623w, 1431w, 1341m, 1206s, 1096s, 954m, 910m, 879s, 797s, 727m, 624m. ^{1}H-NMR (500 MHz, DMSO-d$_6$): δ = 8.08 (s, 5H). ^{13}C-NMR (125.8 MHz, DMSO-d$_6$): δ = 145.77 (br, ipso-C), 134.45, 133.14, 129.85. ^{19}F-NMR (376.5 MHz, DMSO-d$_6$): δ = -131.59, -131.65. ^{11}B-NMR (128.5 MHz, DMSO-d$_6$): δ = 1.16 (q, ^{1}J$_{B-F}$ = 18.5 Hz). UV (MeOH, nm): λ$_{max}$ 261, 30.

2.7. Potassium corannulene trifluoroborate (7)
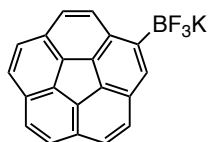
To a suspension of **4** (20 mg, 0.053 mmol) in MeOH (5 ml) was added aq. KHF_2 (4.5 M, 0.04 ml, 1.8 mmol). The suspension was stirred over night at room temperature. The solvent was evaporated and hexane (3 ml) was added. The precipitate was filtered, washed with additional hexane and dried *under vacuo* over night to yield the product as a slightly yellow solid (18.4 mg, 0.052 mmol, 97 %).

M.p.: decomposition above 176 °C. IR (neat, cm^{-1}): 3628*m*, 1607*m*, 1435*w*, 1408*w*, 1323*m*, 1292*w*, 1208*s*, 1186*m*, 1113*s*, 1050*s*, 1022*s*, 928*s*, 888*m*, 863*s*, 827*s* 775*m*, 690*m*, 662*m*. ^{1}H-NMR (500 MHz, MeOH-d_4): δ = 8.27 (dd, 1H, *J* = 8.8 Hz, *J* = 0.85 Hz), 8.03 (s, 1H), 7.81-7.73 (m, 7 H). ^{13}C-NMR (125.8 MHz, MeOH-d_4): δ = 137.08, 136.97, 136.96, 136.82, 136.69, 136.60, 132.53, 131.96, 131.72, 131.70, 131.12 (2 C), 129.92 (q, J = 3.2 Hz, J = 3.4 Hz, *ipso*-C), 128.37, 127.95, 127.76, 127.38, 127.32, 127.25, 126.49. ^{19}F-NMR (376.5 MHz, MeOH-d_4): δ = -153.66. ^{11}B-NMR (128.5 MHz, DMSO-d_6): δ = 1.49 (q, $^1J_{B-F}$ = 11.6 Hz). MS (ESI) *m/z*: 317.0 [M - K]$^+$. HR-MS (ESI) *m/z*: found 317.0760 [M - K]$^+$; calc ($C_{20}H_9BF_3$) 317.0749. UV (MeOH, nm): λ_{max} 254, 288.

2.8. 1,3,5,7,9-*Pentakis*(2-fluorophenyl)corannulene (5) starting from (6)
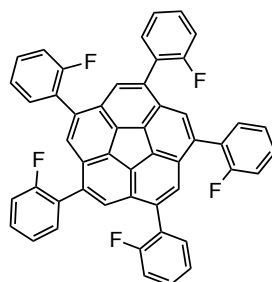
To a flame dried and evacuated pressure tube equipped with magnetic stir bar and septa, **6** (50 mg, 0.064 mmol), 2-bromofluorobenzene (62 mg, 0.353 mmol), $Pd(OAc)_2$ (0.5 mg, 0.002 mmol), K_2CO_3 (133 mg, 0.96 mmol) and MeOH were added. The suspension was degassed with argon for 10 min. The reaction vessel was firmly sealed by a teflon cap and the reaction mixture was allowed to stir at 75 °C for 3 d. After cooling to room temperature the mixture was diluted with dichloromethane and extracted with water three times. The combined organic layers were collected, dried over $MgSO_4$ and concentrated under reduced pressure. The crude mixture was purified by column chromatography with hexane/EtOAc (10:1) as eluent to give the desired compound as a yellow solid (11.5 mg, 0.016 mmol) in 25 % yield.

M.p.: > 400 °C. IR (neat, cm^{-1}): 2987.2*m*, 2970.8*m*, 2901.4*m*, 1576.5*w*, 1492.6*m*, 1450.2*m*, 1435.7*w*, 1394.3*w*, 1318.1*w*, 1263.2*w*, 1245.8*m*, 1209.2*m*, 1102.1*w*, 1065.5*m*, 1056.8*m*, 1037.5*m*, 936.3*w*, 887.1*w*, 826.4*m*, 799.4*w*. ^{1}H-NMR (500 MHz, CD_2Cl_2): δ = 5.68 (d, J = 3 Hz, 5H), 7.52-7.41 (m, 10H), 7.29-7.22 (m, 10H). ^{13}C-NMR (125.8 MHz, CD_2Cl_2): δ = 136.29, 136.02, 133.06, 130.60, 130.50, 128.05, 125.03, 116.63, 116.34, 100.15. HR-MS (APCI) *m/z*: found 721.1953 $[M + H]^+$; calc ($C_{50}H_{25}BF_5$) 720.1995. UV (DCM, nm): $λ_{max}$ 280.

2.9. 1,3,5,7,9-Corannulene pentaboronic acid (8)
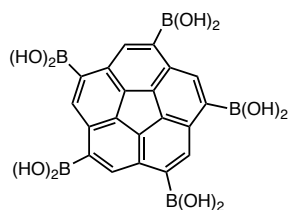
A 50-ml round bottom flask was charged with **3** (100 mg, 0.114 mmol) and polystyrene boronic acid (1.0 g, 2.85 mmol). Acetonitrile (13.5 ml) and 1 M aq. HCl (1.5 ml) were added. The suspension was sonnicated and stirred rigorously for 4 days at room temperature. The mixture was filtered and washed with cold MeOH (10 ml). The recovered resin could be reused with only slight loss of activity. The filtrate was concentrated under reduced pressure at room temperature. Water (5ml) was added and removed at the lyophilizer to afford the desired product (53.12 mg, 0.113 mmol) in 99 % yield.

M.p.: decomposition above 152 °C. IR (neat, cm^{-1}): 3336.3*s* (broad), 2950*w*, 2841*w*, 1646*m*, 1449*w*, 1376*w*, 1014*s*. ^{1}H-NMR (500 MHz, MeOH-d_4): δ = 8.06. ^{13}C-NMR (125.8 MHz, MeOH-d_4): δ = 137.23, 134.80, 133.60. ^{11}B-NMR (128.5 MHz, DMSO-d_6): δ = 19.31.

2.10. Corannulene boronic acid
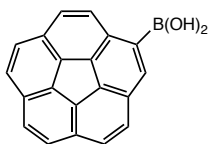
A 10-ml round-bottom flask equipped with magnetic stir bar was charged with **4** (20 mg, 0.053 mmol), polymer-supported benzeneboronic acid (95 mg, 0.266 mmol). Acetonitrile (2.7 ml) and aq. 1M HCl (0.3 ml) were added. The reaction mixture was sonnicated and allowed to stir for 16 hours at room temperature. Water (10 ml) was added and the mixture was filtered. The filtrate was concentrated and redissolved in CH_2Cl_2. The slightly yellow precipitate was collected by vacuum filtration and dried under *vacuo* to afford the desired product (14.2 mg, 0.048 mmol) in 91 % yield.

M.p.: Decomposition above 179.7 − 180.3 °C. IR (neat, cm^{-1}): 3301m (broad), 1662w, 1052s, 1024s, 1005s, 821m, 759m, 680w, 624w. ^{1}H-NMR (500 MHz, DMSO-d_6): δ = 8.44 (s, 2H), 8.42 (d, 3.5 Hz, 1H), 8.41 (d, J = 5 Hz, 1H) 7.97-7.93 (m, 6H). ^{13}C-NMR (125.8 MHz, DMSO-d_6): δ = 135.87, 135.14, 134.99, 134.59, 134.57, 134.53, 134.01, 130.97, 130.54, 130.35, 129.69, 129.34, 127.58, 127.336, 127.27, 127.25, 127.22, 127.09, 126.81. ^{11}B-NMR (128.5 MHz, DMSO-d_6): could not be detected. HR-MS (ESI) *m/z*: found 295.0914 [M + H]$^+$; calc ($C_{26}H_{12}BO_2$) 295.0930. UV (DCM, nm): λ$_{max}$ 257, 29.

2.11. General Procedure for Alcohol Exchange

To a solution of **8** (20 mg, 0.043 mmol) in MeOH (2 ml) an excess of the corresponding diol (0.645 mmol) is added. If the diol is a liquid the reaction was performed in the neat diol. The mixture was stirred over night at room temperature.

2.11.1. 1,3,5,7,9-Corannulene pentaboronic acid, 1,3-propanediol pentaester (9)
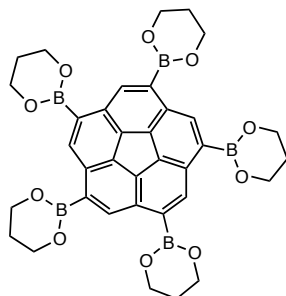
The precipitate was filtered, washed with MeOH and dried *under vacuo* to afford the desired product as colorless powder (26.2 mg, 0.039 mmol) in 91 % yield.

M.p.: 269 °C. IR (neat, cm^{-1}): 2948*w*, 2892*w*, 1481*m*, 1440*m*, 1421*m*, 1348*m*, 1312*m*, 1258*s*, 1208*w*, 1187*s*, 1141*w*, 1098*m*, 953*w*, 989*w*, 841*w* 723*m*, 706*m*. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 8.96 (s, 5H), 4.34 (t, *J* = 6 Hz, 20H), 2.18 (quint, J = 8 Hz, 4 Hz, 10 H). ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 137.25, 136.46, 132.54, 62.12, 27.55. ^{11}B-NMR (128.5 MHz, CDCl$_3$): 18.39. MS (MALDI), *m/z*: 699.3 [M]$^+$. UV (DCM, nm): λ$_{max}$ 275.

2.11.2. 1,3,5,7,9-Corannulene pentaboronic acid, 2,2'-dimethyl-1,3-propanediol pentaester (10)
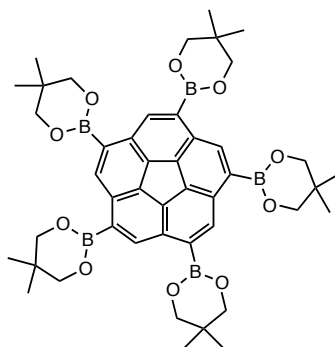
The precipitate was filtered, washed with additional MeOH and dried *under vacuo* to affort the desired product as slightly yellow powder (27.9 mg, 0.034 mmol) in 80 % yield.

M.p.: 305.8 °C. IR (neat, cm^{-1}): 2948*w*, 2892*w*, 1481*m*, 1440*m*, 1421*m*, 1348*m*, 1312*m*, 1258*s*, 1208*w*, 1187*s*, 1141*w*, 1098*m*, 953*w*, 989*w*, 841*w* 723*m*, 706*m*. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 9.02 (s, 5H), 3.95 (s, 20H) 1.13 (s, 30H) ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 137.48, 136.54, 132.69, 72.45, 31.94, 22.15. ^{11}B-NMR (128.5 MHz, CDCl$_3$): 16.67. MS (MALDI), *m/z*: 809.4 [M]$^+$. UV (DCM, nm): λ$_{max}$ 275.

2.11.3. 1,3,5,7,9-Corannulene pentaboronic acid, *cis*-cyclopentanediol pentaester (11)
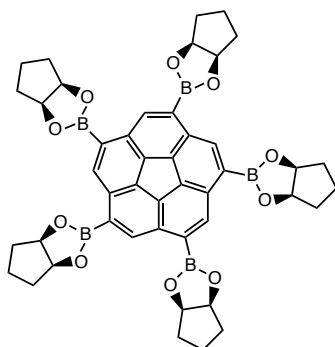
The precipitate was filtered, washed with additional MeOH and dried *under vacuo* to afford the desired product as slightly yellow powder (32.7 mg, 0.041 mmol) in 95 % yield.

M.p.: 341.5-343.8 °C. IR (neat, cm^{-1}): 2963*m*, 2921*m*, 1450*s*, 1365*s*, 1327*w*, 1309*m*, 1274*s*, 1213*m*, 1184*m*, 1101*m*, 1035*s*, 986*w*, 928*w*, 810*w*, 751*w* 723*m*, 723*m*. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 8.97 (s, 5H), 5.51 (d, 10H), 2.21-2.17 (m, 10H), 1.81-1.69 (m, 20H). ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 139.05, 136.72, 132.99, 82.75, 34.95, 21.71. ^{11}B-NMR (128.5 MHz, CDCl$_3$): could not be detected. MS (MALDI), *m/z*: 799.4 [M]$^+$. UV (DCM, nm): λ$_{max}$ 275.

2.11.4. 1,3,5,7,9 -Corannulene pentaboronic acid, *cis*-cyclohexanediol pentaester (12)
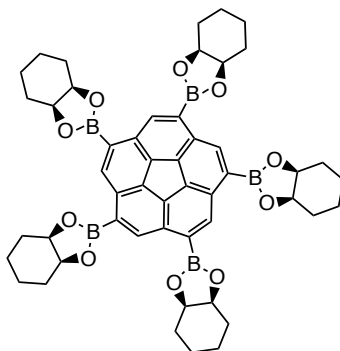
No precipitate occurred after the reaction. The solvent was evaporated and to the crude product cold EtOH was added. The precipitate was filtered, washed with additional cold EtOH and dried *under vacuo* to give the desired product as yellow powder (81.8 mg, 0.037 mmol) in 85 % yield

M.p.: 276 °C. IR (neat, cm^{-1}): 2938.0*m*, 2861.8*w*, 1450.2*s*, 1370.2*m*, 1358.6*m*, 1318.1*m*, 1301.7*w*, 1273.8*s*, 1212.0*w*, 1185.0*m*, 1144.6*w*, 1101.2*w*, 1042.3*w*, 1013.4*m*, 994.1*m*, 926.6*w*, 879.4*w*, 756.9*w*. ^{1}H-NMR (500 MHz, CDCl$_3$): δ = 9.06 (s, 5H), 4.71-4.67 (m, 10H), 1.98 (d, J = 4.5 Hz, 20H), 1.73-1.66 (m, 10H), 1.45-1.42 (m, 10 H). ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 139.10, 136.84, 133.07, 75.65, 28.71, 19.37. ^{11}B-NMR (128.5 MHz, CDCl$_3$): 23.43. MS (MALDI), *m/z*: 870.4 [M]$^+$. [M]$^+$. UV (DCM, nm): λ$_{max}$ 275.

2.11.5. 1,3,5,7,9-Corannulene pentaboronic acid catechol pentaester (13)
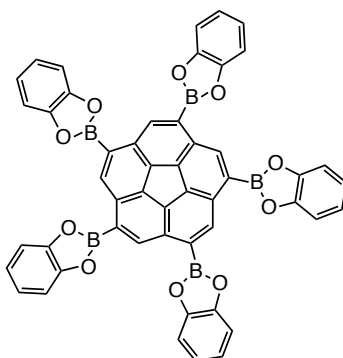
No precipitate occurred after the reaction. The solvent was evaporated and to the crude product cold EtOAc was added. The precipitate was filtered, washed with additional cold EtOAc and dried *under vacuo* to give the desired product as yellow-brown powder (32.2 mg, 0.038 mmol) in 89 % yield

M.p.: decomposition above 311 °C. IR (neat, cm^{-1}): 2365w, 2338w, 1456m, 1374w, 1329w, 1277m, 1237m, 1184w, 956w, 809w, 749s. ^{1}H-NMR (500 MHz, MeOH-d$_4$): δ = 8.06 (s, 5H), 6.77-6.73 (m, 10H), 6.67-6.63 (m, 10H). ^{13}C-NMR (125.8 MHz, CDCl$_3$): δ = 148.63, 143.48, 139.90, 136.32, 132.18, 122.81, 121.26, 115.50, 112.95. ^{11}B-NMR (128.5 MHz, CDCl$_3$): 19.71. MS (MALDI), *m/z*: 838.2 [M]$^+$. UV (DCM, nm): λ$_{max}$ 262.

3. NMR Spectra

3.1. Compound 3

1H-NMR (500 MHz, 300K, CDCl$_3$): 1,3,5,7,9-(Bpin)$_5$-corannulene **3**
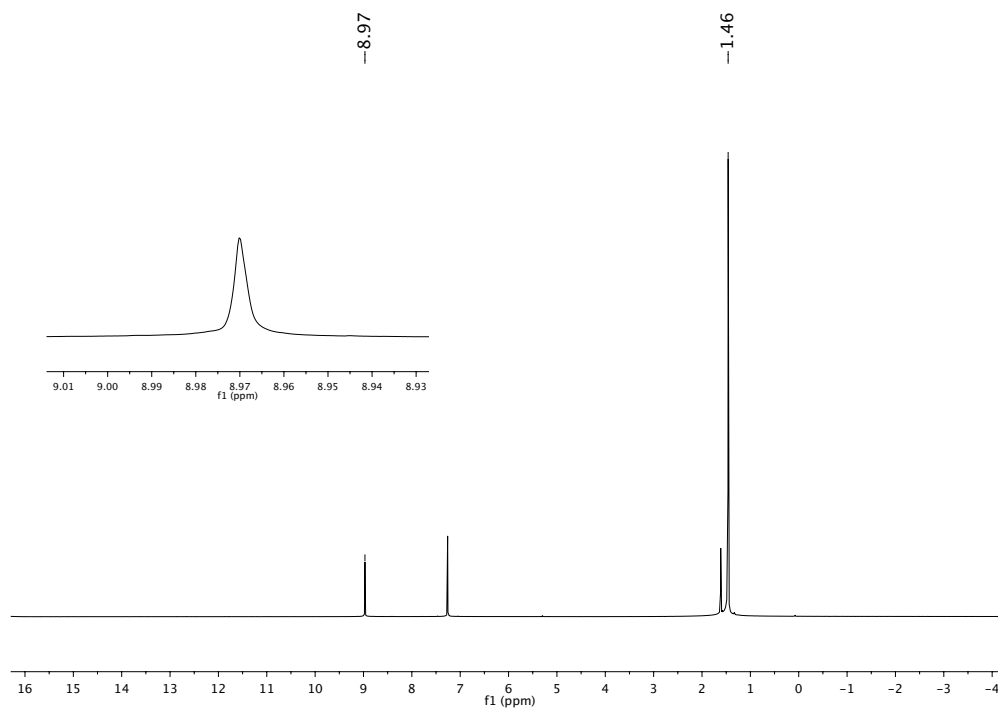
13C-NMR (125.8 MHz, 300K, CDCl$_3$): 1,3,5,7,9-(Bpin)$_5$corannulene **3**
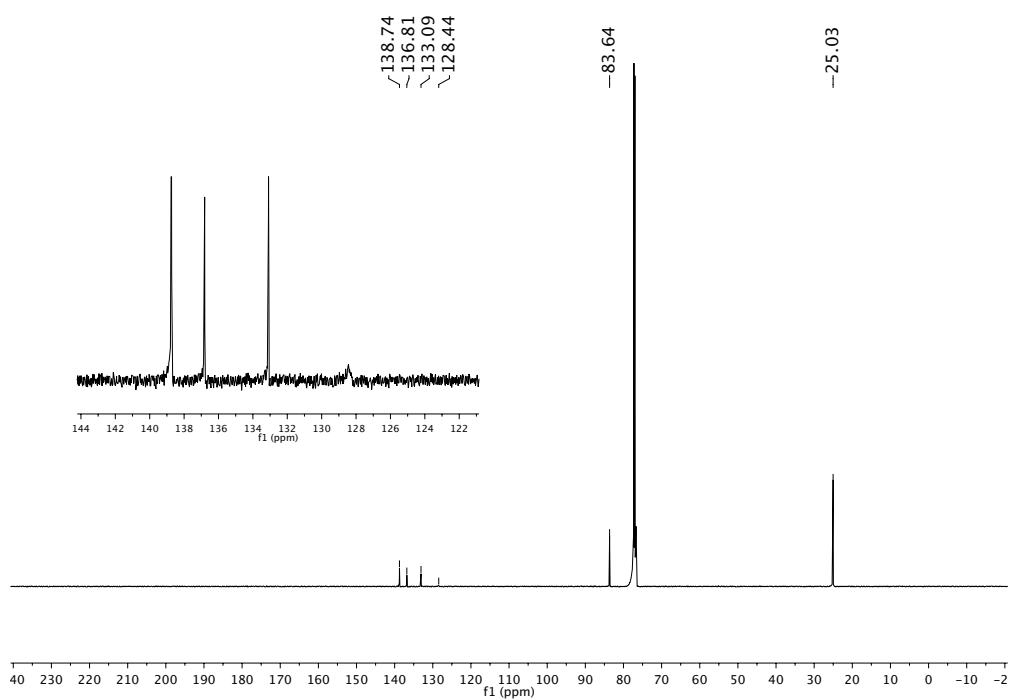
11B-NMR (128.25 MHz, 300K, CDCl$_3$): 1,3,5,7,9-(Bpin)$_5$corannulene **3**
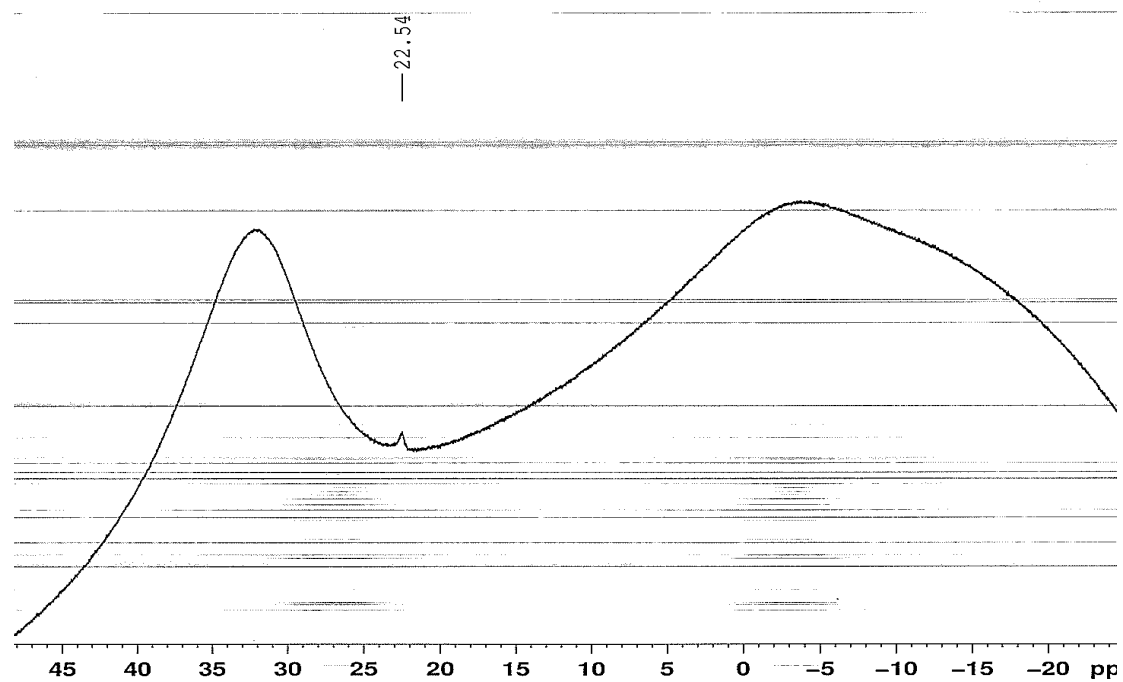
3.2. Compound 4

1H-NMR (500 MHz, 300K, CDCl$_3$) : Bpin-corannulene **4**

18

13C-NMR (125.8 MHz, 300K, CDCl$_3$): Bpin-corannulene **4**

- 137.46
- 136.98
- 136.05
- 135.94
- 135.46
- 135.45
- 134.27
- 131.49
- 130.78
- 130.72
- 129.71
- 128.94
- 127.55
- 127.14
- 127.09
- 127.08
- 127.00
- 126.94
- 126.93
- 126.85
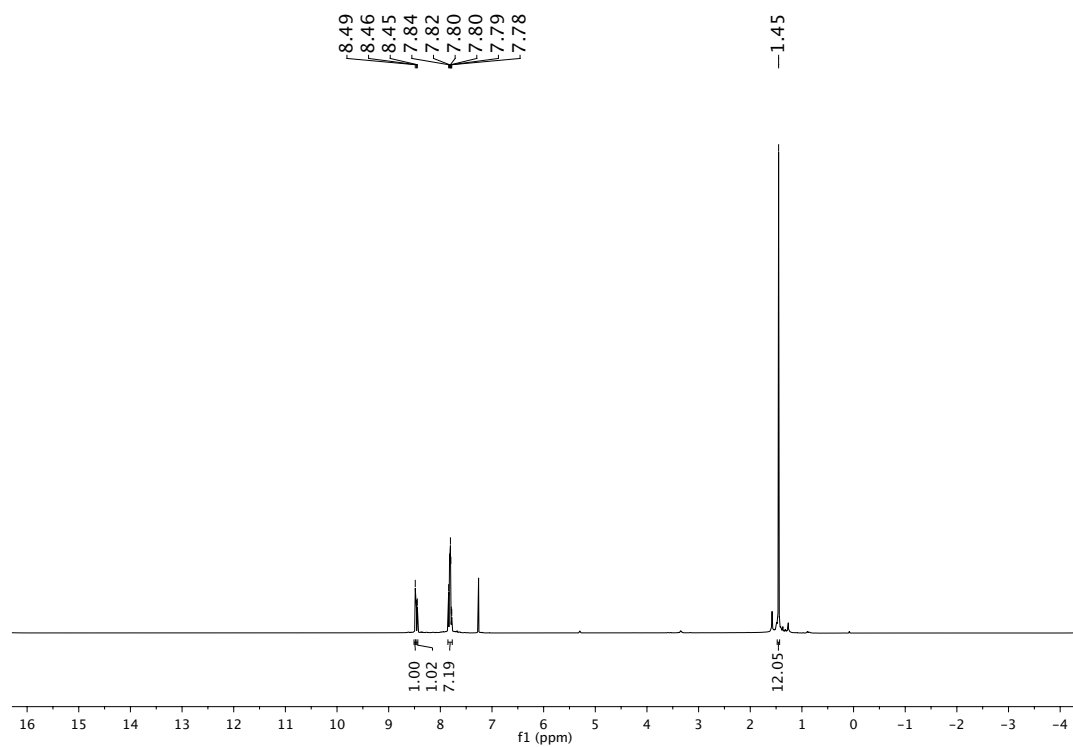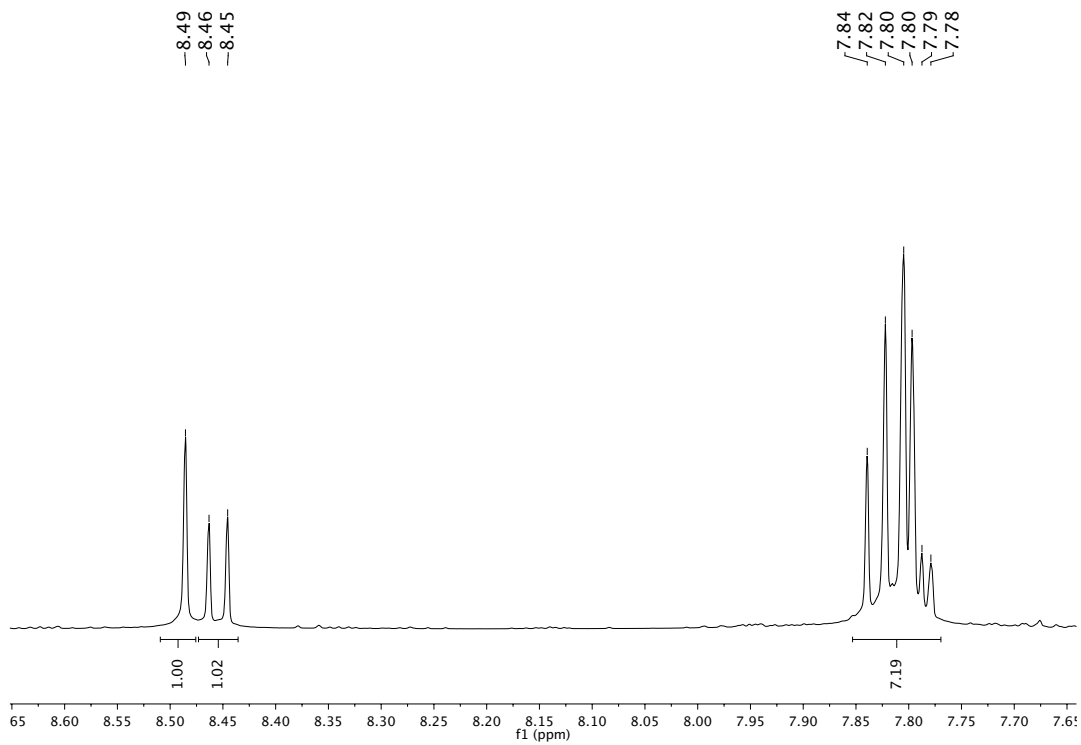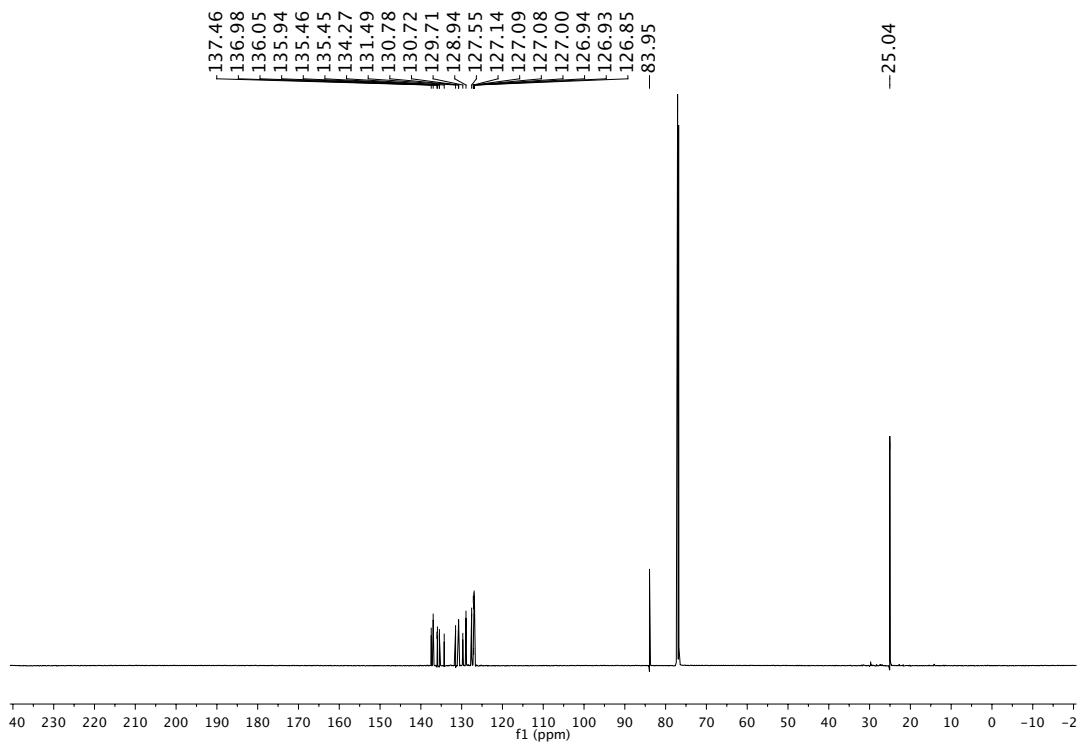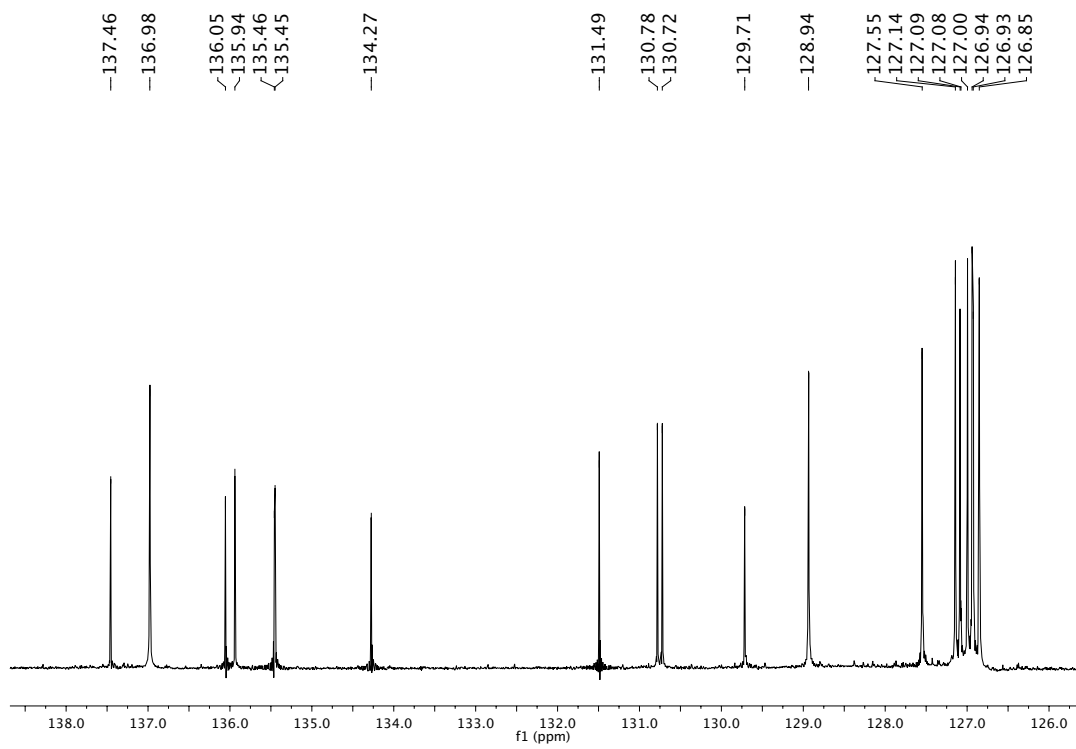
11B-NMR (128.5 MHz, 300K, CDCl$_3$): Bpin-corannulene **4**

- 22.5902

20
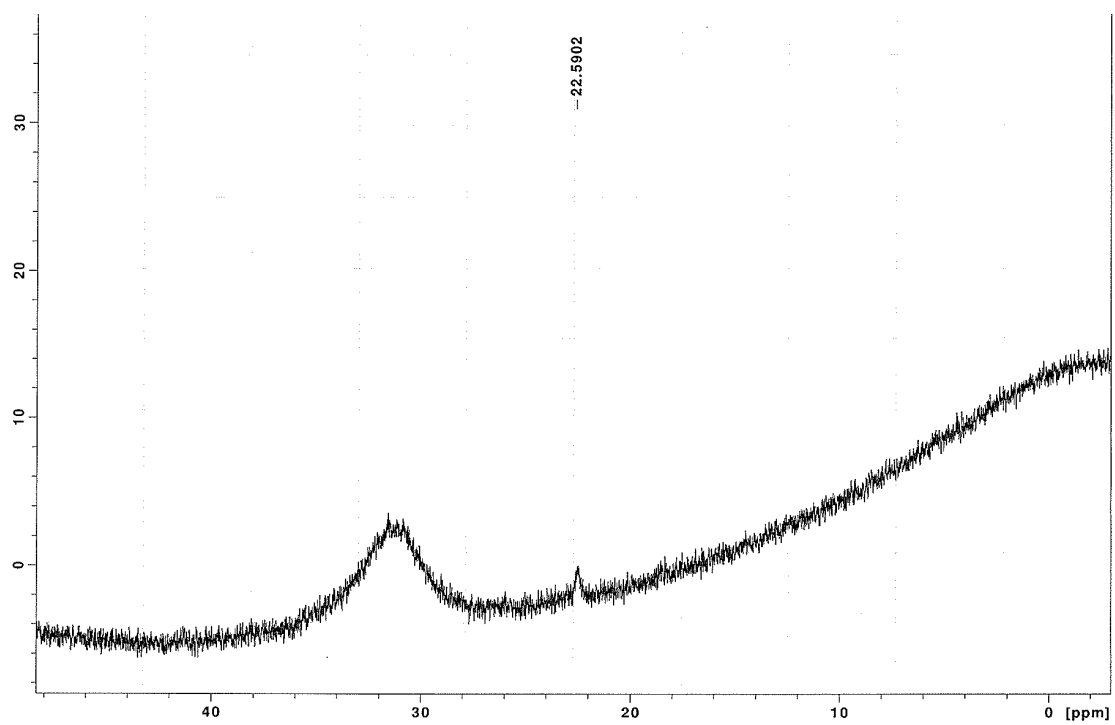
3.3. Compound 5

1H-NMR (500 MHz, 300K, CD$_2$Cl$_2$): 1,3,5,7,9-*Pentakis*(2-fluorophenyl)corannulene **5**
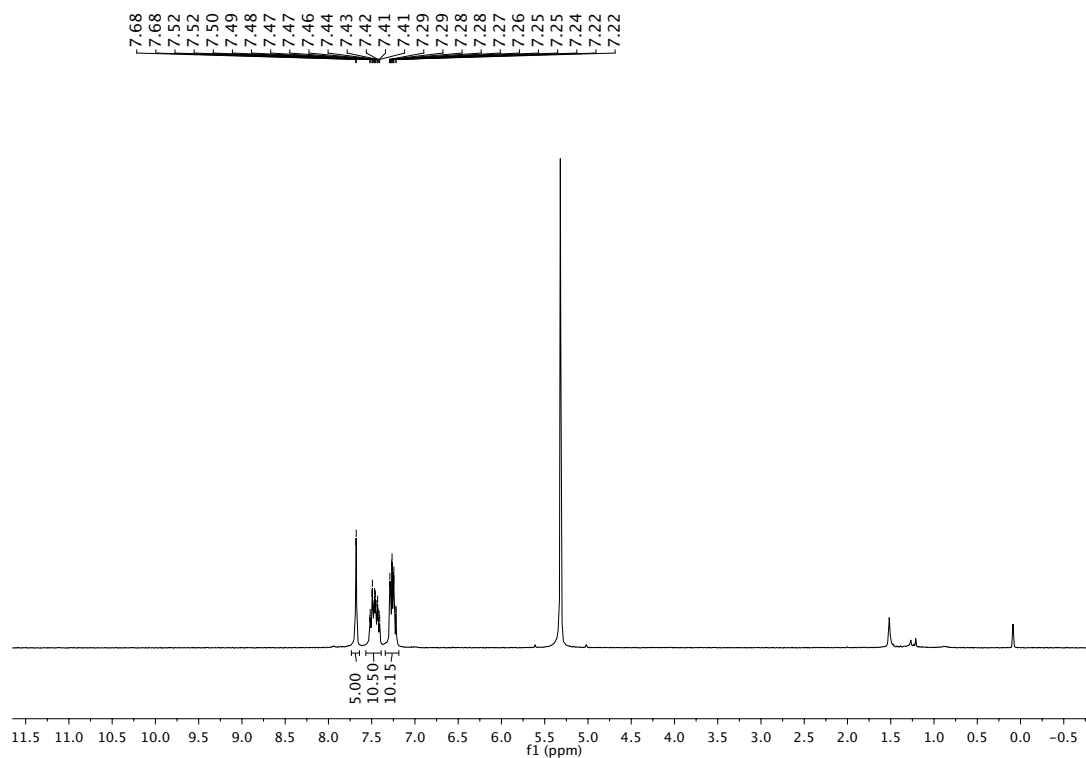
13C-NMR (125.8 MHz, 300K, CD$_2$Cl$_2$): 1,3,5,7,9-*Pentakis*(2-fluorophenyl)corannulene **5**
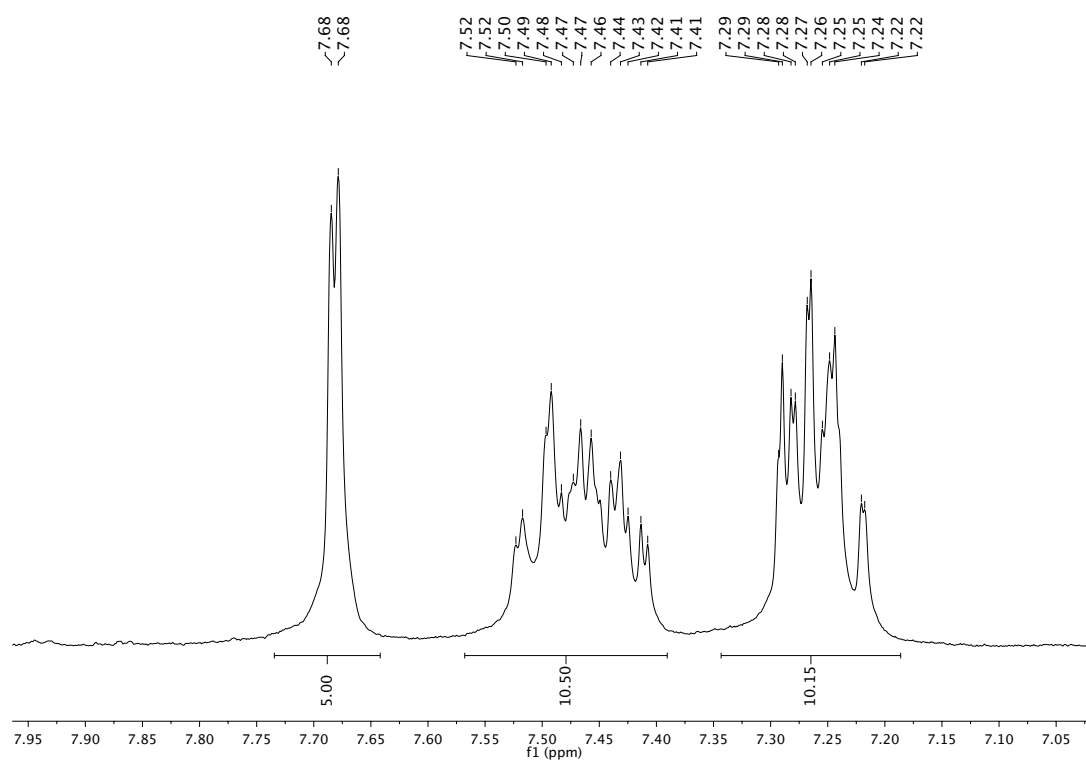
11B-NMR (128.5 MHz, 300K, CD$_2$Cl$_2$): 1,3,5,7,9-*Pentakis*(2-fluorophenyl)corannulene **5**
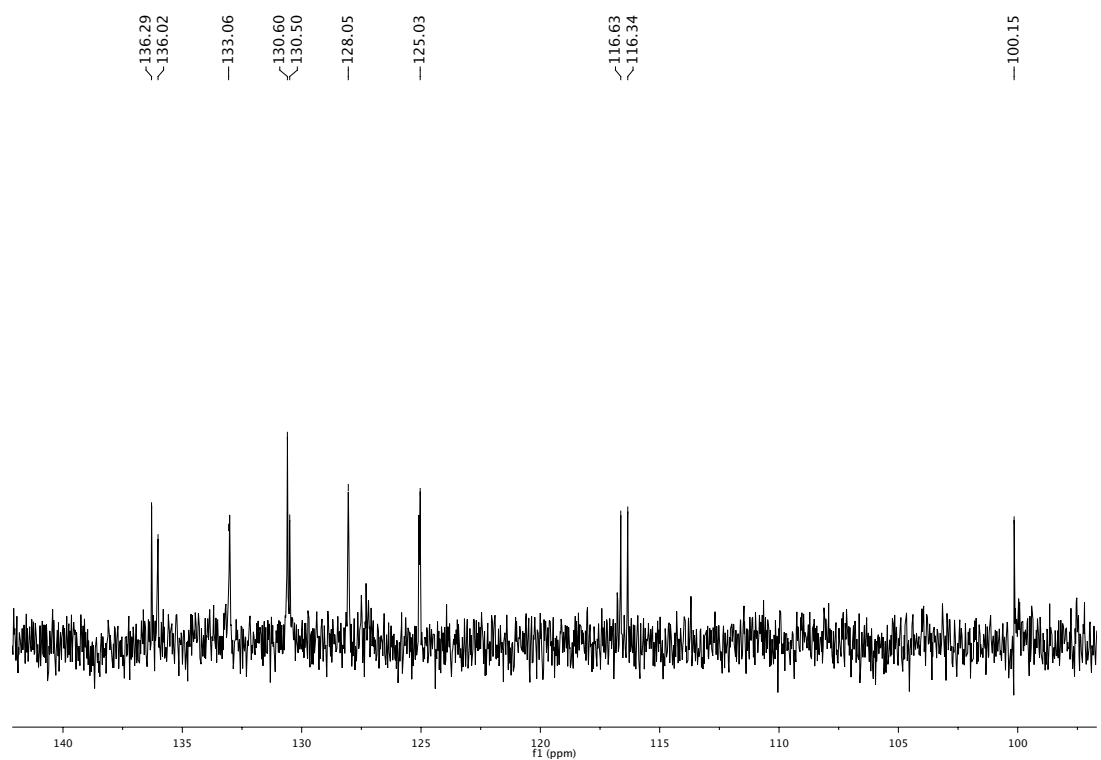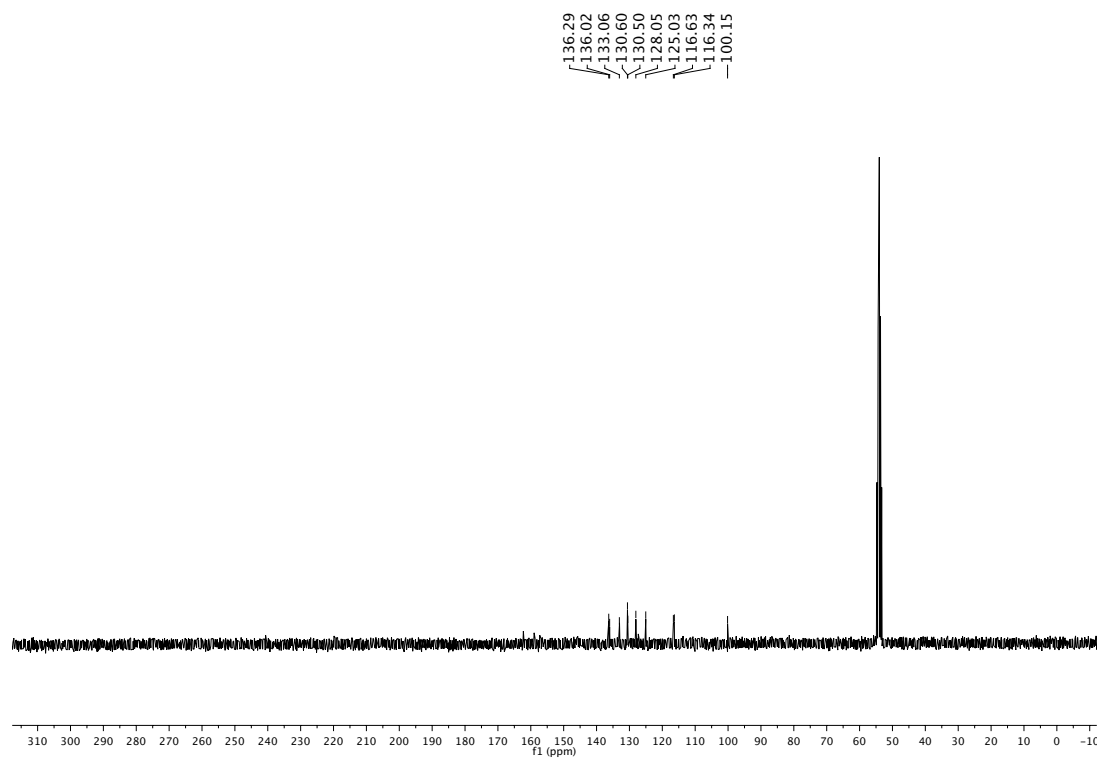
3.4. Compound 6

1H-NMR (500 MHz, 300K, DMSO-d_6): 1,3,5,7,9-(BF$_3$K)$_5$-corannulene **6**

13C-NMR (125.8 MHz, 300K, DMSO-d_6): 1,3,5,7,9-(BF$_3$K)$_5$-corannulene **6**

−145.77

−134.45
−133.14

−129.85

f1 (ppm)
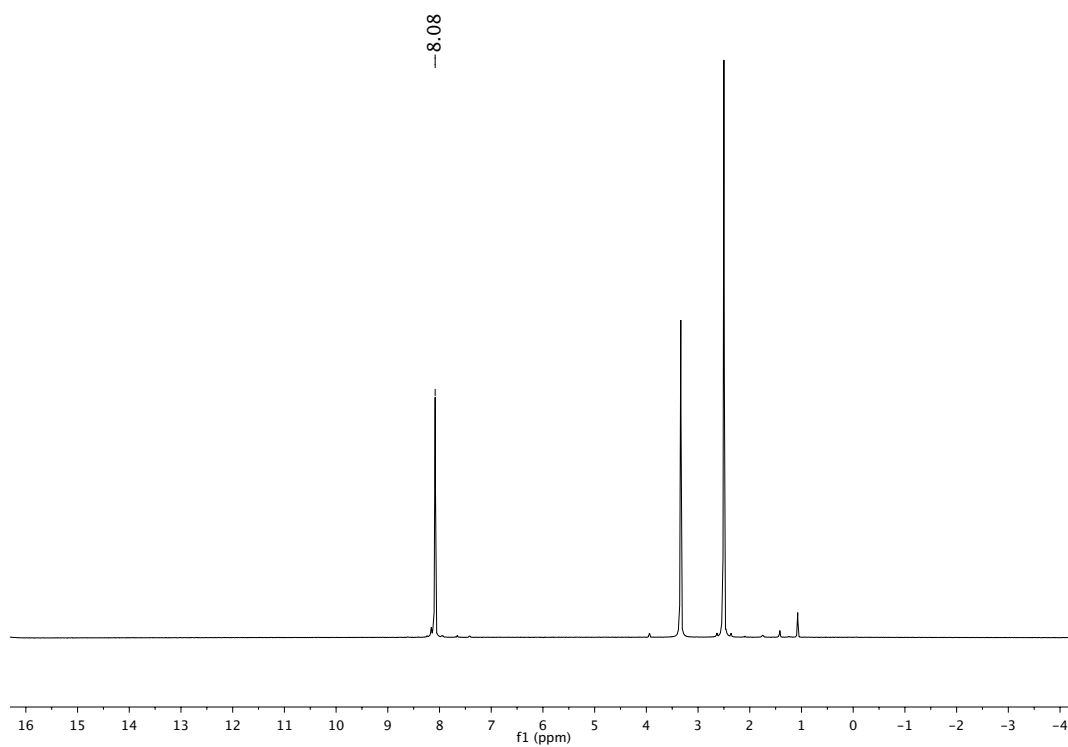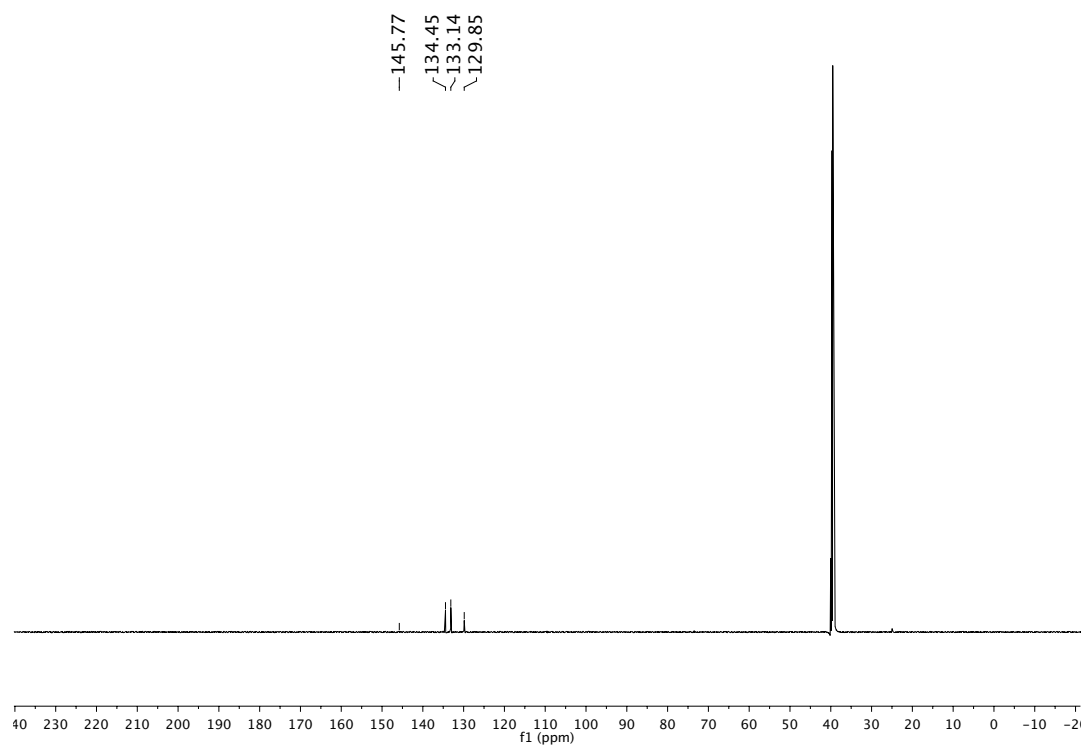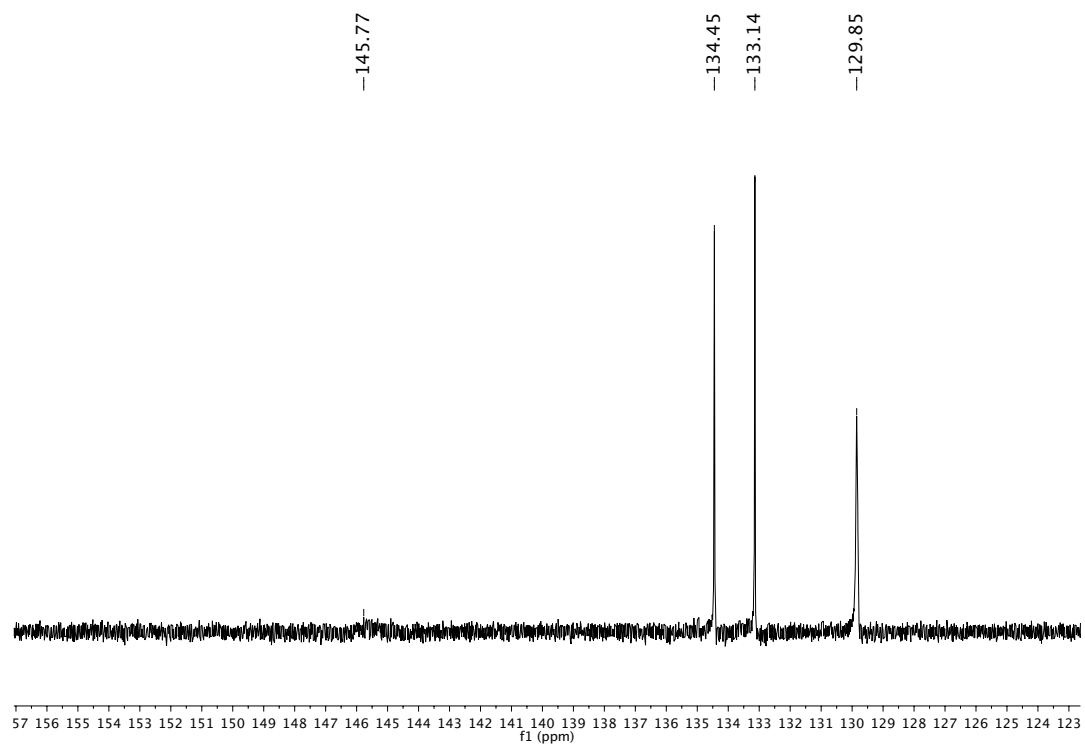
11B-NMR (128.5.5, 300K, DMSO-d_6): 1,3,5,7,9-(BF$_3$K)$_5$-corannulene **6**

1.38
1.24
1.09
0.95

f1 (ppm)

f1 (ppm)

24
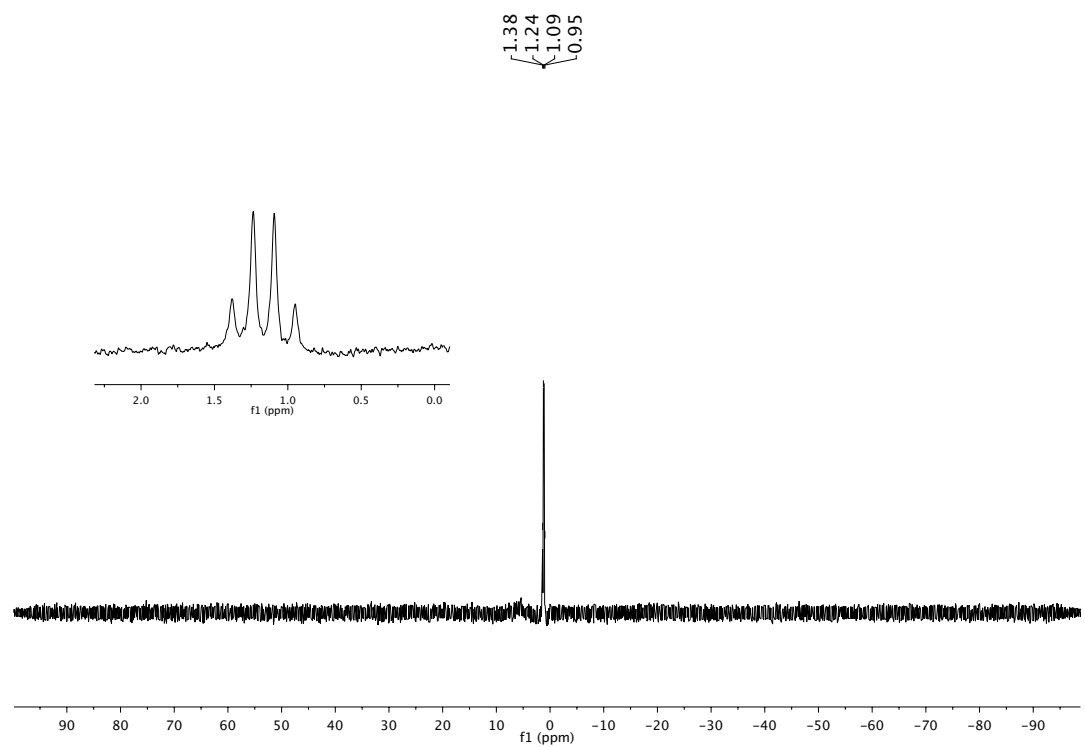
19F-NMR (376.5, 300K, DMSO-d_6): 1,3,5,7,9-(BF$_3$K)$_5$-corannulene **6**
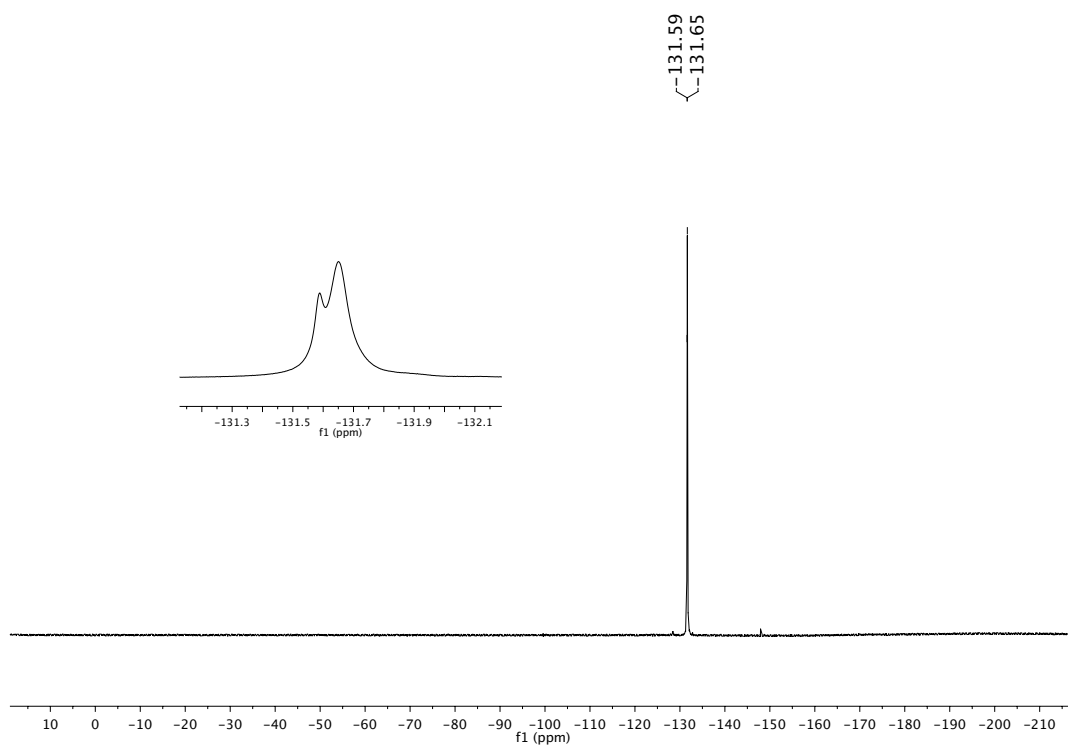
3.5. Compound 7

1H-NMR (500 MHz, 300K, MeOH-d_4): BF$_3$K-corannulene **7**

8.28
8.28
8.27
8.26

8.03

7.81
7.79
7.78
7.77
7.76
7.75
7.73

8.30 8.28 8.26 8.24 8.22 8.20 8.18 8.16 8.14 8.12 8.10 8.08 8.06 8.04 8.02 8.00 7.98 7.96 7.94 7.92 7.90 7.88 7.86 7.84 7.82 7.80 7.78 7.76 7.74 7.72 7.70
f1 (ppm)

13C-NMR (125.8 MHz, 300K, MeOH-d_4): BF$_3$K-corannulene **7**

137.08
136.97
136.96
136.82
136.69
136.60
132.53
131.96
131.72
131.70
131.12
129.94
129.92
129.90
129.87
128.37
127.95
127.76
127.38
127.32
127.25
126.49

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

26
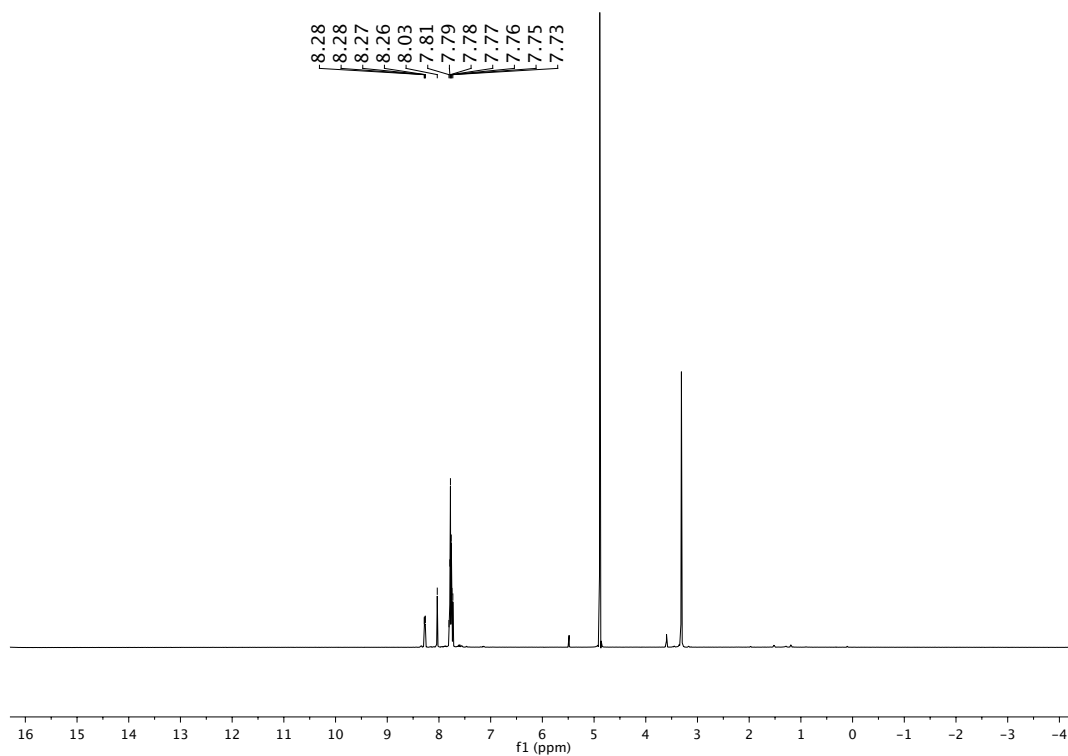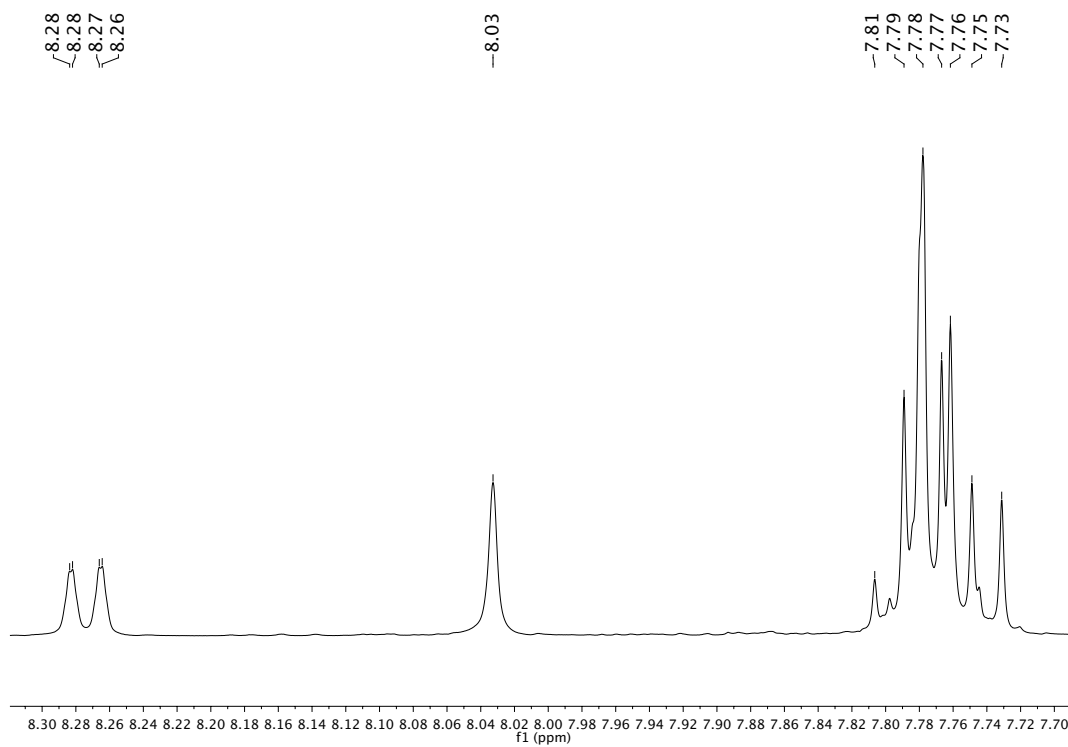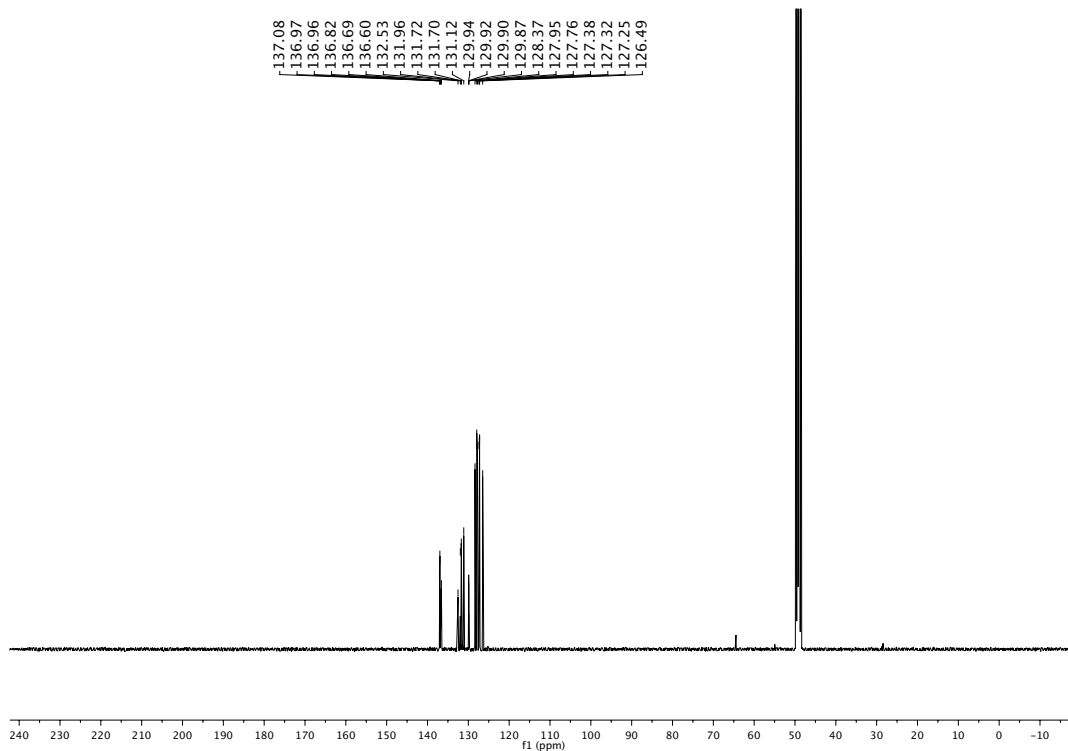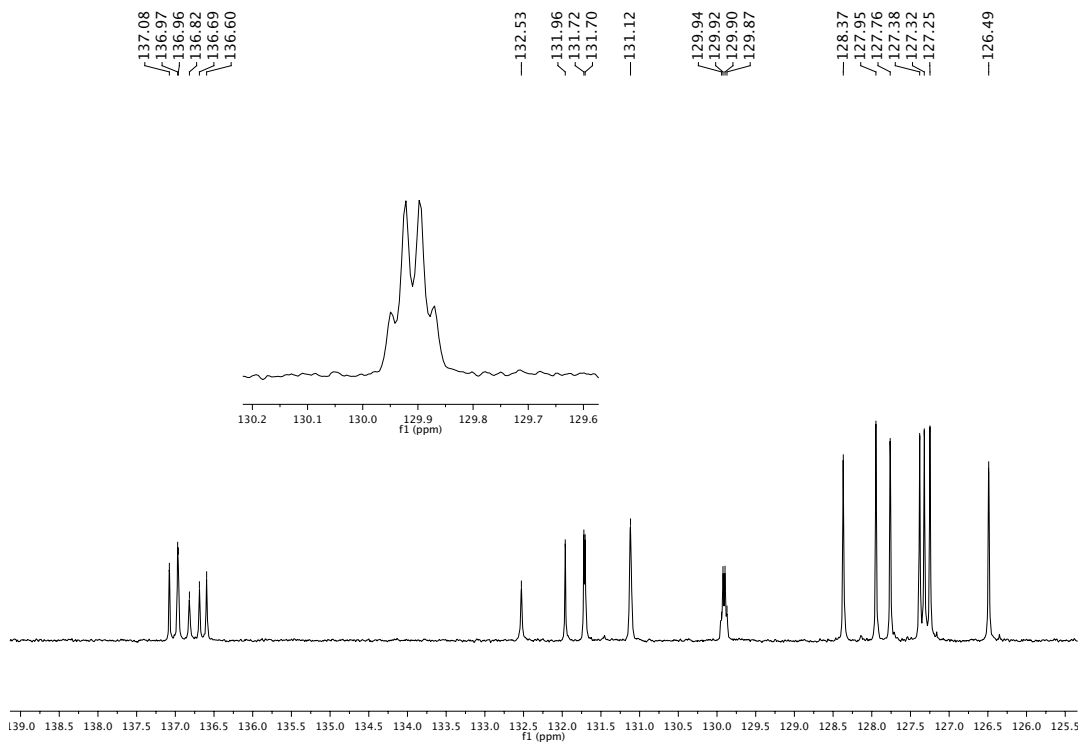
19F-NMR (376.5 MHz, 300K, MeOH-d_4): BF$_3$K-corannulene **7**
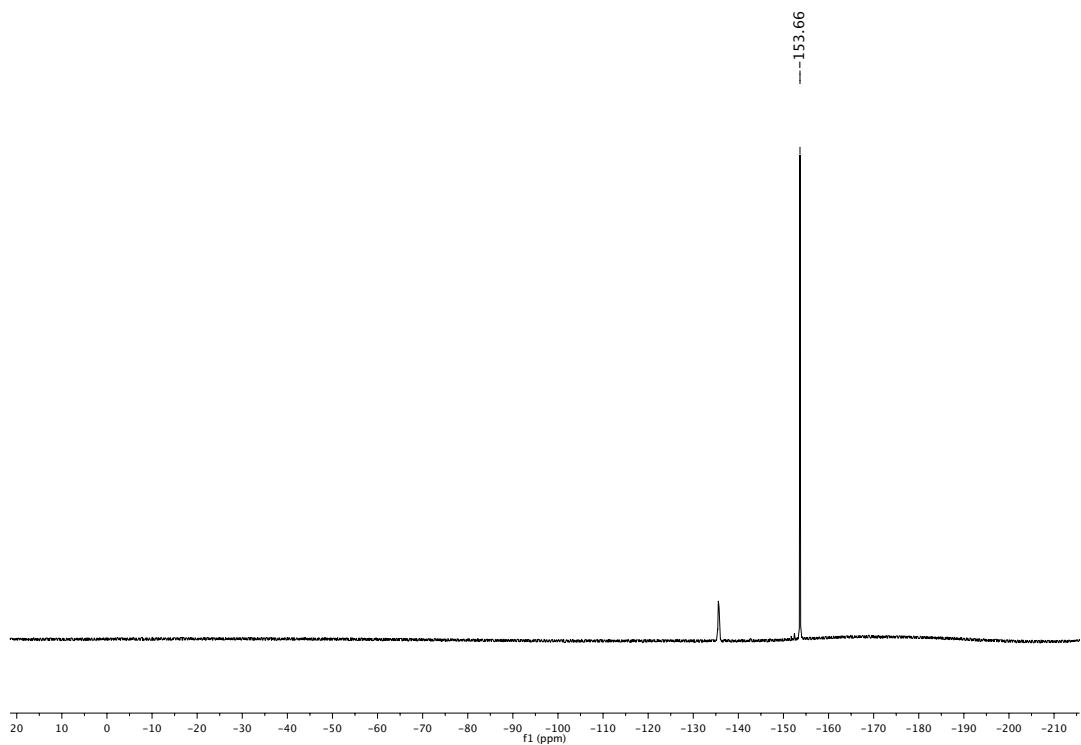
11B-NMR (128.5 MHz, 300K, MeOH-d_4): BF$_3$K-corannulene **7**
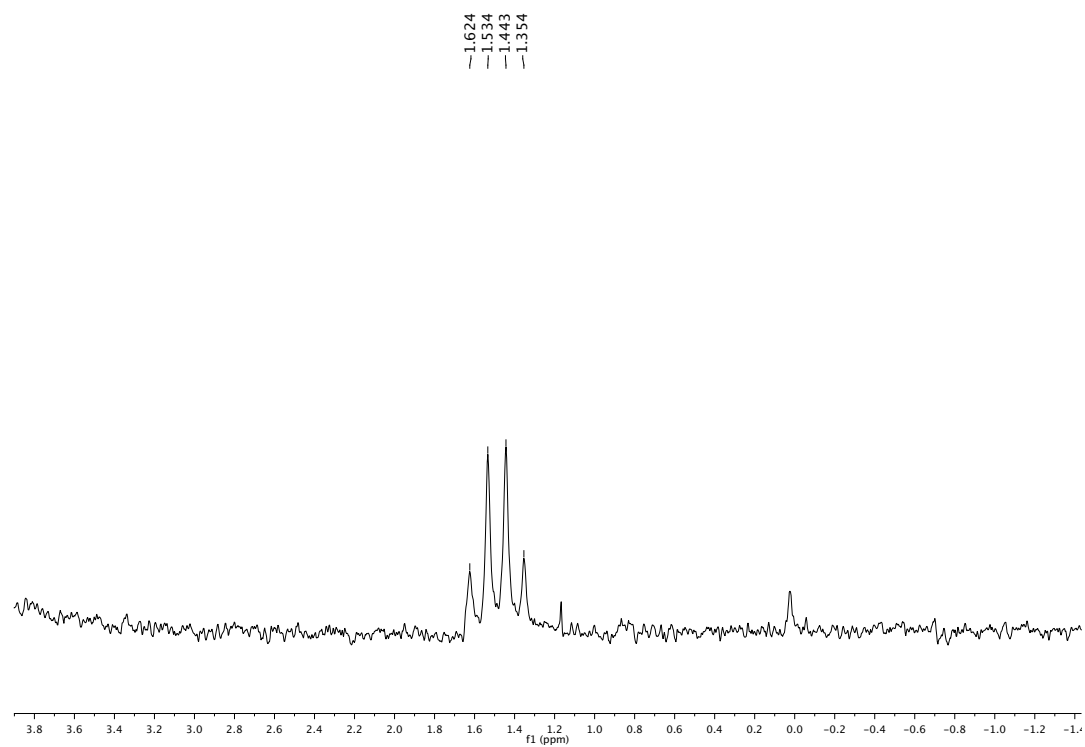
3.6. Compound 8

1H-NMR (500 MHz, 300K, MeOH-d_4): 1,3,5,7,9-corannulene pentaboronic acid **8**
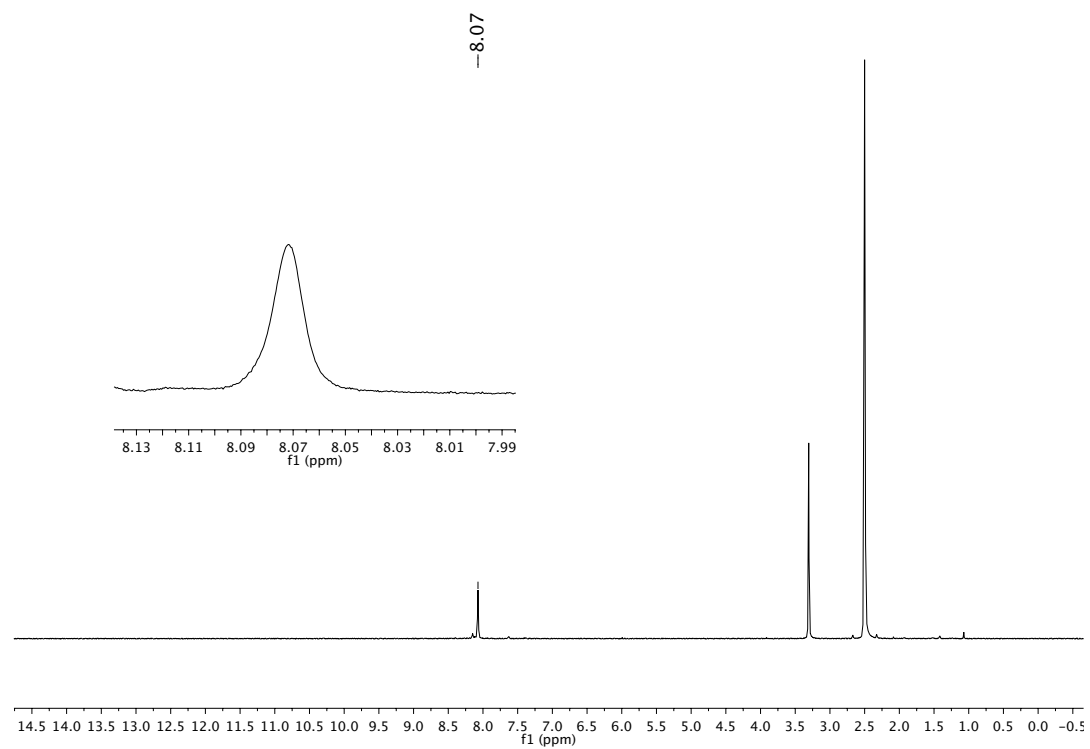
13C-NMR (125.8 MHz, 300K, MeOH-*d*₄): 1,3,5,7,9-corannulene pentaboronic acid **8**

137.21
134.82
133.60

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11B-NMR (128.5 MHz, 300K, MeOH-*d*₄): 1,3,5,7,9-corannulene pentaboronic acid **8**

−19.31

90 90 80 70 60 50 40 30 20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90
f1 (ppm)

29
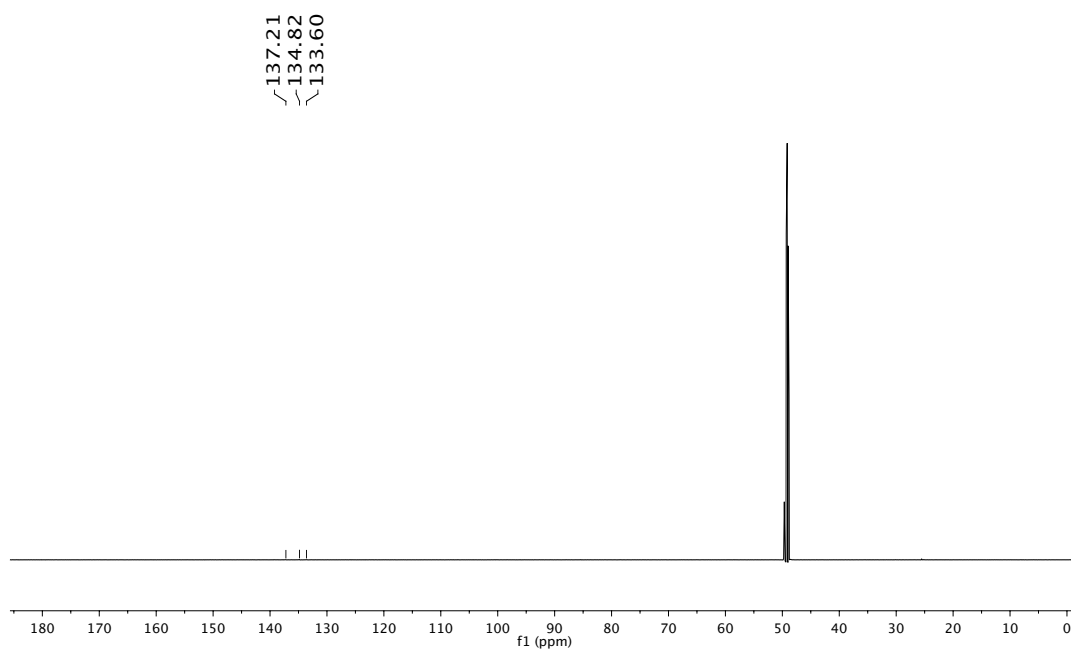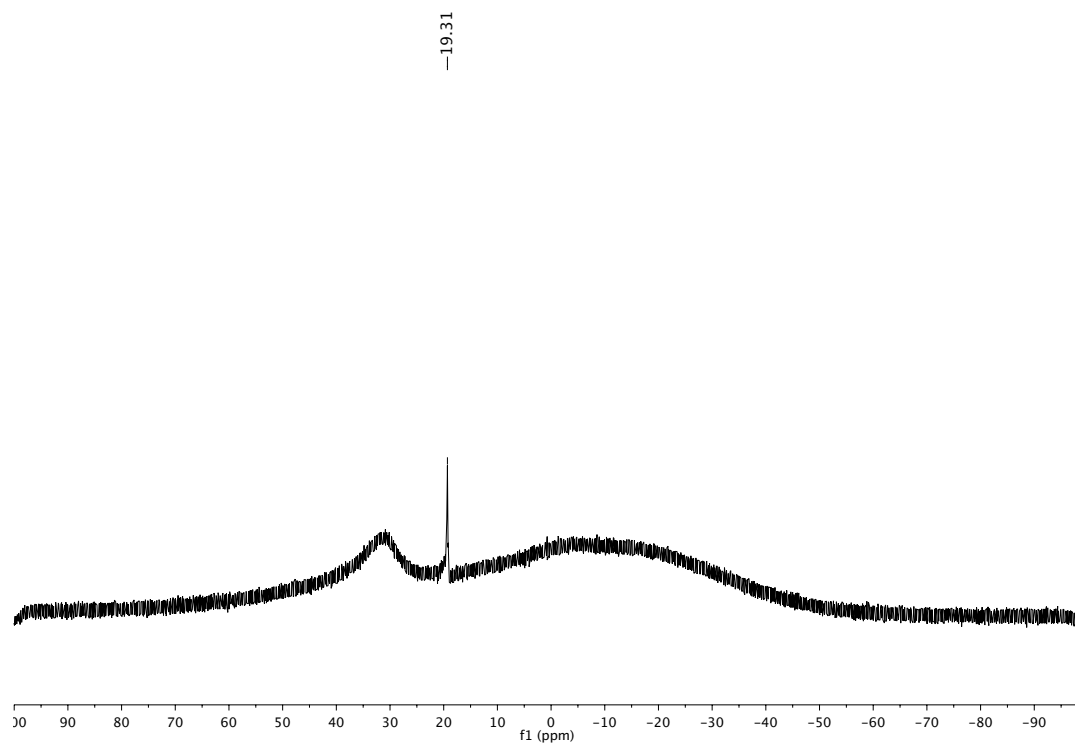
3.7. Compound 8a

1H-NMR (500 MHz, 300K, MeOH-d_4): corannulene boronic acid **8a**
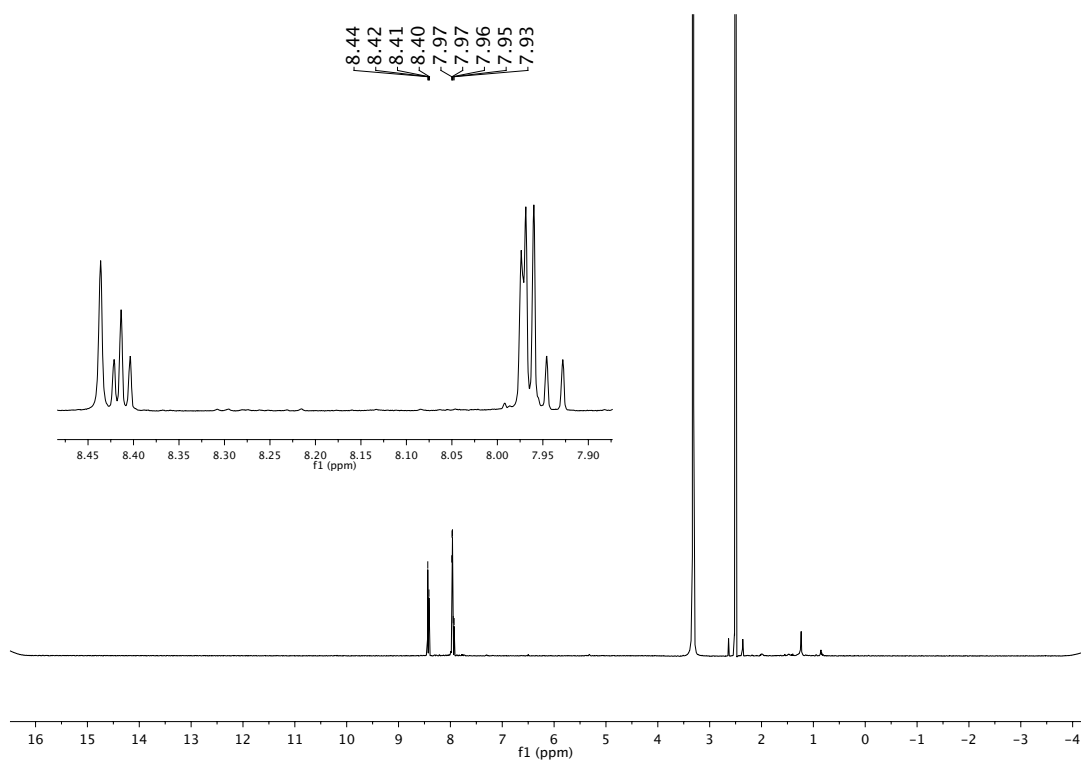
13C-NMR (500 MHz, 300K, D$_2$O): corannulene boronic acid **8a**
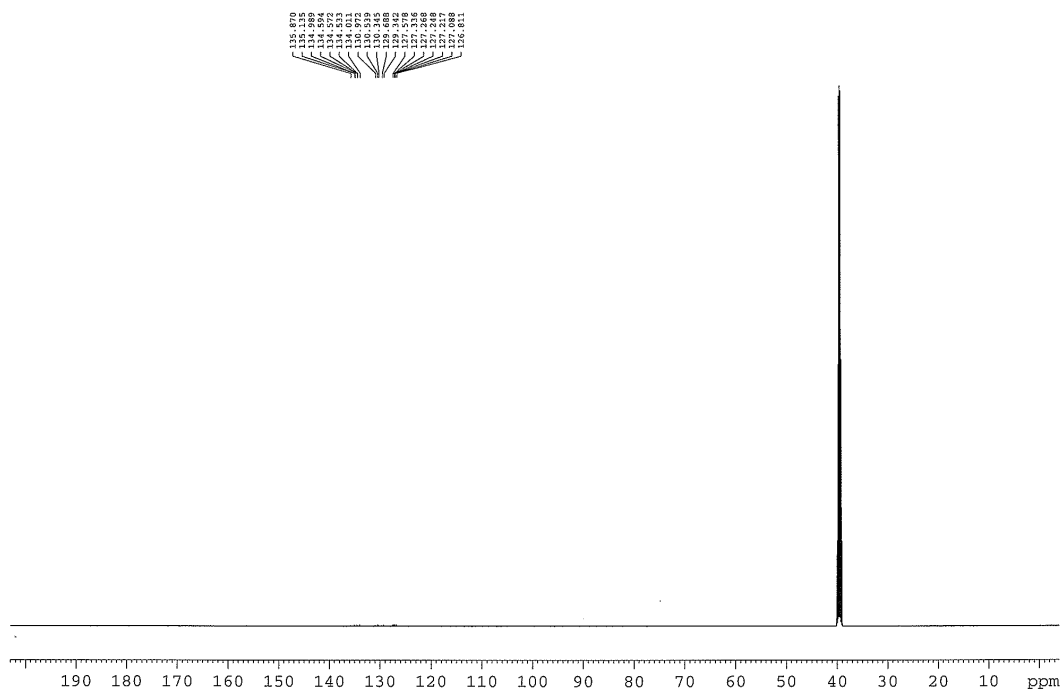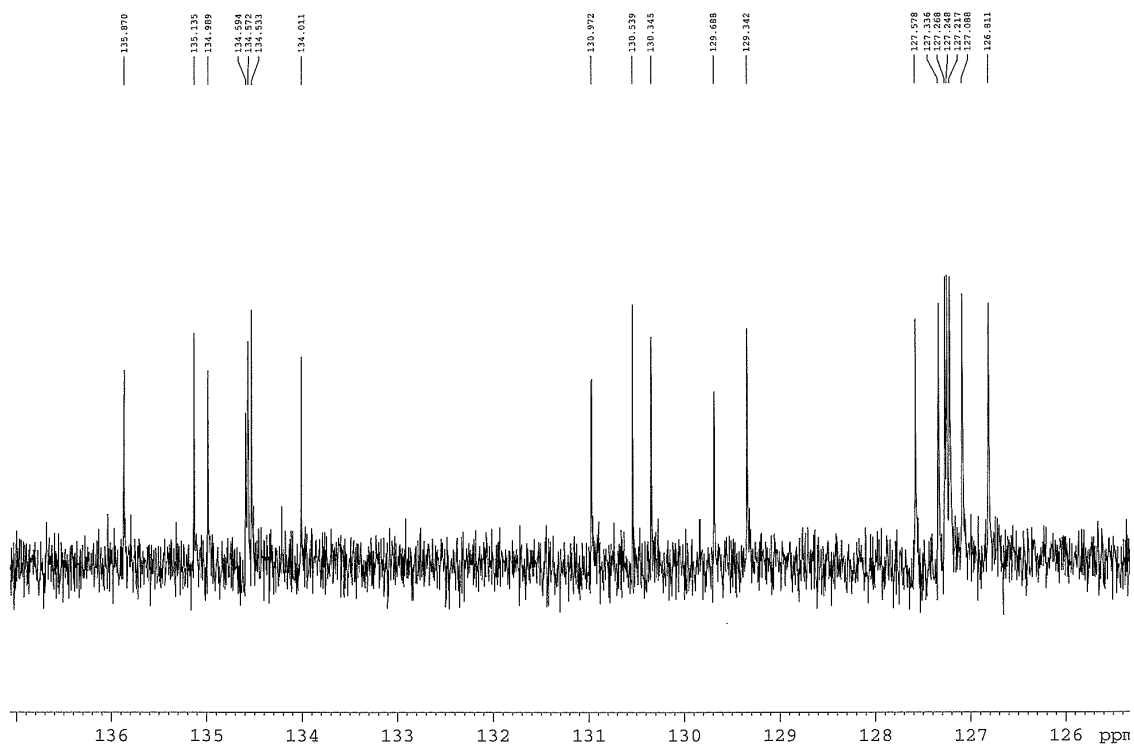
3.8. Compound 9

1H-NMR (500 MHz, 300K, CDCl$_3$): 1,3,5,7,9- corannulene pentaboronic acid, 1,3-propanediol pentaester **9**

13C-NMR (125.8 MHz, 300K, CDCl₃): 1,3,5,7,9- corannulene pentaboronic acid, 1,3-propanediol pentaester **9**

137.25
136.46
132.54
62.12
27.55

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

11B-NMR (128.5 MHz, 300K, CDCl₃): 1,3,5,7,9- corannulene pentaboronic acid, 1,3-propanediol pentaester **9**

18.39

22 21 20 19 18 17 16 15 14
f1 (ppm)

95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 −5 −10 −15 −20 −25
f1 (ppm)

32
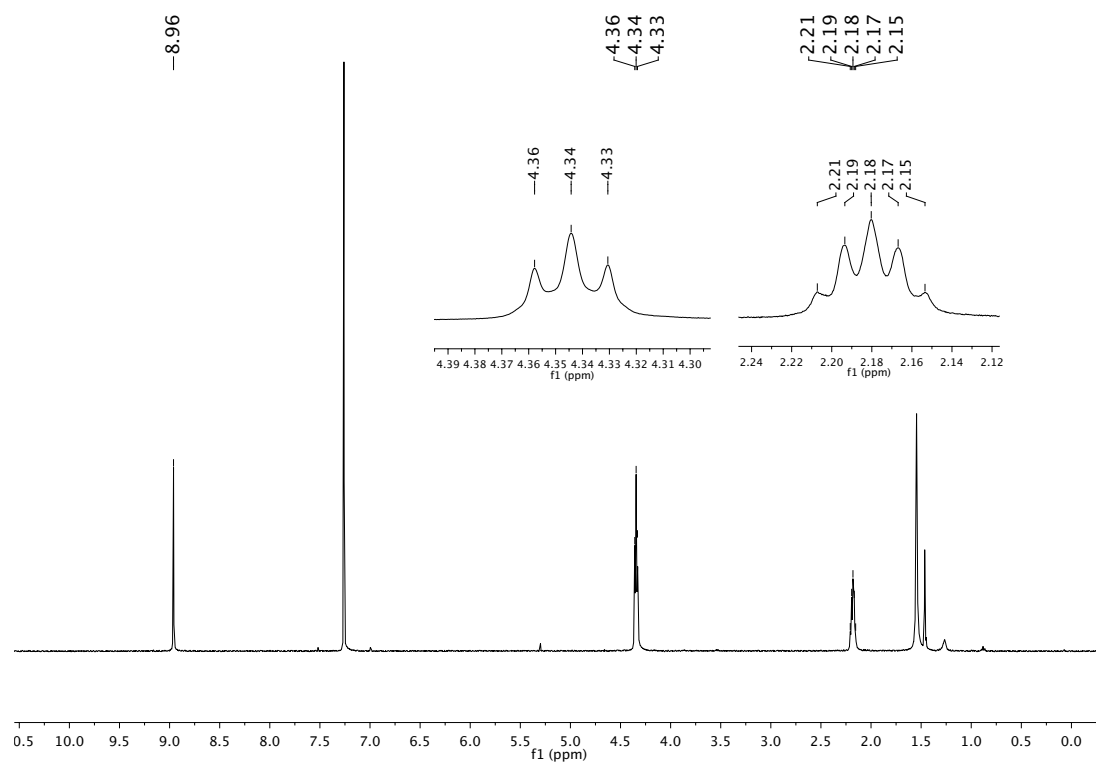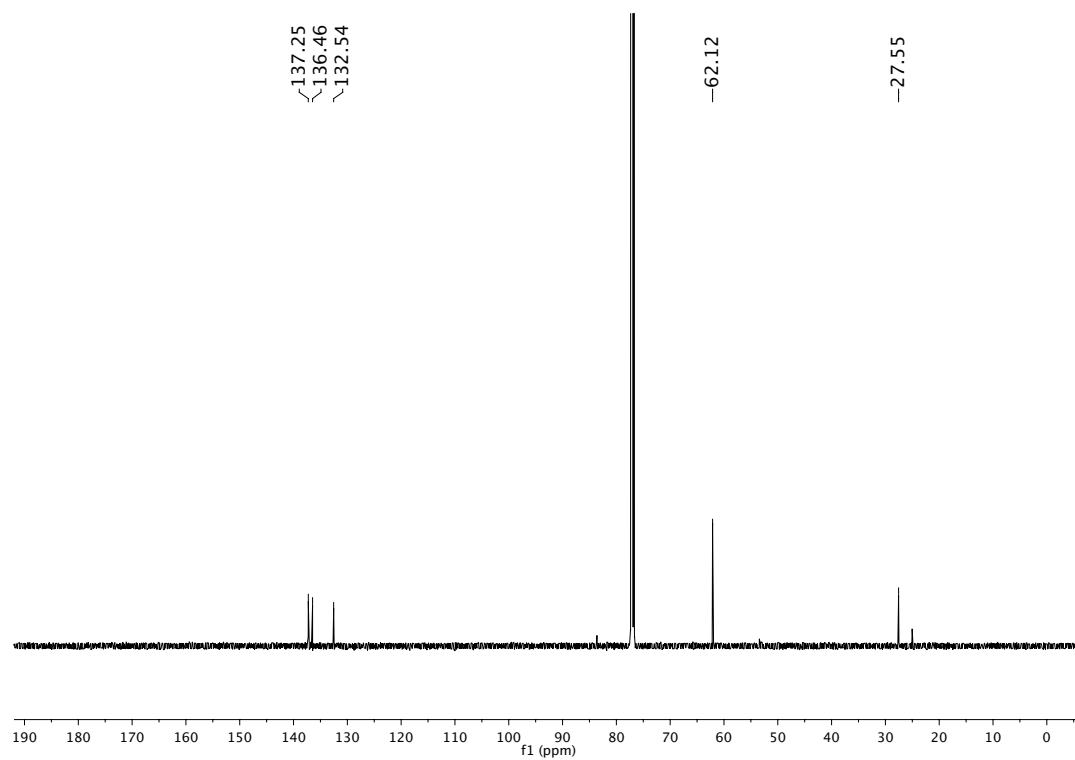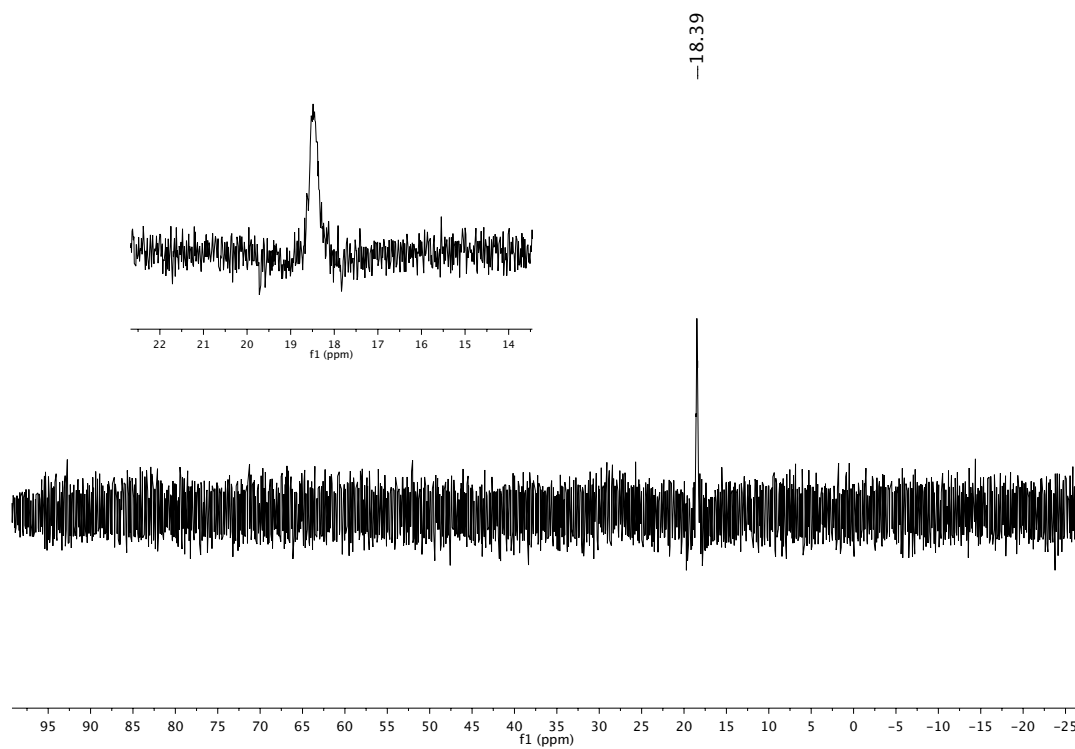
3.9. Compound 10

1H-NMR (500 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, 2,2'-dimethyl-1,3-propanediol pentaester **10**
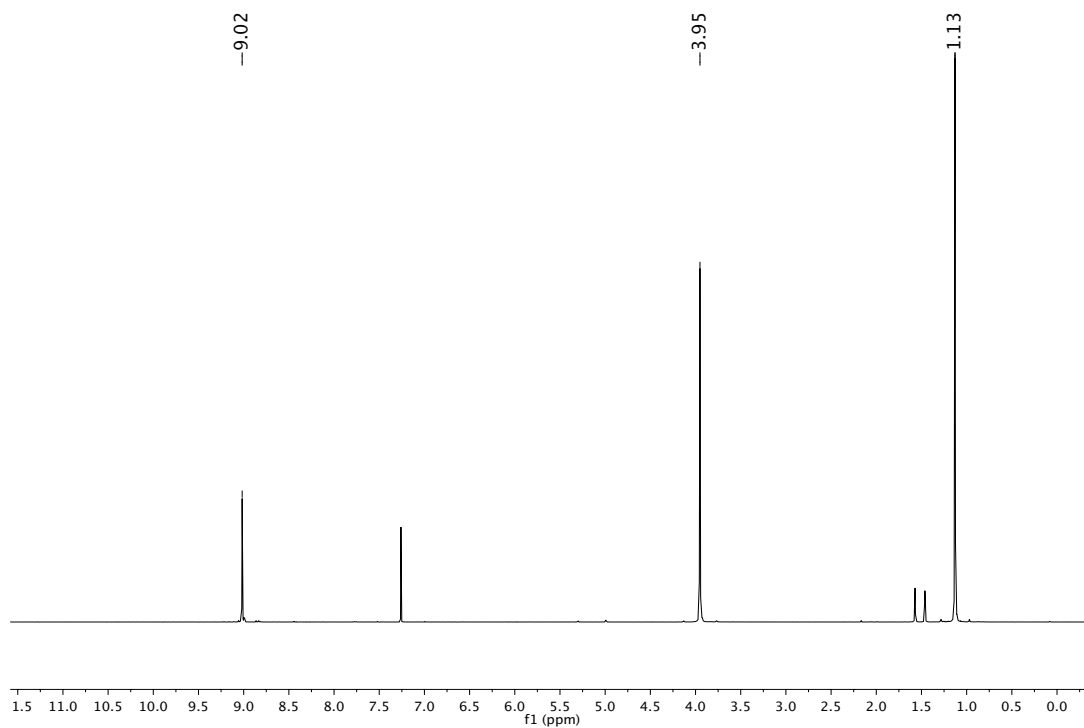
13C-NMR (125.8 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, 2,2'-dimethyl-1,3-propanediol pentaester **10**

11B-NMR (128.5 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, 2,2'-dimethyl-1,3-propanediol pentaester **10**

−16.52
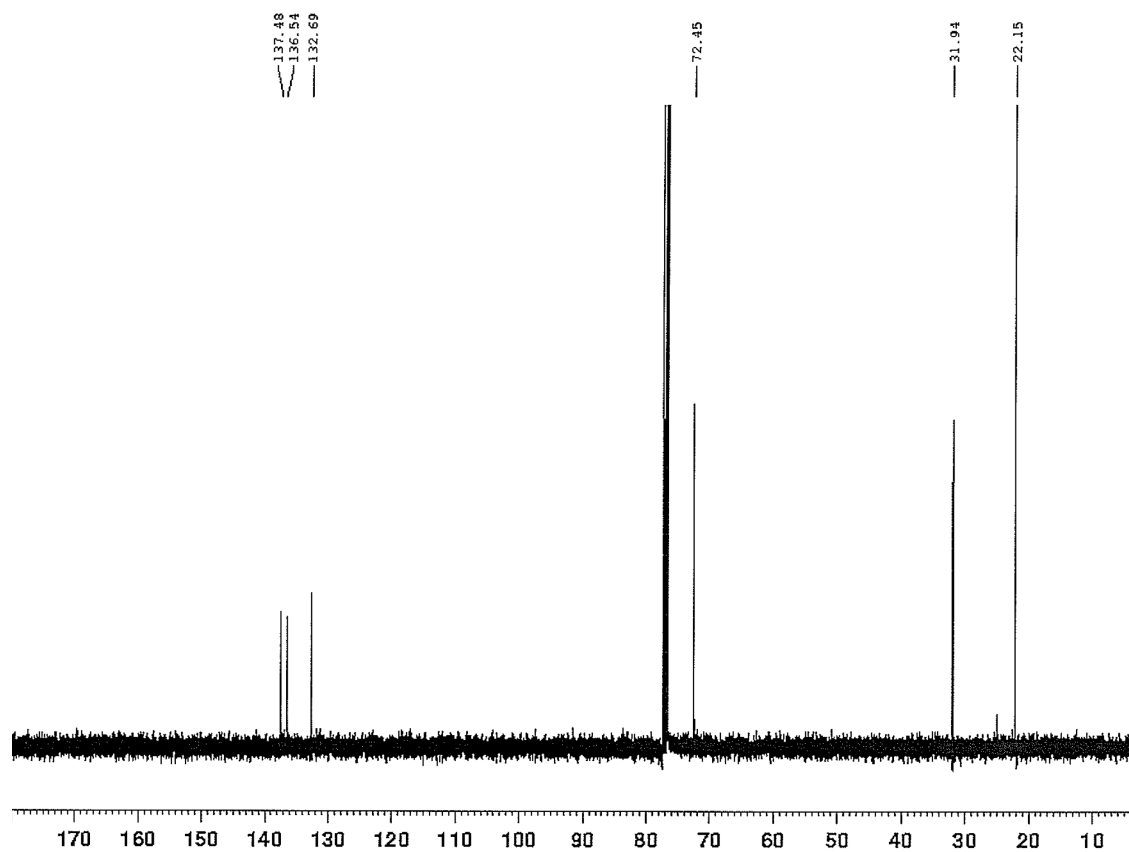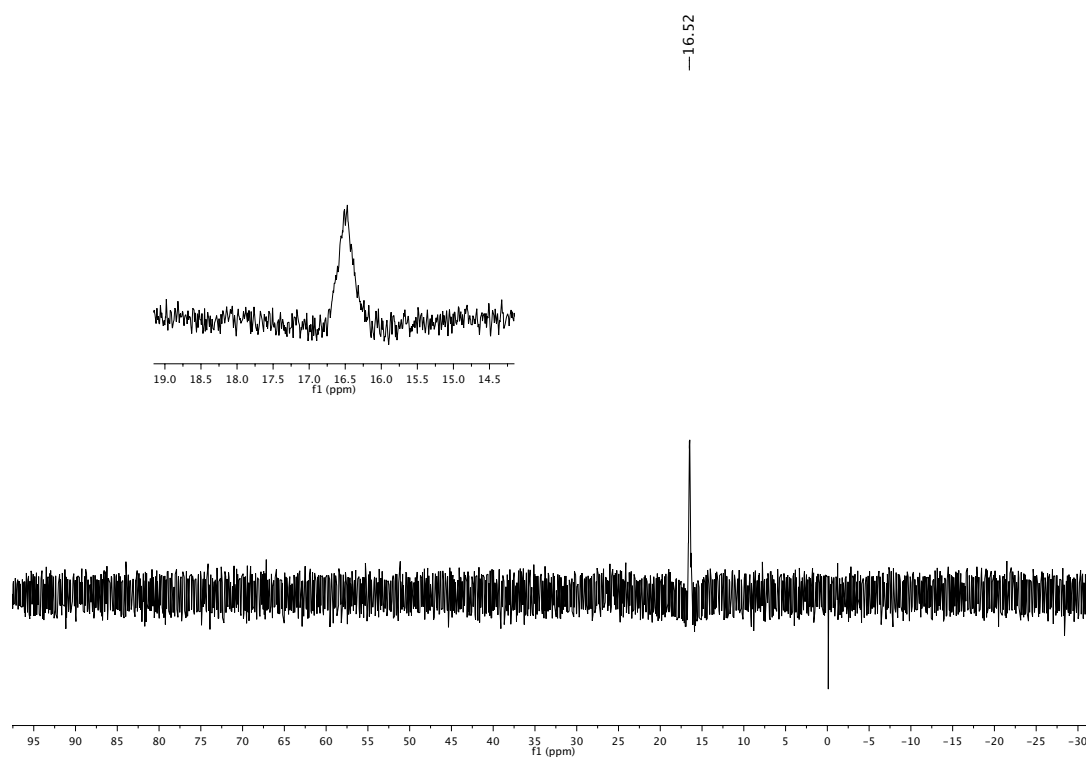
3.10. Compound 11

1H-NMR (125.8 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, *cis*-cyclopentanediol pentaester **11**

−8.97

5.16
5.15
2.21
2.20
2.18
2.17
1.84
1.83
1.81
1.80
1.79
1.78
1.75
1.74
1.71
1.70
1.69

5.00

10.31

10.48
20.34
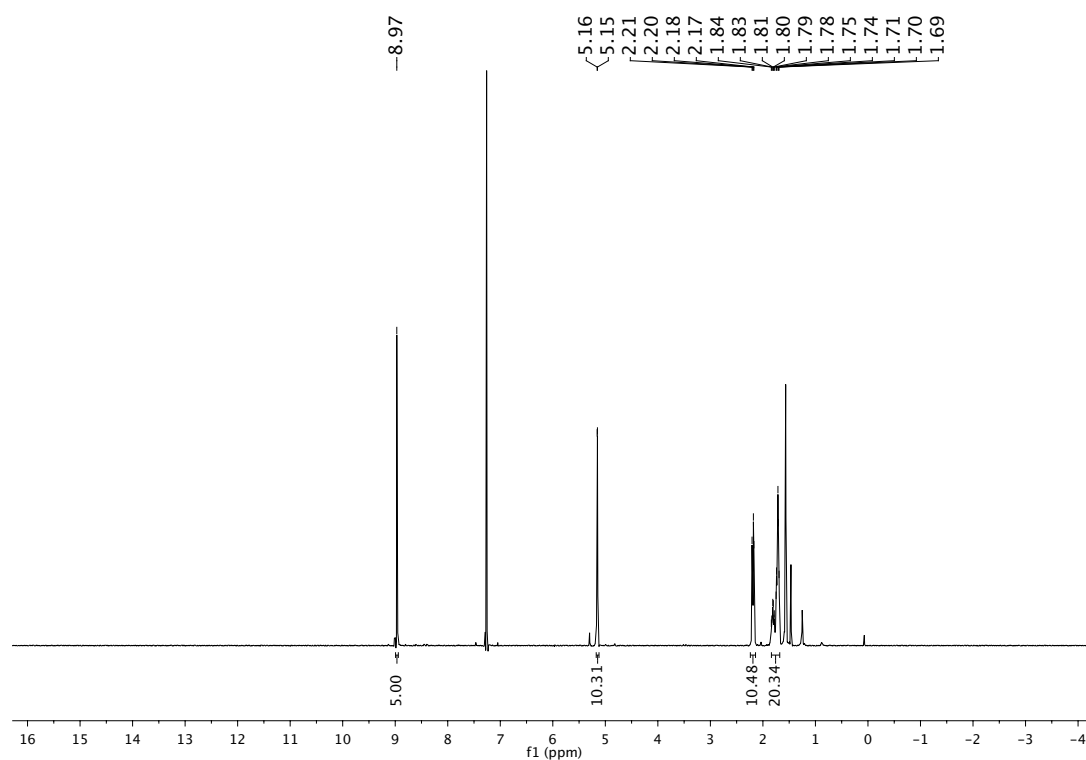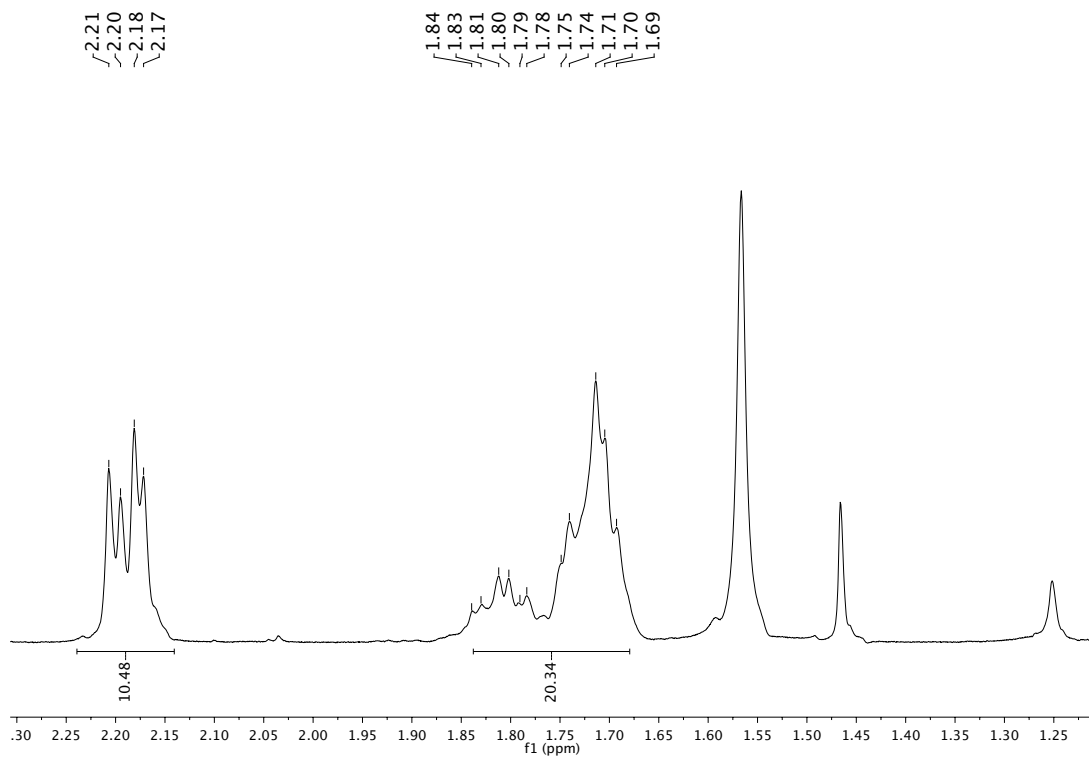
^{13}C-NMR (125.8 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, *cis*-cyclopentanediol pentaester **11**
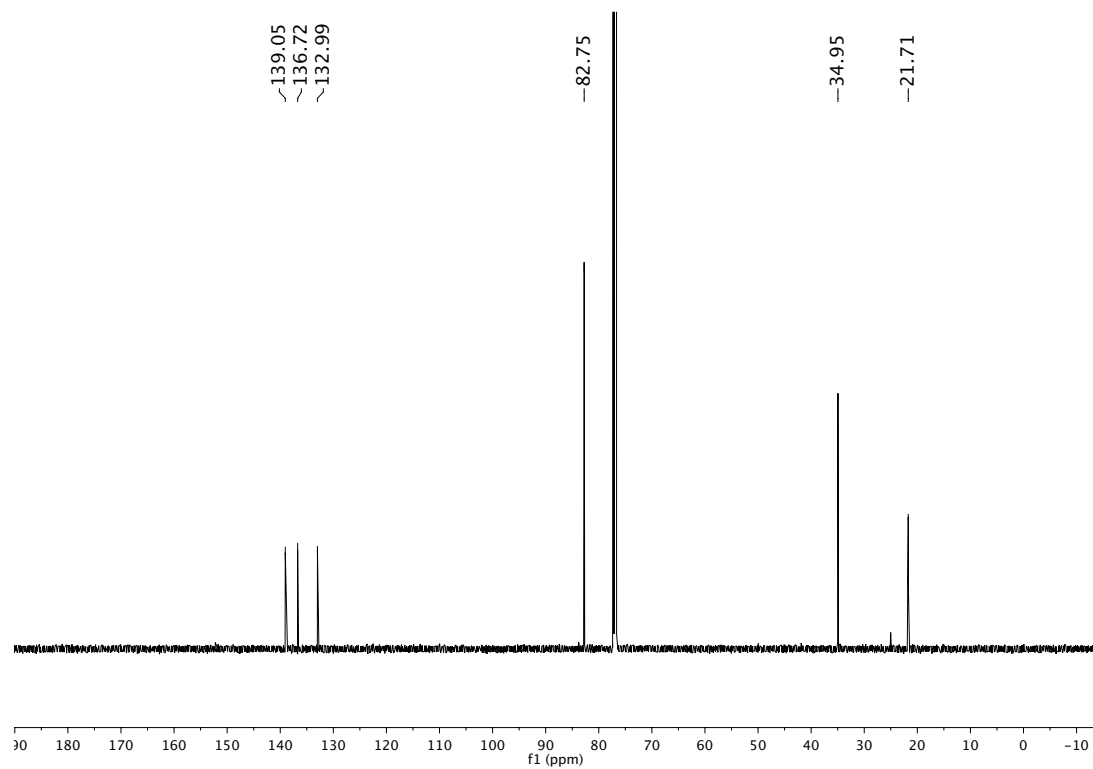
3.11. Compound 12

^{1}H-NMR (500 MHz, 300K, CDCl$_3$): 1,3,5,7,9-corannulene pentaboronic acid, *cis*-cyclohexanediol pentaester **12**
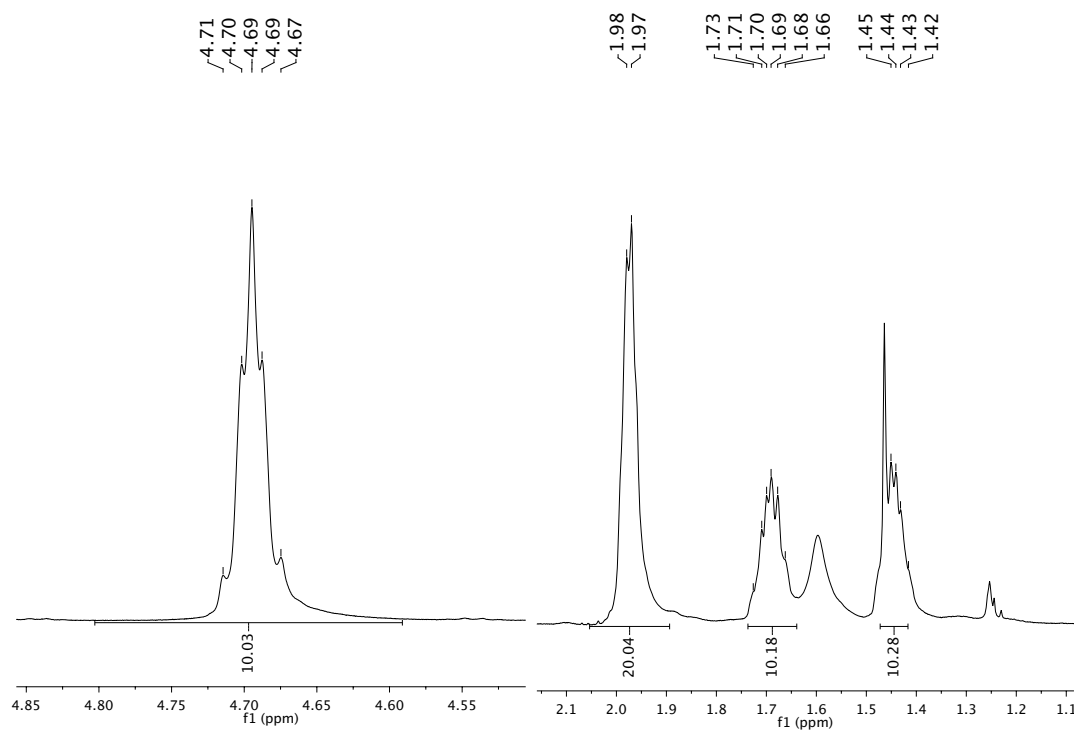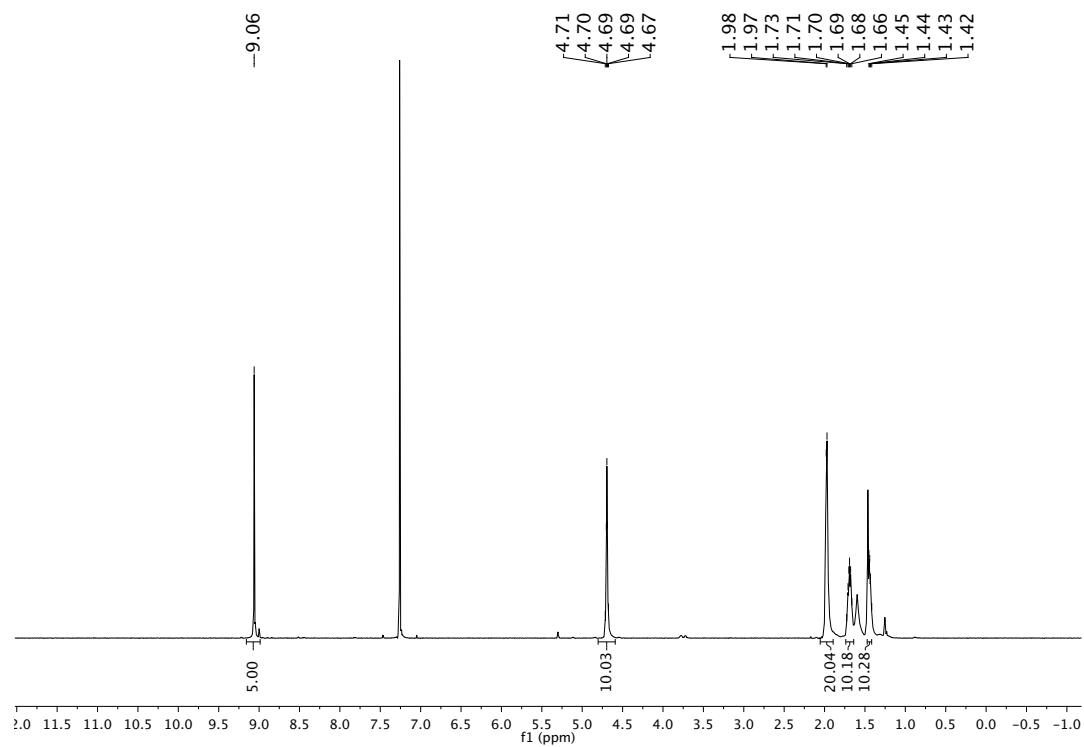
¹³C-NMR (125.8 MHz, 300K, CDCl₃): 1,3,5,7,9-corannulene pentaboronic acid, *cis*-cyclohexanediol pentaester **12**
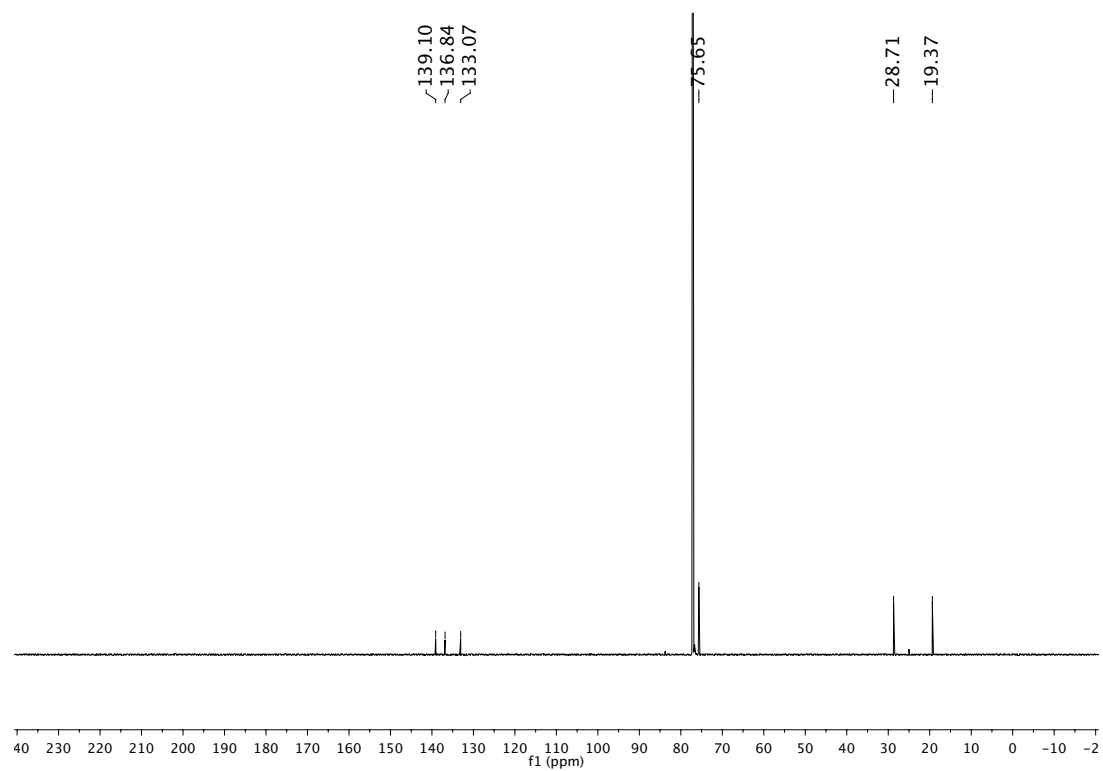
11B-NMR (128.5 MHz, 300K, CDCl₃): 1,3,5,7,9-*Pentakis*(boronic acid)corannulene *cis*-cyclohexanediol ester **12**
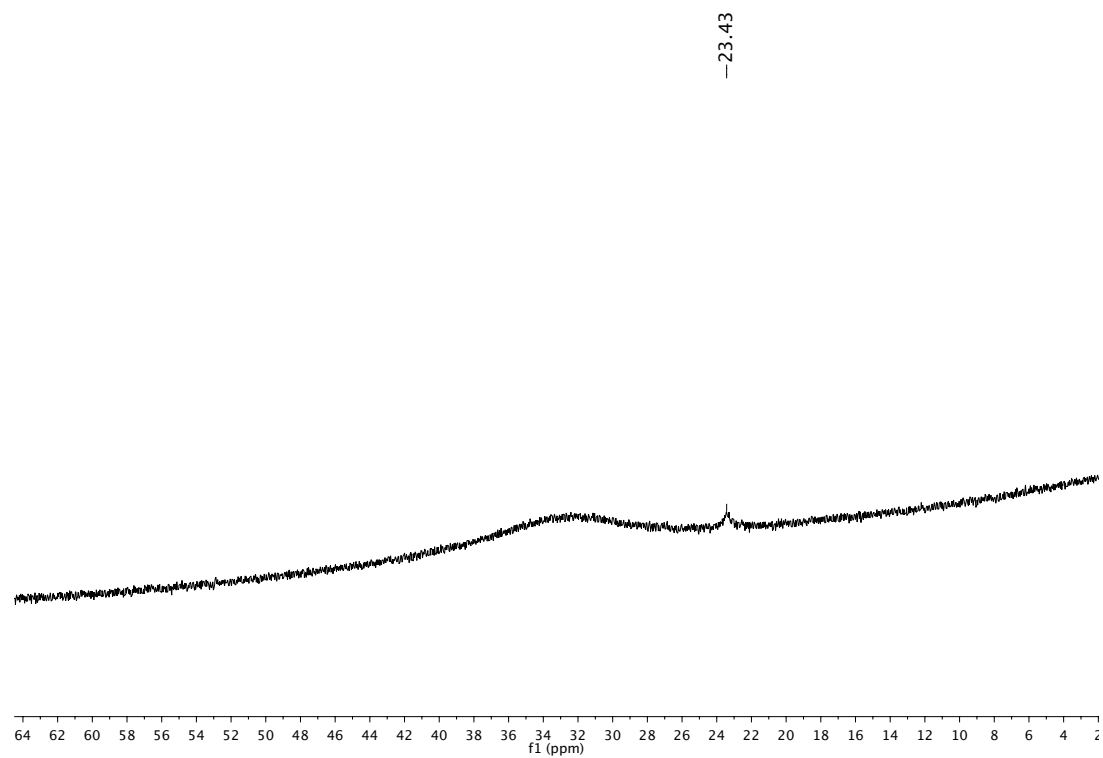
3.12. Compound 13

^{1}H-NMR (500 MHz, 300K, MeOH-d_4): 1,3,5,7,9- corannulene pentaboronic acid, catechol pentaester **13**
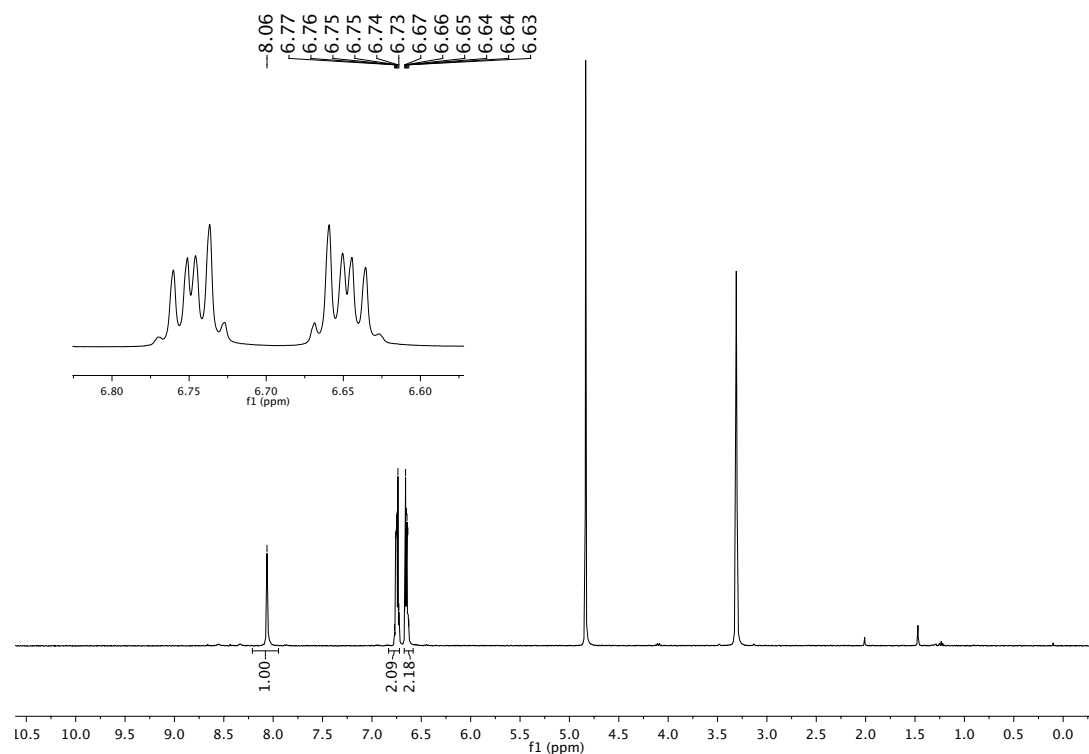
^{13}C-NMR (125.8 MHz, 300K, MeOH-d_4): 1,3,5,7,9- corannulene pentaboronic acid, catechol pentaester **13**

38
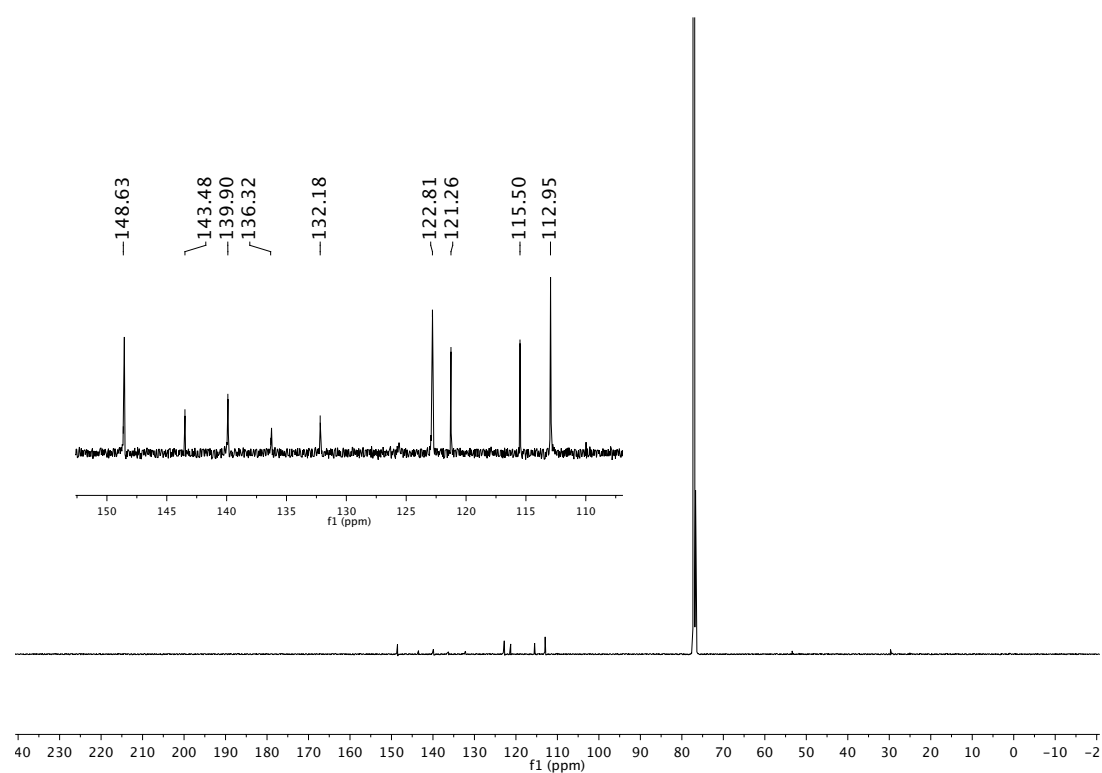
^{11}B-NMR (128.5 MHz, 300K, MeOH-d_4): 1,3,5,7,9- corannulene pentaboronic acid, catechol pentaester **13**
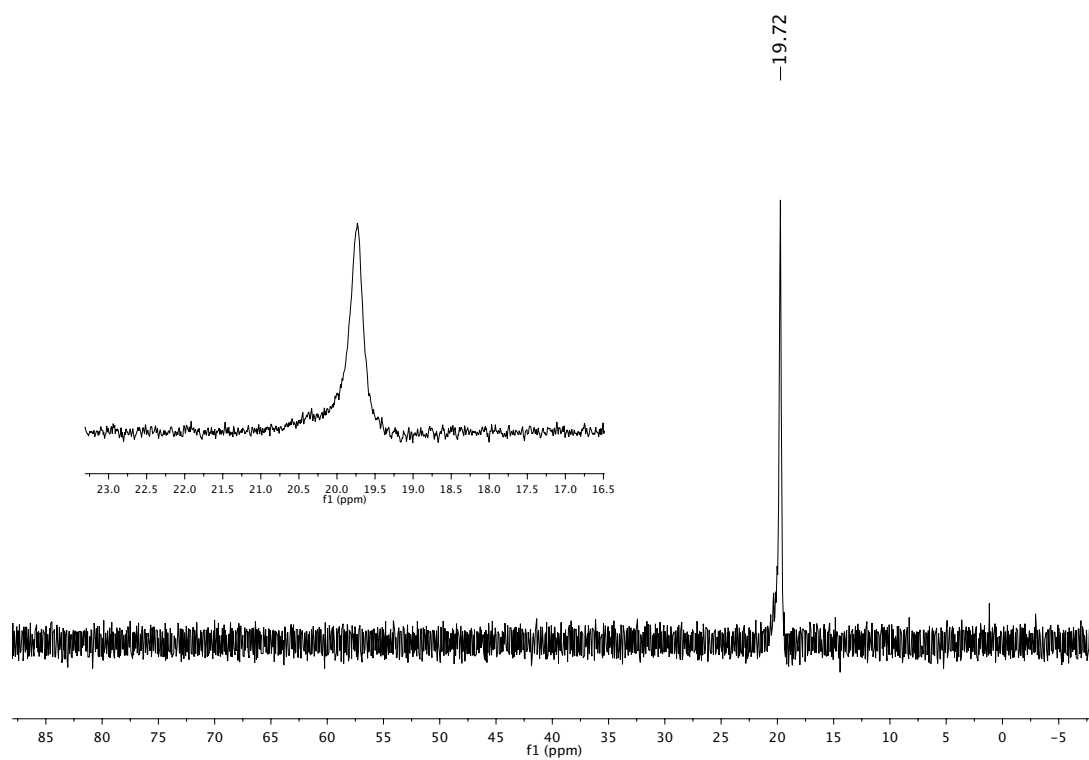
4. Vt-NMR Experiments

4.1. Experimental Procedure

Vt-NMR measurements of boronic ester **3** were performed in dichlorofluoromethane-d_1 (freon-21) from -50 °C to -135 °C on a 500 MHz NMR instrument.
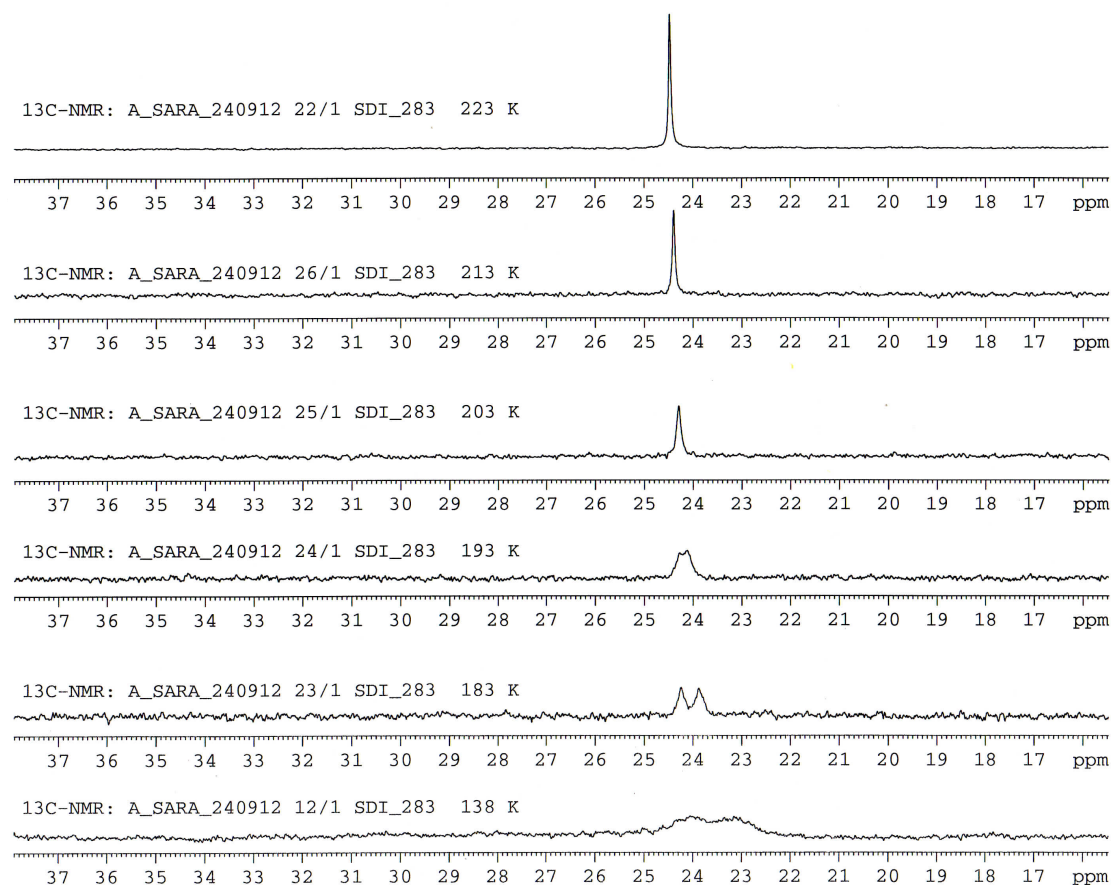
4.2. Calculation and Results

T_c = 195 K, $\Delta\upsilon°_{AB}$ = 50.32 Hz (0.4 ppm)

The rate constant at coalescence, k_c, was calculated by means of the Gutowsky-Holm approximation and was identified to be 111.7 s^{-1}. To calculate the bowl inversion energy of the dynamic bowl-to-bowl inter-conversion of **3**, the Eyring equation was used. The bowl inversion energy turned out to be 9.43 kcal/mol.

4.3. Comparison to Computational DFT-Calculations

	Structure	Bowl Depth [Å]	Bowl Inv. En. [kcal/mol]	Bowl Inv. Freq. [s⁻¹]
Experimental Data	**3**	0.9	9.43	-
	1	0.87	11.5	-
DFT-calculations	**3**	0.872	8.82	-71.4
	1	0.916	10.57	-116.2

5. Cyclic voltammetry

5.1. Experimental

THF for voltammetric measurements was distilled over CaH_2 prior to its use. Electrolyte tetrabutylammonium hexafluorophosphate (TBAHFP) was purchased from *Fluka Chemie AG* and used as received. Cyclic Voltammetry: *CHI600C Electrochemical Analyzer, CH Instruments, Inc.* Electrodes: Non-Aqueous Ag/Ag$^+$ Reference Electrode (10 mM AgNO$_3$ in 0.1 M Bu$_4$NPF$_6$ in acetonitrile); platinum wire counter electrode; glassy carbon working electrode. Experiments were carried out under argon atmosphere with a concentration of 1 mM analyte at a temperature of 298 K. As supporting electrolyte 0.07 M TBAPF$_6$ in THF was used. The measurments were carried out under a scan rate of 0.1 V/s if not otherwise stated. The redox potential were referenced against ferrocinium/ferrocene couple standard potential (+0.085 V for THF[7]) as internal standard. Depicted cyclic voltammograms below do include the correction factor from the internal standard. All $E_{1/2}$ potentials have been directly obtained from cyclic voltammetric curves as averages of the cathodic and anodic peak potentials. For irreversible peaks, the peak potential is given.

5.2. Results

Cyclic voltammetry data was collected for the three bronic esters, *sym-pentakis*(Bpin)corannulene **3**, 1-(Bpin)corannulene **4**, *sym-pentakis*-corannyl boronic (cis-cyclopentane) ester **11**. In the following the electrochemical properties of **3**, **4** and **11** are discussed.

Compounds	Electrochemical reduction potentials ($E_{1/2}$) [V]		
	$^1E_{1/2}$	$^2E_{1/2}$	$^3E_{1/2}$
Corannulene	-2.45	-	-
3	-2.25	-2.38	-2.70
4	-2.42	-2.41	-2.84
11	-2.26	-2.40	-2.72

Table 5.2.1. Electrochemical reduction potentials of boronic ester **3**, **4** and **11** compared to their parent , corannulene.

[7] S. I. Bailey, W.-P. Leung, *Electrochimica Acta* **1985**, *30*, 861–863.
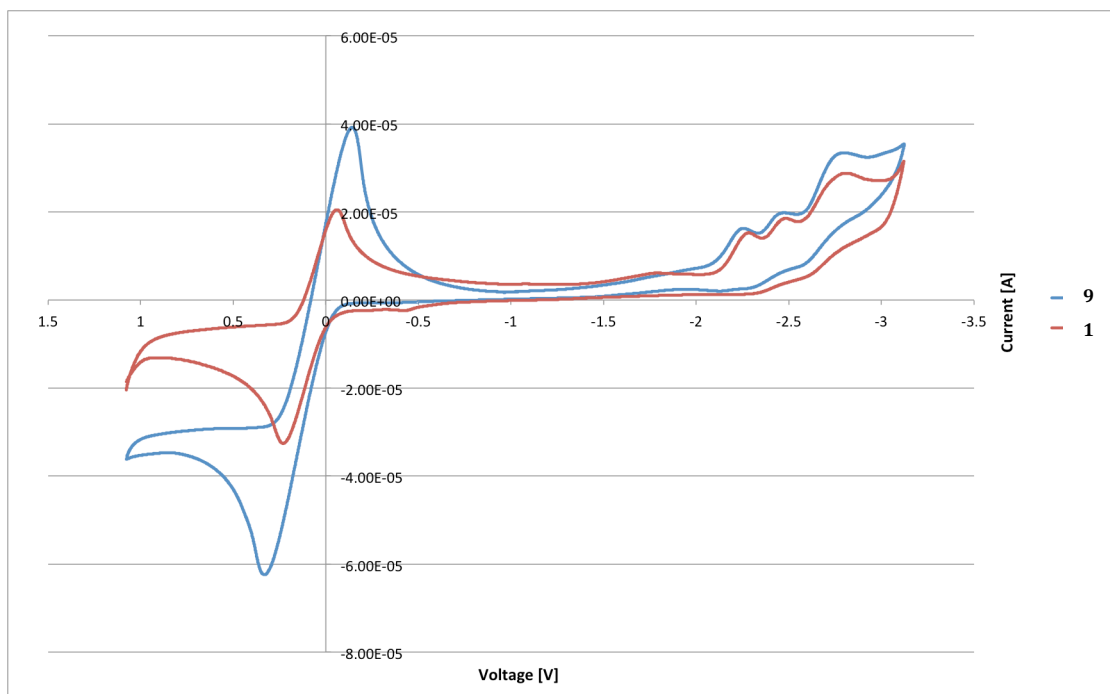
Figure 5.2.1. Comparison of pentapodal boronic ester **3** and **11** (Scan rate 0.1 V/s, solvent THF).
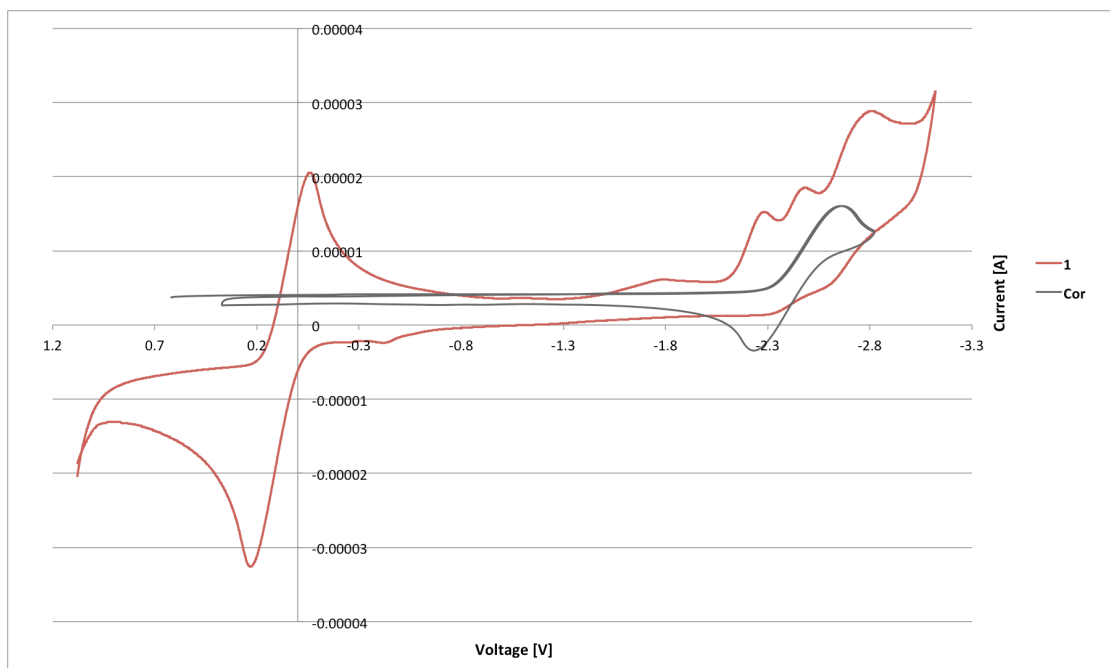
Figure 5.2.2. Comparison of cyclic voltammograms of pentapodal boronic ester **3** with corannulene **1** (Scan rate 0.1 V/s, solvent THF).
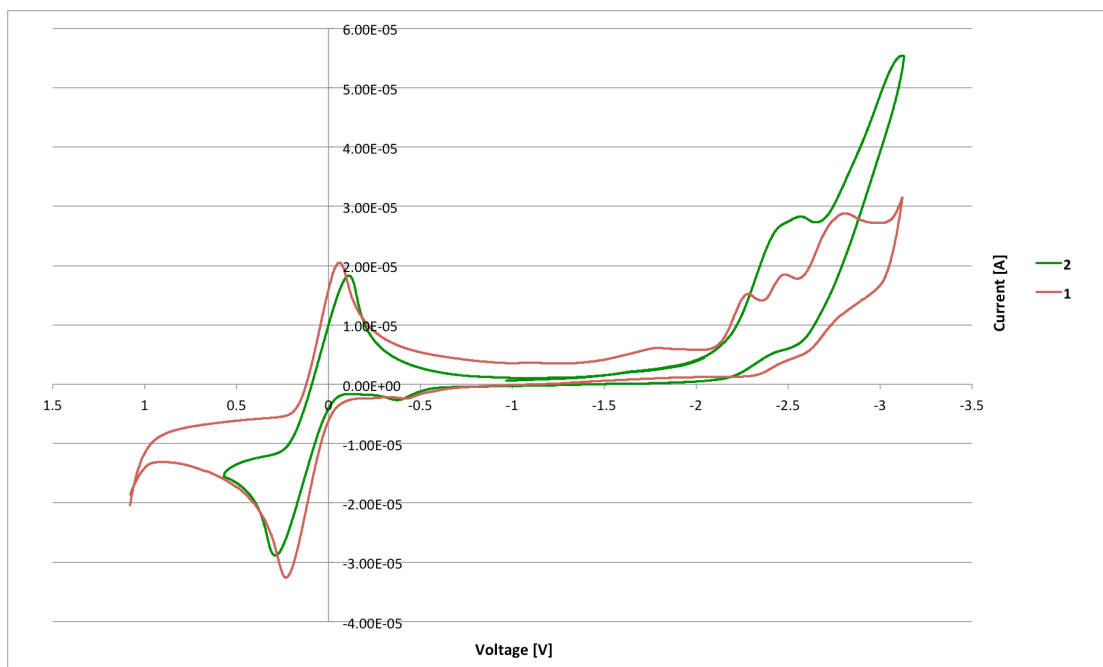
Figure 5.2.3. Comparison of cyclic voltammograms of pentapodal boronic ester **3** and **4** (Scan rate 0.1 V/s, solvent THF).
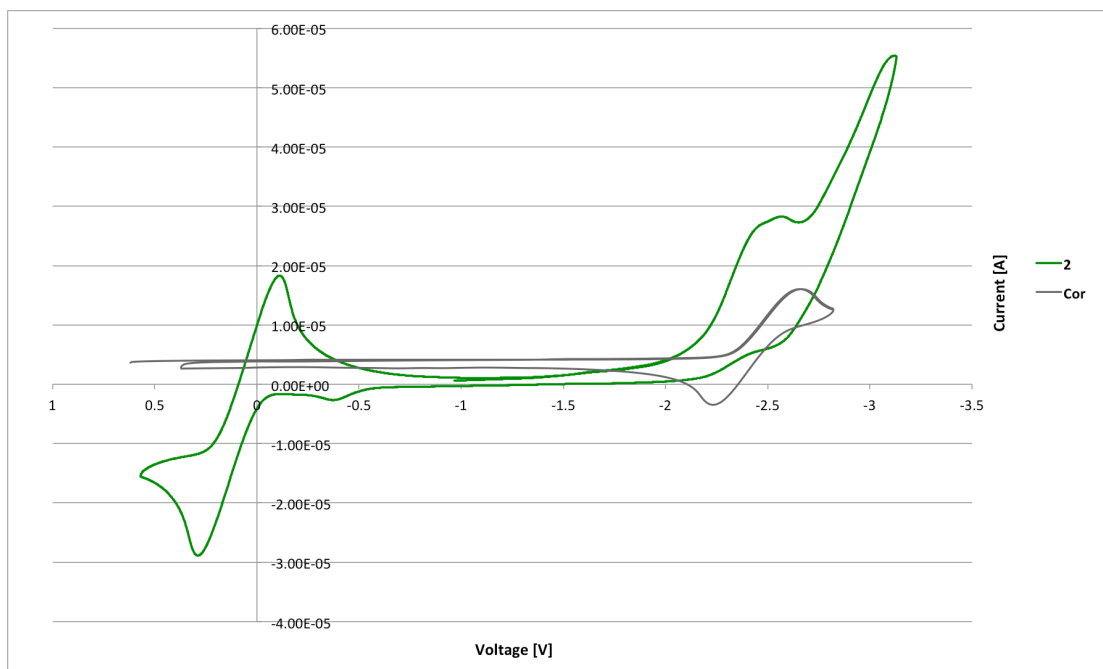
Figure 5.2.4. Comparison of cyclic voltammograms of pentapodal boronic ester **3** and corannulene **1** (Scan rate 0.1 V/s, solvent THF).

5.3. Comparison to Computational Calculations

System	E° (gas phase)	E° (THF)	Expt (THF)
1	-2.97	-2.49	-2.45
11	-3.86	-2.15	-2.25

Table 5.2.1. Comparison of experimental and computational data for the first reduction potentials of **11** and its parent **3**.

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6. HOMO-LUMO Orbitals

In the following the HOMO and LUMO orbitals of **3** are illustrated. An electrophilic HOMO map of **3** reveals that the highest polarity for an electrophilic attack is at the inner cyclopentadienyl ring of corannulene.

a)

b)

c)
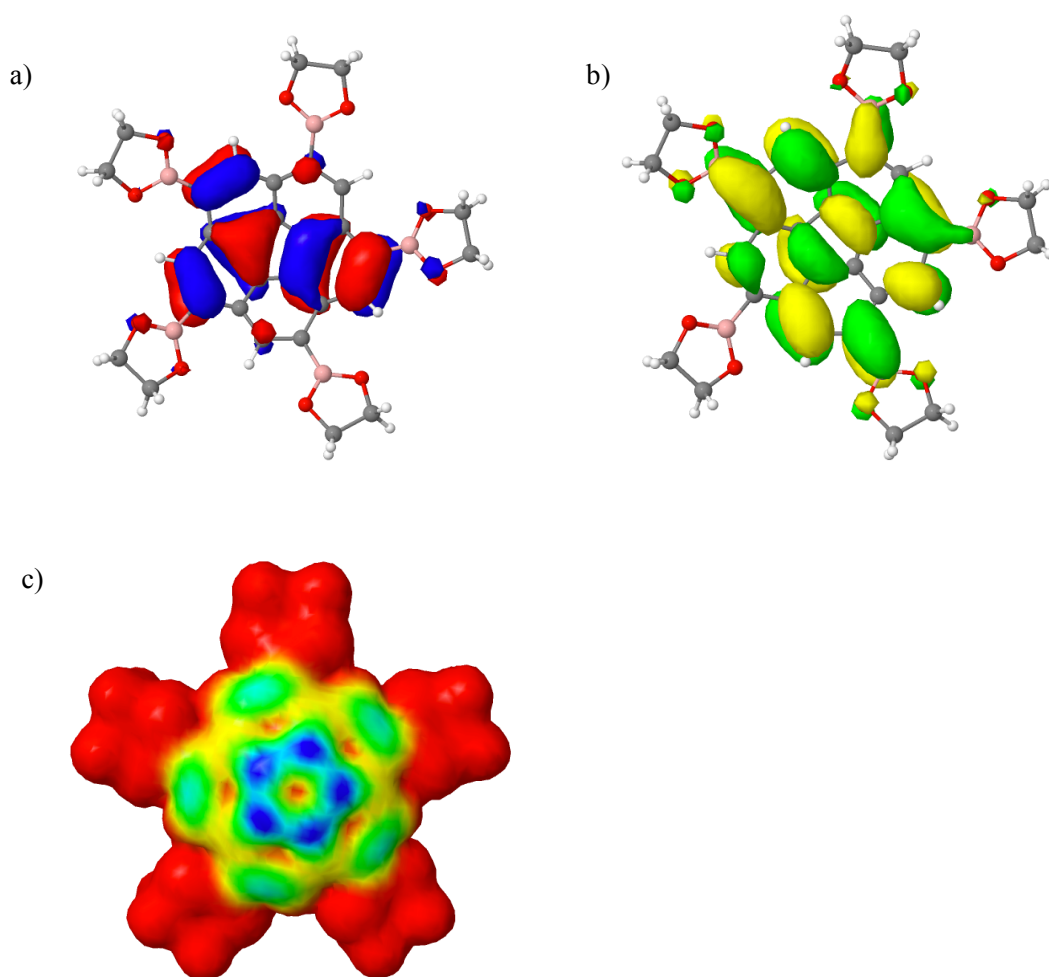
Figure 6.1. Representation of a) HOMO, b) LUMO orbitals of **3** and c) the corresponding electrophilic HOMO map (blue: highest chance for electrophilic attack, red: lowest chance for electrophilic attack).

7. UV-Vis

The collected UV/Vis and emission data reveals that all boronic esters, **9-13** as well as **3**, have similar absorption (λ_{max}: 275 nm, 307 nm) as well as emission (λ_{max}: 439-442 nm) behavior. Furthermore, all boronic esters show a large red shift of roughly 20-24 nm of the π-π* absorption band in the UV/Vis as well as in the emission spectra. The large Stokes shift in boronic ester compounds might be observed due to the significant geometrical distortion in the S1-state as well as contribution from the intramolecular charge transfer.
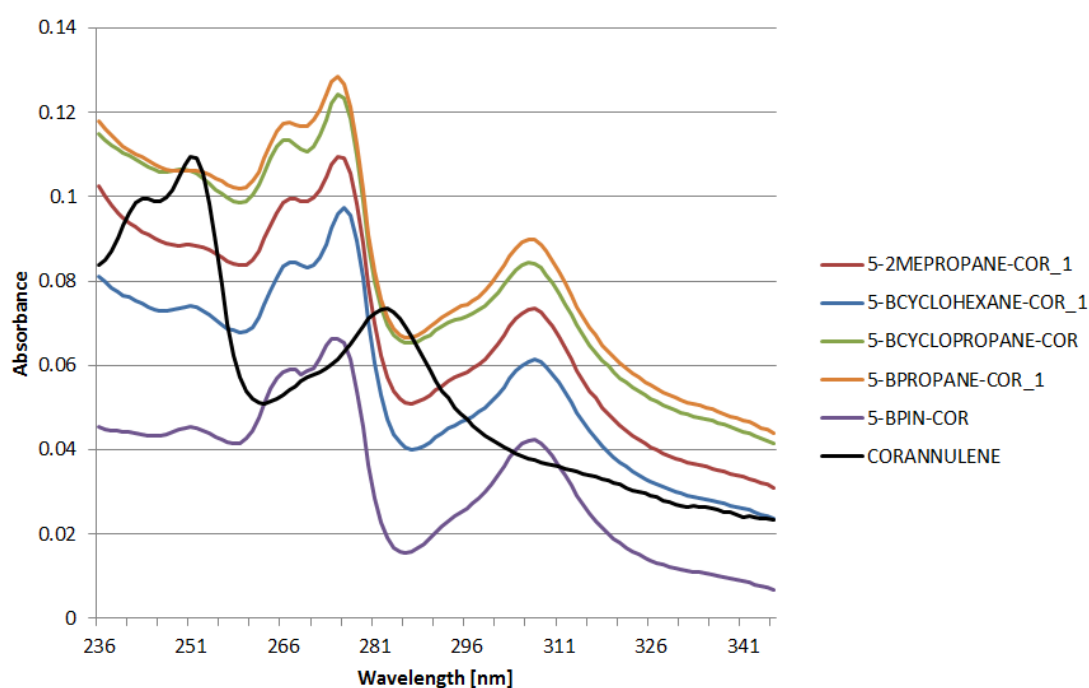
Figure 7.1 Collective UV/Vis spectra of boronic ester derivatives **3**, **9-13** with their parent corannulene.

8. Crystallographic Data

8.1. X-Ray Crystal Structure of Compound 3

8.1.1. Experimental

A crystal of $C_{50}H_{65}B_5O_{10}\cdot C_6H_{14}$, obtained from *n*-hexane / CH_2Cl_2, was mounted on a glass fibre and used for a low-temperature X-ray structure determination. All measurements were made on an *Agilent Technologies SuperNova* area-detector diffractometer[2] using Cu *K*a radiation (l = 1.54184 Å) from a micro-focus X-ray source and an *Oxford Instruments Cryojet XL* cooler. The unit cell constants and an orientation matrix for data collection were obtained from a least-squares refinement of the setting angles of 19130 reflections in the range $3° < 2q < 153°$. A total of 1031 frames were collected using *w* scans with *k* offsets, 2.5-70.0 seconds exposure time and a rotation angle of 1.0° per frame, and a crystal-detector distance of 55.0 mm.

Data reduction was performed with *CrysAlisPro*[2]. The intensities were corrected for Lorentz and polarization effects, and an empirical absorption correction using spherical harmonics[2] was applied. The space group was uniquely determined by the systematic absences. Equivalent reflections, other than Friedel pairs, were merged. The data collection and refinement parameters are given in *Table 1*. A view of the molecule is shown in the *Figure*.

The structure was solved by direct methods using *SHELXS97*[3], which revealed the positions of all non-hydrogen atoms. The asymmetric unit contains one molecule of the corannulene derivative plus one molecule of *n*-hexane. The *n*-hexane molecule is disordered and could not be modelled sufficiently well, so the *SQUEEZE* routine[4] of the program *PLATON*[5] was employed. When the *n*-hexane molecule is omitted from the model, each unit cell contains two cavities of 500 $Å^3$. The electron count in each cavity was calculated to be approximately 113 e, which is a little more than two molecules of *n*-hexane (100 e) per cavity. It was therefore assumed there is one molecule of *n*-hexane per asymmetric unit and this assumption was used in the subsequent calculation of the empirical formula, formula weight, density, linear absorption coefficient and *F*(000). Based on the assumption, the ratio of corannulene derivative molecules to *n*-hexane molecules in the structure is 1:1.

The entire molecule of the corannulene derivative is disordered over two configurations which constitute enantiomeric pairs. Two complete sets of atoms were defined for this molecule and refinement of the site occupation factor led to a value of 0.686(2) for the major configuration. Similarity restraints were applied to all sets of chemically equivalent bond lengths and angles

within and between each configuration of the molecule. Furthermore, neighbouring atoms within and between each configuration were restrained to have similar atomic displacement parameters.

The non-hydrogen atoms were refined anisotropically. The non-hydrogen atoms were refined anisotropically. All of the H-atoms were placed in geometrically calculated positions and refined by using a riding model where each H-atom was assigned a fixed isotropic displacement parameter with a value equal to $1.2U_{eq}$ of its parent atom ($1.5U_{eq}$ for the methyl groups). The refinement of the structure was carried out on F^2 by using full-matrix least-squares procedures, which minimised the function $Sw(F_o^2 - F_c^2)^2$. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. Plots of $Sw(F_o^2 - F_c^2)^2$ versus $F_c/F_c(\max)$ and resolution showed no unusual trends. A correction for secondary extinction was not applied.

Neutral atom scattering factors for non-hydrogen atoms were taken from Maslen, Fox and O'Keefe[6a], and the scattering factors for H-atoms were taken from Stewart, Davidson and Simpson[7]. Anomalous dispersion effects were included in F_c[8]; the values for f' and f'' were those of Creagh and McAuley[6b]. The values of the mass attenuation coefficients are those of Creagh and Hubbel[6c]. The *SHELXL97* program[9] was used for all calculations.

8.1.2. Results

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Crystallised from	n-hexane / CH_2Cl_2
Empirical formula	$C_{56}H_{79}B_5O_{10}$
Formula weight [g mol^{-1}]	966.28
Crystal colour, habit	colourless, prism
Crystal dimensions [mm]	$0.20 \times 0.22 \times 0.38$
Temperature [K]	160(1)
Crystal system	orthorhombic
Space group	$P2_12_12_1$ (#19)
Z	4
Reflections for cell determination	19130
2θ range for cell determination [°]	3–153
Unit cell parameters	a [Å]
	12.38928(14)
	b [Å]	20.5595(3)
	c [Å]	23.6390(3)
	α [°]	90
	β [°]	90
	γ [°]	90
	V [Å^3]	6021.25(12)
$F(000)$	2080
D_x [g cm^{-3}]	1.066
μ(Cu $K\alpha$) [mm^{-1}]	0.555
Scan type	ω
$2\theta_{(max)}$ [°]	153.1
Transmission factors (min; max)	0.711; 1.000
Total reflections measured	32585
Symmetry independent reflections	11894
R_{int}	0.040
Reflections with $I > 2\sigma(I)$	9960
Reflections used in refinement	11894
Parameters refined; restraints	1172; 4120
Final $R(F)$ [$I > 2\sigma(I)$ reflections]	0.1047
$wR(F^2)$ (all data)	0.3220
Weights:	$w = [\sigma^2(F_o^2) + (0.2000P)^2]^{-1}$ where $P = (F_o^2 + 2F_c^2)/3$
Goodness of fit	1.371

Final Δ_{max}/σ		0.001
$\Delta\rho$ (max; min) [e Å^{-3}]		0.42; -0.41
$\sigma(d_{(C-C)})$ [Å]		0.05 – 0.008

TABLE 2. Bond lengths (Å) with standard uncertainties in parentheses.

C(1)	-C(6)	1.374(5)	C(1a)	-C(6a)	1.378(6)
C(1)	-C(2)	1.412(5)	C(1a)	-C(5a)	1.406(6)
C(1)	-C(5)	1.413(5)	C(1a)	-C(2a)	1.410(6)
C(2)	-C(9)	1.384(5)	C(2a)	-C(9a)	1.380(6)
C(2)	-C(3)	1.401(5)	C(2a)	-C(3a)	1.406(6)
C(3)	-C(12)	1.383(5)	C(3a)	-C(12a)	1.379(7)
C(3)	-C(4)	1.405(5)	C(3a)	-C(4a)	1.403(6)
C(4)	-C(15)	1.383(5)	C(4a)	-C(15a)	1.383(6)
C(4)	-C(5)	1.406(5)	C(4a)	-C(5a)	1.403(6)
C(5)	-C(18)	1.379(5)	C(5a)	-C(18a)	1.379(6)
C(6)	-C(20)	1.441(5)	C(6a)	-C(7a)	1.440(6)
C(6)	-C(7)	1.451(5)	C(6a)	-C(20a)	1.441(6)
C(7)	-C(8)	1.401(6)	C(7a)	-C(8a)	1.397(6)
C(7)	-B(1)	1.577(5)	C(7a)	-B(1a)	1.556(7)
C(8)	-C(9)	1.448(5)	C(8a)	-C(9a)	1.449(6)
C(9)	-C(10)	1.451(5)	C(9a)	-C(10a)	1.450(6)
C(10)	-C(11)	1.403(5)	C(10a)	-C(11a)	1.406(7)
C(10)	-B(2)	1.567(6)	C(10a)	-B(2a)	1.578(7)
C(11)	-C(12)	1.449(5)	C(11a)	-C(12a)	1.442(6)
C(12)	-C(13)	1.442(5)	C(12a)	-C(13a)	1.448(6)
C(13)	-C(14)	1.397(5)	C(13a)	-C(14a)	1.400(7)
C(13)	-B(3)	1.568(5)	C(13a)	-B(3a)	1.580(7)
C(14)	-C(15)	1.435(5)	C(14a)	-C(15a)	1.436(6)
C(15)	-C(16)	1.450(5)	C(15a)	-C(16a)	1.447(6)
C(16)	-C(17)	1.391(5)	C(16a)	-C(17a)	1.400(7)
C(16)	-B(4)	1.565(5)	C(16a)	-B(4a)	1.581(7)
C(17)	-C(18)	1.446(5)	C(17a)	-C(18a)	1.448(6)
C(18)	-C(19)	1.456(5)	C(18a)	-C(19a)	1.453(6)
C(19)	-C(20)	1.400(5)	C(19a)	-C(20a)	1.398(7)
C(19)	-B(5)	1.571(5)	C(19a)	-B(5a)	1.564(7)
B(1)	-O(1)	1.343(6)	B(1a)	-O(1a)	1.345(7)
B(1)	-O(2)	1.350(5)	B(1a)	-O(2a)	1.354(7)
O(1)	-C(21)	1.462(6)	O(1a)	-C(21a)	1.465(7)
O(2)	-C(22)	1.450(5)	O(2a)	-C(22a)	1.468(7)
C(21)	-C(24)	1.506(6)	C(21a)	-C(24a)	1.500(7)
C(21)	-C(23)	1.511(6)	C(21a)	-C(23a)	1.513(7)
C(21)	-C(22)	1.544(7)	C(21a)	-C(22a)	1.537(8)
C(22)	-C(25)	1.502(6)	C(22a)	-C(25a)	1.501(7)
C(22)	-C(26)	1.526(6)	C(22a)	-C(26a)	1.518(7)
B(2)	-O(4)	1.344(6)	B(2a)	-O(3a)	1.343(7)
B(2)	-O(3)	1.344(6)	B(2a)	-O(4a)	1.350(7)
O(3)	-C(27)	1.444(6)	O(3a)	-C(27a)	1.452(7)
O(4)	-C(28)	1.450(6)	O(4a)	-C(28a)	1.454(7)

C(27)	−C(29)	1.505(6)	C(27a)−C(29a)	1.513(7)
C(27)	−C(28)	1.525(7)	C(27a)−C(30a)	1.519(7)
C(27)	−C(30)	1.532(6)	C(27a)−C(28a)	1.528(8)
C(28)	−C(32)	1.507(6)	C(28a)−C(32a)	1.514(7)
C(28)	−C(31)	1.535(7)	C(28a)−C(31a)	1.520(7)
B(3)	−O(6)	1.336(6)	B(3a) −O(6a)	1.343(7)
B(3)	−O(5)	1.349(5)	B(3a) −O(5a)	1.351(7)
O(5)	−C(33)	1.450(6)	O(5a) −C(33a)	1.453(7)
O(6)	−C(34)	1.462(6)	O(6a) −C(34a)	1.459(7)
C(33)	−C(34)	1.514(7)	C(33a)−C(36a)	1.515(7)
C(33)	−C(36)	1.518(6)	C(33a)−C(35a)	1.518(7)
C(33)	−C(35)	1.523(6)	C(33a)−C(34a)	1.525(8)
C(34)	−C(38)	1.525(6)	C(34a)−C(38a)	1.518(7)
C(34)	−C(37)	1.528(6)	C(34a)−C(37a)	1.520(7)
B(4)	−O(8)	1.337(6)	B(4a) −O(8a)	1.366(7)
B(4)	−O(7)	1.350(6)	B(4a) −O(7a)	1.368(7)
O(7)	−C(39)	1.439(5)	O(7a) −C(39a)	1.463(7)
O(8)	−C(40)	1.431(6)	O(8a) −C(40a)	1.463(7)
C(39)	−C(42)	1.512(6)	C(39a)−C(41a)	1.515(7)
C(39)	−C(40)	1.527(7)	C(39a)−C(40a)	1.518(8)
C(39)	−C(41)	1.532(6)	C(39a)−C(42a)	1.521(7)
C(40)	−C(44)	1.512(6)	C(40a)−C(43a)	1.520(7)
C(40)	−C(43)	1.540(7)	C(40a)−C(44a)	1.525(7)
B(5)	−O(9)	1.342(6)	B(5a) −O(9a)	1.341(7)
B(5)	−O(10)	1.352(5)	B(5a) −O(10a)	1.344(7)
O(9)	−C(45)	1.455(5)	O(9a) −C(45a)	1.461(7)
O(10)	−C(46)	1.454(5)	O(10a)−C(46a)	1.465(7)
C(45)	−C(48)	1.506(6)	C(45a)−C(47a)	1.514(7)
C(45)	−C(47)	1.518(6)	C(45a)−C(48a)	1.516(7)
C(45)	−C(46)	1.530(7)	C(45a)−C(46a)	1.524(8)
C(46)	−C(49)	1.514(6)	C(46a)−C(50a)	1.512(7)
C(46)	−C(50)	1.523(6)	C(46a)−C(49a)	1.520(7)

TABLE 3. Bond angles (°) with standard uncertainties in parentheses.

C(6) −C(1) −C(2) 122.0(4)	C(6a) −C(1a) −C(5a) 124.1(5)	
C(6) −C(1) −C(5) 123.4(4)	C(6a) −C(1a) −C(2a) 121.8(5)	
C(2) −C(1) −C(5) 108.4(3)	C(5a) −C(1a) −C(2a) 108.4(5)	
C(9) −C(2) −C(3) 123.3(4)	C(9a) −C(2a) −C(3a) 123.0(5)	
C(9) −C(2) −C(1) 122.5(4)	C(9a) −C(2a) −C(1a) 122.1(5)	
C(3) −C(2) −C(1) 107.6(4)	C(3a) −C(2a) −C(1a) 107.3(5)	
C(12) −C(3) −C(2) 122.7(4)	C(12a)−C(3a) −C(4a) 122.6(5)	
C(12) −C(3) −C(4) 122.0(4)	C(12a)−C(3a) −C(2a) 122.9(5)	
C(2) −C(3) −C(4) 108.3(4)	C(4a) −C(3a) −C(2a) 108.4(5)	
C(15) −C(4) −C(3) 122.6(4)	C(15a)−C(4a) −C(3a) 122.5(5)	
C(15) −C(4) −C(5) 122.9(4)	C(15a)−C(4a) −C(5a) 123.2(5)	
C(3) −C(4) −C(5) 108.5(4)	C(3a) −C(4a) −C(5a) 108.1(5)	
C(18) −C(5) −C(4) 123.1(4)	C(18a)−C(5a) −C(4a) 122.9(6)	
C(18) −C(5) −C(1) 122.4(4)	C(18a)−C(5a) −C(1a) 122.4(6)	
C(4) −C(5) −C(1) 107.2(3)	C(4a) −C(5a) −C(1a) 107.7(4)	
C(1) −C(6) −C(20) 114.6(4)	C(1a) −C(6a) −C(7a) 116.7(5)	
C(1) −C(6) −C(7) 117.0(3)	C(1a) −C(6a) −C(20a) 113.7(5)	
C(20) −C(6) −C(7) 127.1(4)	C(7a) −C(6a) −C(20a) 128.5(6)	
C(8) −C(7) −C(6) 119.1(4)	C(8a) −C(7a) −C(6a) 120.1(5)	
C(8) −C(7) −B(1) 118.2(4)	C(8a) −C(7a) −B(1a) 115.8(6)	
C(6) −C(7) −B(1) 122.3(4)	C(6a) −C(7a) −B(1a) 123.4(6)	
C(7) −C(8) −C(9) 122.5(5)	C(7a) −C(8a) −C(9a) 121.1(6)	
C(2) −C(9) −C(8) 115.0(4)	C(2a) −C(9a) −C(8a) 115.5(5)	
C(2) −C(9) −C(10) 115.2(4)	C(2a) −C(9a) −C(10a) 115.8(5)	

C(8) –C(9) –C(10)	128.8(4)	C(8a) –C(9a) –C(10a)		128.2(5)
C(11) –C(10) –C(9)	120.1(4)	C(11a)–C(10a)–C(9a)		119.5(6)
C(11) –C(10) –B(2)	115.6(5)	C(11a)–C(10a)–B(2a)		118.5(6)
C(9) –C(10) –B(2)	123.5(4)	C(9a) –C(10a)–B(2a)		120.3(7)
C(10) –C(11) –C(12)	122.5(4)	C(10a)–C(11a)–C(12a)		123.0(6)
C(3) –C(12) –C(13)	117.0(4)	C(3a) –C(12a)–C(11a)		114.6(5)
C(3) –C(12) –C(11)	114.6(4)	C(3a) –C(12a)–C(13a)		116.4(6)
C(13) –C(12) –C(11)	126.7(4)	C(11a)–C(12a)–C(13a)		127.2(6)
C(14) –C(13) –C(12)	119.0(4)	C(14a)–C(13a)–C(12a)		118.4(6)
C(14) –C(13) –B(3)	120.5(4)	C(14a)–C(13a)–B(3a)		120.1(7)
C(12) –C(13) –B(3)	119.8(4)	C(12a)–C(13a)–B(3a)		120.8(8)
C(13) –C(14) –C(15)	123.2(4)	C(13a)–C(14a)–C(15a)		123.7(6)
C(4) –C(15) –C(14)	115.0(4)	C(4a) –C(15a)–C(14a)		114.4(5)
C(4) –C(15) –C(16)	115.0(4)	C(4a) –C(15a)–C(16a)		115.3(5)
C(14) –C(15) –C(16)	128.5(4)	C(14a)–C(15a)–C(16a)		129.3(6)
C(17) –C(16) –C(15)	120.5(4)	C(17a)–C(16a)–C(15a)		119.5(6)
C(17) –C(16) –B(4)	117.7(4)	C(17a)–C(16a)–B(4a)		121.3(7)
C(15) –C(16) –B(4)	121.7(4)	C(15a)–C(16a)–B(4a)		119.2(7)
C(16) –C(17) –C(18)	122.7(4)	C(16a)–C(17a)–C(18a)		123.4(7)
C(5) –C(18) –C(17)	114.0(4)	C(5a) –C(18a)–C(17a)		113.8(6)
C(5) –C(18) –C(19)	115.8(4)	C(5a) –C(18a)–C(19a)		115.2(5)
C(17) –C(18) –C(19)	128.8(4)	C(17a)–C(18a)–C(19a)		129.1(7)
C(20) –C(19) –C(18)	119.9(4)	C(20a)–C(19a)–C(18a)		120.7(6)
C(20) –C(19) –B(5)	119.3(4)	C(20a)–C(19a)–B(5a)		122.4(8)
C(18) –C(19) –B(5)	120.2(4)	C(18a)–C(19a)–B(5a)		116.6(9)

C(19) –C(20) –C(6)	122.8(4)	C(19a)–C(20a)–C(6a)	122.6(7)
O(1) –B(1) –O(2)	113.2(4)	O(1a) –B(1a) –O(2a)	113.3(5)
O(1) –B(1) –C(7)	123.6(4)	O(1a) –B(1a) –C(7a)	117.4(8)
O(2) –B(1) –C(7)	123.1(4)	O(2a) –B(1a) –C(7a)	128.5(8)
B(1) –O(1) –C(21)	107.4(4)	B(1a) –O(1a) –C(21a)	106.3(5)
B(1) –O(2) –C(22)	106.7(4)	B(1a) –O(2a) –C(22a)	104.9(5)
O(1) –C(21) –C(24)	107.9(5)	O(1a) –C(21a)–C(24a)	108.0(7)
O(1) –C(21) –C(23)	107.3(5)	O(1a) –C(21a)–C(23a)	106.9(7)
C(24) –C(21) –C(23)	107.5(5)	C(24a)–C(21a)–C(23a)	107.9(6)
O(1) –C(21) –C(22)	100.7(4)	O(1a) –C(21a)–C(22a)	99.1(5)
C(24) –C(21) –C(22)	116.4(5)	C(24a)–C(21a)–C(22a)	118.1(7)
C(23) –C(21) –C(22)	116.2(5)	C(23a)–C(21a)–C(22a)	115.7(7)
O(2) –C(22) –C(25)	109.8(5)	O(2a) –C(22a)–C(25a)	108.6(6)
O(2) –C(22) –C(26)	107.5(5)	O(2a) –C(22a)–C(26a)	107.6(6)
C(25) –C(22) –C(26)	110.4(5)	C(25a)–C(22a)–C(26a)	111.0(7)
O(2) –C(22) –C(21)	102.2(3)	O(2a) –C(22a)–C(21a)	101.3(5)
C(25) –C(22) –C(21)	110.3(5)	C(25a)–C(22a)–C(21a)	111.5(7)
C(26) –C(22) –C(21)	116.1(5)	C(26a)–C(22a)–C(21a)	116.0(7)
O(4) –B(2) –O(3)	112.9(4)	O(3a) –B(2a) –O(4a)	112.0(5)
O(4) –B(2) –C(10)	120.2(5)	O(3a) –B(2a) –C(10a)	123.3(7)
O(3) –B(2) –C(10)	127.0(5)	O(4a) –B(2a) –C(10a)	124.6(7)
B(2) –O(3) –C(27)	108.8(4)	B(2a) –O(3a) –C(27a)	108.9(5)
B(2) –O(4) –C(28)	107.0(4)	B(2a) –O(4a) –C(28a)	106.7(6)
O(3) –C(27) –C(29)	108.2(5)	O(3a) –C(27a)–C(29a)	107.7(7)
O(3) –C(27) –C(28)	102.1(4)	O(3a) –C(27a)–C(30a)	106.9(6)

C(29) –C(27) –C(28)	117.7(5)	C(29a)–C(27a)–C(30a)	106.9(6)
O(3) –C(27) –C(30)	105.4(5)	O(3a) –C(27a)–C(28a)	101.5(4)
C(29) –C(27) –C(30)	106.6(5)	C(29a)–C(27a)–C(28a)	116.2(7)
C(28) –C(27) –C(30)	115.9(6)	C(30a)–C(27a)–C(28a)	116.8(7)
O(4) –C(28) –C(32)	110.0(5)	O(4a) –C(28a)–C(32a)	108.6(6)
O(4) –C(28) –C(27)	103.5(4)	O(4a) –C(28a)–C(31a)	107.6(6)
C(32) –C(28) –C(27)	117.7(5)	C(32a)–C(28a)–C(31a)	109.8(6)
O(4) –C(28) –C(31)	105.6(5)	O(4a) –C(28a)–C(27a)	102.3(4)
C(32) –C(28) –C(31)	109.3(5)	C(32a)–C(28a)–C(27a)	117.1(7)
C(27) –C(28) –C(31)	110.1(5)	C(31a)–C(28a)–C(27a)	110.8(7)
O(6) –B(3) –O(5)	110.8(4)	O(6a) –B(3a) –O(5a)	112.5(5)
O(6) –B(3) –C(13)	117.9(5)	O(6a) –B(3a) –C(13a)	124.1(8)
O(5) –B(3) –C(13)	129.4(5)	O(5a) –B(3a) –C(13a)	122.8(9)
B(3) –O(5) –C(33)	107.6(4)	B(3a) –O(5a) –C(33a)	107.6(5)
B(3) –O(6) –C(34)	106.8(4)	B(3a) –O(6a) –C(34a)	107.3(5)
O(5) –C(33) –C(34)	101.6(4)	O(5a) –C(33a)–C(36a)	107.6(7)
O(5) –C(33) –C(36)	106.2(5)	O(5a) –C(33a)–C(35a)	107.8(7)
C(34) –C(33) –C(36)	119.3(6)	C(36a)–C(33a)–C(35a)	106.3(6)
O(5) –C(33) –C(35)	107.0(5)	O(5a) –C(33a)–C(34a)	101.2(4)
C(34) –C(33) –C(35)	115.8(6)	C(36a)–C(33a)–C(34a)	117.5(7)
C(36) –C(33) –C(35)	105.9(5)	C(35a)–C(33a)–C(34a)	115.8(7)
O(6) –C(34) –C(33)	105.4(4)	O(6a) –C(34a)–C(38a)	107.9(7)
O(6) –C(34) –C(38)	106.9(6)	O(6a) –C(34a)–C(37a)	107.1(6)
C(33) –C(34) –C(38)	117.3(6)	C(38a)–C(34a)–C(37a)	109.8(6)
O(6) –C(34) –C(37)	106.3(6)	O(6a) –C(34a)–C(33a)	103.0(5)

C(33) –C(34) –C(37)	111.2(6)	C(38a)–C(34a)–C(33a)
117.4(7)		
C(38) –C(34) –C(37)	109.1(6)	C(37a)–C(34a)–C(33a)
111.0(7)		
O(8) –B(4) –O(7)	112.8(4)	O(8a) –B(4a) –O(7a)
107.1(7)		
O(8) –B(4) –C(16)	122.4(5)	O(8a) –B(4a) –C(16a)
148.6(8)		
O(7) –B(4) –C(16)	124.5(5)	O(7a) –B(4a) –C(16a)
103.9(8)		
B(4) –O(7) –C(39)	108.8(4)	B(4a) –O(7a) –C(39a)
105.1(6)		
B(4) –O(8) –C(40)	108.5(4)	B(4a) –O(8a) –C(40a)
105.2(5)		
O(7) –C(39) –C(42)	107.5(5)	O(7a) –C(39a)–C(41a)
107.3(7)		
O(7) –C(39) –C(40)	103.8(4)	O(7a) –C(39a)–C(40a)
101.6(4)		
C(42) –C(39) –C(40)	118.4(5)	C(41a)–C(39a)–C(40a)
117.2(7)		
O(7) –C(39) –C(41)	107.2(5)	O(7a) –C(39a)–C(42a)
105.8(6)		
C(42) –C(39) –C(41)	106.0(5)	C(41a)–C(39a)–C(42a)
106.2(6)		
C(40) –C(39) –C(41)	113.3(6)	C(40a)–C(39a)–C(42a)
117.6(7)		
O(8) –C(40) –C(44)	110.7(6)	O(8a) –C(40a)–C(39a)
104.9(4)		
O(8) –C(40) –C(39)	104.8(4)	O(8a) –C(40a)–C(43a)
106.1(7)		
C(44) –C(40) –C(39)	116.5(6)	C(39a)–C(40a)–C(43a)
111.2(7)		
O(8) –C(40) –C(43)	106.7(5)	O(8a) –C(40a)–C(44a)
107.3(7)		
C(44) –C(40) –C(43)	108.6(6)	C(39a)–C(40a)–C(44a)
116.9(7)		
C(39) –C(40) –C(43)	109.2(6)	C(43a)–C(40a)–C(44a)
109.6(6)		
O(9) –B(5) –O(10)	112.6(3)	O(9a) –B(5a) –O(10a)
113.2(5)		
O(9) –B(5) –C(19)	127.1(4)	O(9a) –B(5a) –C(19a)
118.3(9)		
O(10) –B(5) –C(19)	119.9(5)	O(10a)–B(5a) –C(19a)
128.3(9)		
B(5) –O(9) –C(45)	108.1(4)	B(5a) –O(9a) –C(45a)
108.0(5)		
B(5) –O(10) –C(46)	106.8(4)	B(5a) –O(10a)–C(46a)
105.9(6)		
O(9) –C(45) –C(48)	108.0(5)	O(9a) –C(45a)–C(47a)
106.9(7)		

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O(9)  -C(45) -C(47)    106.6(5)        O(9a) -C(45a)-C(48a)
106.6(7)
C(48) -C(45) -C(47)    106.7(5)        C(47a)-C(45a)-C(48a)
106.8(6)
O(9)  -C(45) -C(46)    101.3(3)        O(9a) -C(45a)-C(46a)
100.7(5)
C(48) -C(45) -C(46)    117.4(5)        C(47a)-C(45a)-C(46a)
116.8(7)
C(47) -C(45) -C(46)    116.0(5)        C(48a)-C(45a)-C(46a)
118.0(7)
O(10) -C(46) -C(49)    109.2(5)        O(10a)-C(46a)-C(50a)
107.5(7)
O(10) -C(46) -C(50)    107.9(5)        O(10a)-C(46a)-C(49a)
106.2(7)
C(49) -C(46) -C(50)    109.5(5)        C(50a)-C(46a)-C(49a)
110.1(6)
O(10) -C(46) -C(45)    102.4(3)        O(10a)-C(46a)-C(45a)
102.7(5)
C(49) -C(46) -C(45)    110.7(5)        C(50a)-C(46a)-C(45a)
118.4(7)
C(50) -C(46) -C(45)    116.7(5)        C(49a)-C(46a)-C(45a)
110.9(7)


TABLE  4.   Torsion  angles  (°)  with  standard  uncertainties  in
parentheses.


C(6)  -C(1)  -C(2)  -C(9)     -1.2(7)      C(6a) -C(1a) -C(2a) -C(9a)
4(1)
C(5)  -C(1)  -C(2)  -C(9)    151.8(4)      C(5a) -C(1a) -C(2a) -C(9a)
-150.4(8)
C(6)  -C(1)  -C(2)  -C(3)   -153.5(4)      C(6a) -C(1a) -C(2a) -C(3a)
154.3(9)
C(5)  -C(1)  -C(2)  -C(3)     -0.5(5)      C(5a) -C(1a) -C(2a) -C(3a)
-0(1)
C(9)  -C(2)  -C(3)  -C(12)     0.0(7)      C(9a) -C(2a) -C(3a) -C(12a)
-4(2)
C(1)  -C(2)  -C(3)  -C(12)   152.0(4)      C(1a) -C(2a) -C(3a) -C(12a)
-153.6(8)
C(9)  -C(2)  -C(3)  -C(4)   -151.1(4)      C(9a) -C(2a) -C(3a) -C(4a)
149.4(8)
C(1)  -C(2)  -C(3)  -C(4)      0.9(5)      C(1a) -C(2a) -C(3a) -C(4a)
-1(1)
C(12) -C(3)  -C(4)  -C(15)     0.9(7)      C(12a)-C(3a) -C(4a) -C(15a)
1(1)
C(2)  -C(3)  -C(4)  -C(15)   152.2(4)      C(2a) -C(3a) -C(4a) -C(15a)
-152.2(9)
C(12) -C(3)  -C(4)  -C(5)   -152.3(4)      C(12a)-C(3a) -C(4a) -C(5a)
154.1(8)
C(2)  -C(3)  -C(4)  -C(5)     -1.0(5)      C(2a) -C(3a) -C(4a) -C(5a)
1(1)
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C(15)	−C(4)	−C(5)	−C(18)	−1.7(7)	C(15a)−C(4a) −C(5a) −C(18a)	1(1)
C(3)	−C(4)	−C(5)	−C(18)	151.4(4)	C(3a) −C(4a) −C(5a) −C(18a)	−152.3(9)
C(15)	−C(4)	−C(5)	−C(1)	−152.5(4)	C(15a)−C(4a) −C(5a) −C(1a)	151.9(9)
C(3)	−C(4)	−C(5)	−C(1)	0.6(5)	C(3a) −C(4a) −C(5a) −C(1a)	−1(1)
C(6)	−C(1)	−C(5)	−C(18)	1.5(7)	C(6a) −C(1a) −C(5a) −C(18a)	−2(1)
C(2)	−C(1)	−C(5)	−C(18)	−151.0(4)	C(2a) −C(1a) −C(5a) −C(18a)	152.1(9)
C(6)	−C(1)	−C(5)	−C(4)	152.5(4)	C(6a) −C(1a) −C(5a) −C(4a)	−153.0(9)
C(2)	−C(1)	−C(5)	−C(4)	−0.1(5)	C(2a) −C(1a) −C(5a) −C(4a)	1(1)
C(2)	−C(1)	−C(6)	−C(20)	156.6(4)	C(5a) −C(1a) −C(6a) −C(7a)	161.0(9)
C(5)	−C(1)	−C(6)	−C(20)	7.7(7)	C(2a) −C(1a) −C(6a) −C(7a)	11(1)
C(2)	−C(1)	−C(6)	−C(7)	−11.1(6)	C(5a) −C(1a) −C(6a) −C(20a)	−8(1)
C(5)	−C(1)	−C(6)	−C(7)	−160.1(4)	C(2a) −C(1a) −C(6a) −C(20a)	−158(1)
C(1)	−C(6)	−C(7)	−C(8)	12.9(7)	C(1a) −C(6a) −C(7a) −C(8a)	−13(2)
C(20)	−C(6)	−C(7)	−C(8)	−153.1(5)	C(20a)−C(6a) −C(7a) −C(8a)	154(1)
C(1)	−C(6)	−C(7)	−B(1)	−174.8(5)	C(1a) −C(6a) −C(7a) −B(1a)	176(1)
C(20)	−C(6)	−C(7)	−B(1)	19.2(8)	C(20a)−C(6a) −C(7a) −B(1a)	−17(2)
C(6)	−C(7)	−C(8)	−C(9)	−2.8(8)	C(6a) −C(7a) −C(8a) −C(9a)	2(2)
B(1)	−C(7)	−C(8)	−C(9)	−175.5(6)	B(1a) −C(7a) −C(8a) −C(9a)	173(1)
C(3)	−C(2)	−C(9)	−C(8)	159.2(5)	C(3a) −C(2a) −C(9a) −C(8a)	−161.2(9)
C(1)	−C(2)	−C(9)	−C(8)	11.2(7)	C(1a) −C(2a) −C(9a) −C(8a)	−16(1)
C(3)	−C(2)	−C(9)	−C(10)	−10.6(6)	C(3a) −C(2a) −C(9a) −C(10a)	11(1)
C(1)	−C(2)	−C(9)	−C(10)	−158.5(4)	C(1a) −C(2a) −C(9a) −C(10a)	156.5(8)
C(7)	−C(8)	−C(9)	−C(2)	−9.0(8)	C(7a) −C(8a) −C(9a) −C(2a)	13(2)
C(7)	−C(8)	−C(9)	−C(10)	159.0(5)	C(7a) −C(8a) −C(9a) −C(10a)	−158(1)
C(2)	−C(9)	−C(10)	−C(11)	11.3(7)	C(2a) −C(9a) −C(10a)−C(11a)	−9(1)

C(8) -C(9) -C(10)-C(11)	-156.8(5)	C(8a) -C(9a) -C(10a)-C(11a)	162(1)
C(2) -C(9) -C(10)-B(2)	-179.5(7)	C(2a) -C(9a) -C(10a)-B(2a)	-174(2)
C(8) -C(9) -C(10)-B(2)	12.4(9)	C(8a) -C(9a) -C(10a)-B(2a)	-3(2)
C(9) -C(10)-C(11)-C(12)	-2.0(8)	C(9a) -C(10a)-C(11a)-C(12a)	0(1)
B(2) -C(10)-C(11)-C(12)	-172.1(7)	B(2a) -C(10a)-C(11a)-C(12a)	166(2)
C(2) -C(3) -C(12)-C(13)	-156.6(5)	C(4a) -C(3a) -C(12a)-C(11a)	-154.7(8)
C(4) -C(3) -C(12)-C(13)	-9.4(7)	C(2a) -C(3a) -C(12a)-C(11a)	-5(1)
C(2) -C(3) -C(12)-C(11)	9.5(7)	C(4a) -C(3a) -C(12a)-C(13a)	12(1)
C(4) -C(3) -C(12)-C(11)	156.7(4)	C(2a) -C(3a) -C(12a)-C(13a)	161(1)
C(10)-C(11)-C(12)-C(3)	-8.3(7)	C(10a)-C(11a)-C(12a)-C(3a)	7(1)
C(10)-C(11)-C(12)-C(13)	156.2(6)	C(10a)-C(11a)-C(12a)-C(13a)	-158(1)
C(3) -C(12)-C(13)-C(14)	8.4(8)	C(3a) -C(12a)-C(13a)-C(14a)	-14(2)
C(11)-C(12)-C(13)-C(14)	-155.8(5)	C(11a)-C(12a)-C(13a)-C(14a)	150(1)
C(3) -C(12)-C(13)-B(3)	179.1(5)	C(3a) -C(12a)-C(13a)-B(3a)	176(2)
C(11)-C(12)-C(13)-B(3)	14.9(9)	C(11a)-C(12a)-C(13a)-B(3a)	-20(2)
C(12)-C(13)-C(14)-C(15)	0.9(9)	C(12a)-C(13a)-C(14a)-C(15a)	4(2)
B(3) -C(13)-C(14)-C(15)	-169.7(5)	B(3a) -C(13a)-C(14a)-C(15a)	175(2)
C(3) -C(4) -C(15)-C(14)	8.2(6)	C(3a) -C(4a) -C(15a)-C(14a)	-10(1)
C(5) -C(4) -C(15)-C(14)	157.6(4)	C(5a) -C(4a) -C(15a)-C(14a)	-159.5(9)
C(3) -C(4) -C(15)-C(16)	-159.0(5)	C(3a) -C(4a) -C(15a)-C(16a)	160(1)
C(5) -C(4) -C(15)-C(16)	-9.6(7)	C(5a) -C(4a) -C(15a)-C(16a)	11(2)
C(13)-C(14)-C(15)-C(4)	-9.1(7)	C(13a)-C(14a)-C(15a)-C(4a)	8(2)
C(13)-C(14)-C(15)-C(16)	156.1(6)	C(13a)-C(14a)-C(15a)-C(16a)	-161(1)
C(4) -C(15)-C(16)-C(17)	9.6(8)	C(4a) -C(15a)-C(16a)-C(17a)	-11(2)
C(14)-C(15)-C(16)-C(17)	-155.5(5)	C(14a)-C(15a)-C(16a)-C(17a)	157(1)

C(4)	−C(15)	−C(16)	−B(4)	−173.6(7)	C(4a) −C(15a)−C(16a)−B(4a) 170(1)
C(14)	−C(15)	−C(16)	−B(4)	21(1)	C(14a)−C(15a)−C(16a)−B(4a) −21(2)
C(15)	−C(16)	−C(17)	−C(18)	1.2(9)	C(15a)−C(16a)−C(17a)−C(18a) 1(2)
B(4)	−C(16)	−C(17)	−C(18)	−175.8(6)	B(4a) −C(16a)−C(17a)−C(18a) 180(1)
C(4)	−C(5)	−C(18)	−C(17)	12.3(6)	C(4a) −C(5a) −C(18a)−C(17a) −11(1)
C(1)	−C(5)	−C(18)	−C(17)	158.7(4)	C(1a) −C(5a) −C(18a)−C(17a) −157.9(9)
C(4)	−C(5)	−C(18)	−C(19)	−155.1(4)	C(4a) −C(5a) −C(18a)−C(19a) 155.0(9)
C(1)	−C(5)	−C(18)	−C(19)	−8.7(6)	C(1a) −C(5a) −C(18a)−C(19a) 8(1)
C(16)	−C(17)	−C(18)	−C(5)	−12.0(7)	C(16a)−C(17a)−C(18a)−C(5a) 10(2)
C(16)	−C(17)	−C(18)	−C(19)	153.4(5)	C(16a)−C(17a)−C(18a)−C(19a) −154(1)
C(5)	−C(18)	−C(19)	−C(20)	6.3(6)	C(5a) −C(18a)−C(19a)−C(20a) −4(1)
C(17)	−C(18)	−C(19)	−C(20)	−158.8(4)	C(17a)−C(18a)−C(19a)−C(20a) 159(1)
C(5)	−C(18)	−C(19)	−B(5)	177.8(6)	C(5a) −C(18a)−C(19a)−B(5a) −179(2)
C(17)	−C(18)	−C(19)	−B(5)	12.7(8)	C(17a)−C(18a)−C(19a)−B(5a) −15(2)
C(18)	−C(19)	−C(20)	−C(6)	3.0(7)	C(18a)−C(19a)−C(20a)−C(6a) −6(2)
B(5)	−C(19)	−C(20)	−C(6)	−168.6(6)	B(5a) −C(19a)−C(20a)−C(6a) 168(2)
C(1)	−C(6)	−C(20)	−C(19)	−9.8(7)	C(1a) −C(6a) −C(20a)−C(19a) 12(2)
C(7)	−C(6)	−C(20)	−C(19)	156.5(5)	C(7a) −C(6a) −C(20a)−C(19a) −156(1)
C(8)	−C(7)	−B(1)	−O(1)	−164.4(8)	C(8a) −C(7a) −B(1a) −O(1a) 9(2)
C(6)	−C(7)	−B(1)	−O(1)	23(1)	C(6a) −C(7a) −B(1a) −O(1a) −180(2)
C(8)	−C(7)	−B(1)	−O(2)	17(1)	C(8a) −C(7a) −B(1a) −O(2a) 179(2)
C(6)	−C(7)	−B(1)	−O(2)	−155.0(7)	C(6a) −C(7a) −B(1a) −O(2a) −11(3)
O(2)	−B(1)	−O(1)	−C(21)	11(1)	O(2a) −B(1a) −O(1a) −C(21a) 15(2)
C(7)	−B(1)	−O(1)	−C(21)	−167.7(7)	C(7a) −B(1a) −O(1a) −C(21a) −174(2)
O(1)	−B(1)	−O(2)	−C(22)	11(1)	O(1a) −B(1a) −O(2a) −C(22a) 11(2)

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C(7)  -B(1)  -O(2)  -C(22)   -171.1(7)    C(7a) -B(1a) -O(2a) -C(22a)
-159(2)
B(1)  -O(1)  -C(21) -C(24)   -147.8(7)    B(1a) -O(1a) -C(21a)-C(24a)
-156(1)
B(1)  -O(1)  -C(21) -C(23)    96.7(7)     B(1a) -O(1a) -C(21a)-C(23a)
88(2)
B(1)  -O(1)  -C(21) -C(22)   -25.3(7)     B(1a) -O(1a) -C(21a)-C(22a)
-32(1)
B(1)  -O(2)  -C(22) -C(25)   -142.7(7)    B(1a) -O(2a) -C(22a)-C(25a)
-148(1)
B(1)  -O(2)  -C(22) -C(26)    97.2(7)     B(1a) -O(2a) -C(22a)-C(26a)
92(1)
B(1)  -O(2)  -C(22) -C(21)   -25.5(7)     B(1a) -O(2a) -C(22a)-C(21a)
-30(1)
O(1)  -C(21) -C(22) -O(2)     30.2(6)     O(1a) -C(21a)-C(22a)-O(2a)
37.3(8)
C(24) -C(21) -C(22) -O(2)    146.5(6)     C(24a)-C(21a)-C(22a)-O(2a)
153.4(9)
C(23) -C(21) -C(22) -O(2)    -85.2(6)     C(23a)-C(21a)-C(22a)-O(2a)
-76.6(9)
O(1)  -C(21) -C(22) -C(25)   147.0(6)     O(1a) -C(21a)-C(22a)-C(25a)
152.7(9)
C(24) -C(21) -C(22) -C(25)   -96.7(7)     C(24a)-C(21a)-C(22a)-C(25a)
-91(1)
C(23) -C(21) -C(22) -C(25)    31.6(7)     C(23a)-C(21a)-C(22a)-C(25a)
39(1)
O(1)  -C(21) -C(22) -C(26)   -86.4(6)     O(1a) -C(21a)-C(22a)-C(26a)
-79(1)
C(24) -C(21) -C(22) -C(26)    29.9(7)     C(24a)-C(21a)-C(22a)-C(26a)
37(1)
C(23) -C(21) -C(22) -C(26)   158.2(6)     C(23a)-C(21a)-C(22a)-C(26a)
167(1)
C(11) -C(10) -B(2)  -O(4)    -15(1)       C(11a)-C(10a)-B(2a) -O(3a)
-2(4)
C(9)  -C(10) -B(2)  -O(4)    175.2(7)     C(9a) -C(10a)-B(2a) -O(3a)
163(2)
C(11) -C(10) -B(2)  -O(3)    166(1)       C(11a)-C(10a)-B(2a) -O(4a)
174(2)
C(9)  -C(10) -B(2)  -O(3)     -4(2)       C(9a) -C(10a)-B(2a) -O(4a)
-21(4)
O(4)  -B(2)  -O(3)  -C(27)    -5(1)       O(4a) -B(2a) -O(3a) -C(27a)
-3(3)
C(10) -B(2)  -O(3)  -C(27)   174.3(9)     C(10a)-B(2a) -O(3a) -C(27a)
174(2)
O(3)  -B(2)  -O(4)  -C(28)   -12(1)       O(3a) -B(2a) -O(4a) -C(28a)
-17(3)
C(10) -B(2)  -O(4)  -C(28)   169.6(8)     C(10a)-B(2a) -O(4a) -C(28a)
167(2)
B(2)  -O(3)  -C(27) -C(29)   142.3(8)     B(2a) -O(3a) -C(27a)-C(29a)
142(2)
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B(2)	−O(3)	−C(27)	−C(28)	17.5(9)	B(2a)	−O(3a)	−C(27a)−C(30a)	−104(2)
B(2)	−O(3)	−C(27)	−C(30)	−104.0(9)	B(2a)	−O(3a)	−C(27a)−C(28a)	19(2)
B(2)	−O(4)	−C(28)	−C(32)	148.1(8)	B(2a)	−O(4a)	−C(28a)−C(32a)	152(2)
B(2)	−O(4)	−C(28)	−C(27)	21.5(8)	B(2a)	−O(4a)	−C(28a)−C(31a)	−89(2)
B(2)	−O(4)	−C(28)	−C(31)	−94.2(8)	B(2a)	−O(4a)	−C(28a)−C(27a)	28(2)
O(3)	−C(27)	−C(28)	−O(4)	−23.2(6)	O(3a)	−C(27a)	−C(28a)−O(4a)	−27.7(8)
C(29)	−C(27)	−C(28)	−O(4)	−141.4(6)	C(29a)−C(27a)	−C(28a)−O(4a)		−144.2(8)
C(30)	−C(27)	−C(28)	−O(4)	90.7(6)	C(30a)−C(27a)	−C(28a)−O(4a)		88.1(8)
O(3)	−C(27)	−C(28)	−C(32)	−144.7(6)	O(3a)	−C(27a)	−C(28a)−C(32a)	−146.2(9)
C(29)	−C(27)	−C(28)	−C(32)	97.1(8)	C(29a)−C(27a)	−C(28a)−C(32a)		97(1)
C(30)	−C(27)	−C(28)	−C(32)	−30.7(8)	C(30a)−C(27a)	−C(28a)−C(32a)		−31(1)
O(3)	−C(27)	−C(28)	−C(31)	89.3(6)	O(3a)	−C(27a)	−C(28a)−C(31a)	86.8(9)
C(29)	−C(27)	−C(28)	−C(31)	−29.0(8)	C(29a)−C(27a)	−C(28a)−C(31a)		−30(1)
C(30)	−C(27)	−C(28)	−C(31)	−156.8(6)	C(30a)−C(27a)	−C(28a)−C(31a)		−157.4(9)
C(14)	−C(13)	−B(3)	−O(6)	16(1)	C(14a)−C(13a)	−B(3a)	−O(6a)	165(2)
C(12)	−C(13)	−B(3)	−O(6)	−154.5(7)	C(12a)−C(13a)	−B(3a)	−O(6a)	−25(4)
C(14)	−C(13)	−B(3)	−O(5)	178.5(7)	C(14a)−C(13a)	−B(3a)	−O(5a)	−24(4)
C(12)	−C(13)	−B(3)	−O(5)	8(1)	C(12a)−C(13a)	−B(3a)	−O(5a)	146(2)
O(6)	−B(3)	−O(5)	−C(33)	−30.2(8)	O(6a)	−B(3a)	−O(5a)	−C(33a)	−15(3)
C(13)	−B(3)	−O(5)	−C(33)	166.3(7)	C(13a)−B(3a)	−O(5a)	−C(33a)	173(2)
O(5)	−B(3)	−O(6)	−C(34)	22.1(9)	O(5a)	−B(3a)	−O(6a)	−C(34a)	−5(3)
C(13)	−B(3)	−O(6)	−C(34)	−172.4(6)	C(13a)−B(3a)	−O(6a)	−C(34a)	167(2)
B(3)	−O(5)	−C(33)	−C(34)	24.1(7)	B(3a)	−O(5a)	−C(33a)−C(36a)	−98(2)
B(3)	−O(5)	−C(33)	−C(36)	−101.3(7)	B(3a)	−O(5a)	−C(33a)−C(35a)	148(2)
B(3)	−O(5)	−C(33)	−C(35)	145.9(6)	B(3a)	−O(5a)	−C(33a)−C(34a)	26(2)

B(3) –O(6) –C(34) –C(33) –5.6(8)	B(3a) –O(6a) –C(34a)–C(38a)	145(2)
B(3) –O(6) –C(34) –C(38) 119.9(7)	B(3a) –O(6a) –C(34a)–C(37a)	–96(2)
B(3) –O(6) –C(34) –C(37) –123.7(7)	B(3a) –O(6a) –C(34a)–C(33a)	21(2)
O(5) –C(33) –C(34) –O(6) –10.9(6)	O(5a) –C(33a)–C(34a)–O(6a)	–27.8(8)
C(36) –C(33) –C(34) –O(6) 105.3(7)	C(36a)–C(33a)–C(34a)–O(6a)	88.9(9)
C(35) –C(33) –C(34) –O(6) –126.4(6)	C(35a)–C(33a)–C(34a)–O(6a)	–144.0(9)
O(5) –C(33) –C(34) –C(38) –129.7(7)	O(5a) –C(33a)–C(34a)–C(38a)	–146.2(9)
C(36) –C(33) –C(34) –C(38) –13.5(8)	C(36a)–C(33a)–C(34a)–C(38a)	–30(1)
C(35) –C(33) –C(34) –C(38) 114.8(7)	C(35a)–C(33a)–C(34a)–C(38a)	98(1)
O(5) –C(33) –C(34) –C(37) 103.8(6)	O(5a) –C(33a)–C(34a)–C(37a)	86.5(9)
C(36) –C(33) –C(34) –C(37) –140.0(6)	C(36a)–C(33a)–C(34a)–C(37a)	–157(1)
C(35) –C(33) –C(34) –C(37) –11.7(8)	C(35a)–C(33a)–C(34a)–C(37a)	–30(1)
C(17) –C(16) –B(4) –O(8) –5(1)	C(17a)–C(16a)–B(4a) –O(8a)	–171(3)
C(15) –C(16) –B(4) –O(8) 178.1(8)	C(15a)–C(16a)–B(4a) –O(8a)	7(4)
C(17) –C(16) –B(4) –O(7) –178.2(8)	C(17a)–C(16a)–B(4a) –O(7a)	17(2)
C(15) –C(16) –B(4) –O(7) 5(1)	C(15a)–C(16a)–B(4a) –O(7a)	–164(1)
O(8) –B(4) –O(7) –C(39) 8(1)	O(8a) –B(4a) –O(7a) –C(39a)	42(2)
C(16) –B(4) –O(7) –C(39) –178.4(8)	C(16a)–B(4a) –O(7a) –C(39a)	–143(1)
O(7) –B(4) –O(8) –C(40) –12(1)	O(7a) –B(4a) –O(8a) –C(40a)	–36(2)
C(16) –B(4) –O(8) –C(40) 174.1(8)	C(16a)–B(4a) –O(8a) –C(40a)	153(3)
B(4) –O(7) –C(39) –C(42) –126.9(8)	B(4a) –O(7a) –C(39a)–C(41a)	94(1)
B(4) –O(7) –C(39) –C(40) –0.6(8)	B(4a) –O(7a) –C(39a)–C(40a)	–30(1)
B(4) –O(7) –C(39) –C(41) 119.5(8)	B(4a) –O(7a) –C(39a)–C(42a)	–153(1)
B(4) –O(8) –C(40) –C(44) 137.0(8)	B(4a) –O(8a) –C(40a)–C(39a)	15(1)
B(4) –O(8) –C(40) –C(39) 10.7(9)	B(4a) –O(8a) –C(40a)–C(43a)	–103(1)

B(4) –O(8) –C(40) –C(43) –105.0(8)	B(4a) –O(8a) –C(40a)–C(44a) 140(1)
O(7) –C(39) –C(40) –O(8) –6.0(7)	O(7a) –C(39a)–C(40a)–O(8a) 8.5(9)
C(42) –C(39) –C(40) –O(8) 113.0(7)	C(41a)–C(39a)–C(40a)–O(8a) –108.0(9)
C(41) –C(39) –C(40) –O(8) –121.9(7)	C(42a)–C(39a)–C(40a)–O(8a) 123.4(9)
O(7) –C(39) –C(40) –C(44) –128.6(7)	O(7a) –C(39a)–C(40a)–C(43a) 122.8(9)
C(42) –C(39) –C(40) –C(44) –9.6(8)	C(41a)–C(39a)–C(40a)–C(43a) 6(1)
C(41) –C(39) –C(40) –C(44) 115.5(7)	C(42a)–C(39a)–C(40a)–C(43a) –122(1)
O(7) –C(39) –C(40) –C(43) 108.0(6)	O(7a) –C(39a)–C(40a)–C(44a) –110(1)
C(42) –C(39) –C(40) –C(43) –133.0(7)	C(41a)–C(39a)–C(40a)–C(44a) 133(1)
C(41) –C(39) –C(40) –C(43) –7.9(7)	C(42a)–C(39a)–C(40a)–C(44a) 5(1)
C(20) –C(19) –B(5) –O(9) –172.1(9)	C(20a)–C(19a)–B(5a) –O(9a) –24(4)
C(18) –C(19) –B(5) –O(9) 16(1)	C(18a)–C(19a)–B(5a) –O(9a) 150(2)
C(20) –C(19) –B(5) –O(10) 15(1)	C(20a)–C(19a)–B(5a) –O(10a) 161(2)
C(18) –C(19) –B(5) –O(10) –156.4(7)	C(18a)–C(19a)–B(5a) –O(10a) –25(4)
O(10) –B(5) –O(9) –C(45) 9(1)	O(10a)–B(5a) –O(9a) –C(45a) –8(3)
C(19) –B(5) –O(9) –C(45) –164.6(9)	C(19a)–B(5a) –O(9a) –C(45a) 176(2)
O(9) –B(5) –O(10) –C(46) 11(1)	O(9a) –B(5a) –O(10a)–C(46a) –13(3)
C(19) –B(5) –O(10) –C(46) –174.9(7)	C(19a)–B(5a) –O(10a)–C(46a) 163(3)
B(5) –O(9) –C(45) –C(48) –147.3(7)	B(5a) –O(9a) –C(45a)–C(47a) 146(2)
B(5) –O(9) –C(45) –C(47) 98.3(8)	B(5a) –O(9a) –C(45a)–C(48a) –100(2)
B(5) –O(9) –C(45) –C(46) –23.3(7)	B(5a) –O(9a) –C(45a)–C(46a) 24(2)
B(5) –O(10) –C(46) –C(49) –142.4(7)	B(5a) –O(10a)–C(46a)–C(50a) 152(2)
B(5) –O(10) –C(46) –C(50) 98.7(7)	B(5a) –O(10a)–C(46a)–C(49a) –90(2)
B(5) –O(10) –C(46) –C(45) –25.1(7)	B(5a) –O(10a)–C(46a)–C(45a) 27(2)
O(9) –C(45) –C(46) –O(10) 28.7(5)	O(9a) –C(45a)–C(46a)–O(10a) –29.9(9)

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C(48) –C(45) –C(46) –O(10)     146.0(5)     C(47a)–C(45a)–C(46a)–O(10a)
–145.1(9)
C(47) –C(45) –C(46) –O(10)     –86.2(5)     C(48a)–C(45a)–C(46a)–O(10a)
86(1)
O(9)  –C(45) –C(46) –C(49)     145.0(5)     O(9a) –C(45a)–C(46a)–C(50a)
–148.1(9)
C(48) –C(45) –C(46) –C(49)     –97.8(6)     C(47a)–C(45a)–C(46a)–C(50a)
97(1)
C(47) –C(45) –C(46) –C(49)      30.1(6)     C(48a)–C(45a)–C(46a)–C(50a)
–33(1)
O(9)  –C(45) –C(46) –C(50)     –88.9(5)     O(9a) –C(45a)–C(46a)–C(49a)
83(1)
C(48) –C(45) –C(46) –C(50)      28.4(7)     C(47a)–C(45a)–C(46a)–C(49a)
–32(1)
C(47) –C(45) –C(46) –C(50)     156.2(5)     C(48a)–C(45a)–C(46a)–C(49a)
–161(1)
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8.2.   X-Ray Crystal Structure of Compound 11

8.2.1.   Experimental

A crystal of $C_{45}H_{45}B_5O_{10} \cdot CHCl_3$, obtained from $CDCl_3$, was mounted on a glass fibre and used for a low-temperature X-ray structure determination. All measurements were made on an *Agilent Technologies SuperNova* area-detector diffractometer[2] using Cu *K*a radiation (*l* = 1.54180 Å) from a micro-focus X-ray source and an *Oxford Instruments Cryojet XL* cooler. The unit cell constants and an orientation matrix for data collection were obtained from a least-squares refinement of the setting angles of 8066 reflections in the range $4° < 2q < 148°$. A total of 1876 frames were collected using *w* scans with *k* offsets, 0.5-4.0 seconds exposure time and a rotation angle of 0.5° per frame, and a crystal-detector distance of 55.0 mm.

Data reduction was performed with *CrysAlisPro*[2]. The intensities were corrected for Lorentz and polarization effects, and an empirical absorption correction using spherical harmonics[2] was applied. The space group was determined from the systematic absences, packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure. Equivalent reflections, other than Friedel pairs, were merged. The data collection and refinement parameters are given in *Table 1*. A view of the molecule is shown in the *Figure*.

The structure was solved by direct methods using *SHELXS-2013* [3], which revealed the

positions of all non-hydrogen atoms. The entire molecule is disordered over two positions related by a crystallographic mirror plane passing through the molecule, which arise from the superposition of the enantiomorphs of the axially chiral corannulene molecule on the same crystallographic site. One set of atomic positions were defined for the entire molecule and the mirror symmetry generates the other orientation. The site occupation factor of each orientation is 0.5 by definition. Similarity restraints were applied to the chemically equivalent bond lengths involving all atoms in the corannulene core and the C–B bonds. The five peripheral substituents were also restrained to have similar bond lengths and angles. Neighbouring atoms within and between each orientation of the molecule were restrained to have similar atomic displacement parameters. The non-hydrogen atoms were refined anisotropically. All of the H-atoms were placed in geometrically calculated positions and refined by using a riding model where each H-atom was assigned a fixed isotropic displacement parameter with a value equal to $1.2U_{eq}$ of its parent atom. The refinement of the structure was carried out on F^2 by using full-matrix least-squares procedures, which minimised the function $Sw(F_o{}^2 - F_c{}^2)^2$. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. Plots of $Sw(F_o{}^2 - F_c{}^2)^2$ versus $F_c/F_c(max)$ and resolution showed no unusual trends. A correction for secondary extinction was not applied. Refinement of the absolute structure parameter[4] yielded a value of 0.030(6), which confidently confirms that the refined model represents the true absolute structure.

Neutral atom scattering factors for non-hydrogen atoms were taken from Maslen, Fox and O'Keefe[5a], and the scattering factors for H-atoms were taken from Stewart, Davidson and Simpson[6]. Anomalous dispersion effects were included in F_c[7]; the values for f' and f'' were those of Creagh and McAuley[5b]. The values of the mass attenuation coefficients are those of Creagh and Hubbel[5c]. The *SHELXL-2013* program[3] was used for all calculations.

8.2.2. Results

Crystallised from	$CDCl_3$
Empirical formula	$C_{46}H_{46}B_5Cl_3O_{10}$
Formula weight [g mol^{-1}]	919.27
Crystal colour, habit	yellow, prism
Crystal dimensions [mm]	0.14 x 0.17 x 0.25
Temperature [K]	160(1)
Crystal system	orthorhombic
Space group	$Pmn2_1$ (#31)
Z	2
Reflections for cell determination	8066
2θ range for cell determination [°]	4−148
Unit cell parameters a [Å]	20.2644(2)
b [Å]	13.18215(13)
c [Å]	8.24990(8)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	2203.78(4)
$F(000)$	956
D_x [g cm^{-3}]	1.385
μ(Cu $K\alpha$) [mm^{-1}]	2.373
Scan type	ω
$2\theta_{(max)}$ [°]	148.5
Transmission factors (min; max)	0.610; 1.000
Total reflections measured	11867
Symmetry independent reflections	4240
R_{int}	0.016
Reflections with $I > 2\sigma(I)$	4195
Reflections used in refinement	4240
Parameters refined; restraints	562; 750
Final $R(F)$ [$I > 2\sigma(I)$ reflections]	0.0531
$wR(F^2)$ (all data)	0.1442
Weights: $w = [\sigma^2(F_o^2) + (0.0675P)^2 + 2.2122P]^{-1}$ where $P = (F_o^2 + 2F_c^2)/3$	
Goodness of fit	1.059
Final Δ_{max}/σ	0.000
$\Delta\rho$ (max; min) [e Å^{-3}]	0.92; -0.82

$\sigma(d_{(C-C)})$ [Å] $0.005 - 0.014$

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TABLE 2. Bond lengths (Å) with standard uncertainties in parentheses.

C(1)	-C(6)	1.383(6)		B(2)	-O(4)	1.361(6)
C(1)	-C(2)	1.395(9)		B(2)	-O(3)	1.364(7)
C(1)	-C(5)	1.409(10)		O(3)	-C(26)	1.482(13)
C(2)	-C(9)	1.385(6)		O(4)	-C(30)	1.435(13)
C(2)	-C(3)	1.418(7)		C(26)	-C(27)	1.521(14)
C(3)	-C(12)	1.380(6)		C(26)	-C(30)	1.542(6)
C(3)	-C(4)	1.418(7)		C(27)	-C(28)	1.547(9)
C(4)	-C(15)	1.386(6)		C(28)	-C(29)	1.519(9)
C(4)	-C(5)	1.398(9)		C(29)	-C(30)	1.547(14)
C(5)	-C(18)	1.386(6)		B(3)	-O(6)	1.361(6)
C(6)	-C(7)	1.445(5)		B(3)	-O(5)	1.365(7)
C(6)	-C(20)	1.446(5)		O(5)	-C(31)	1.478(12)
C(7)	-C(8)	1.396(7)		O(6)	-C(35)	1.429(13)
C(7)	-B(1)	1.563(7)		C(31)	-C(32)	1.511(14)
C(8)	-C(9)	1.445(5)		C(31)	-C(35)	1.544(6)
C(9)	-C(10)	1.446(5)		C(32)	-C(33)	1.543(9)
C(10)	-C(11)	1.396(7)		C(33)	-C(34)	1.518(10)
C(10)	-B(2)	1.563(6)		C(34)	-C(35)	1.546(14)
C(11)	-C(12)	1.447(6)		B(4)	-O(8)	1.359(6)
C(12)	-C(13)	1.447(5)		B(4)	-O(7)	1.364(7)
C(13)	-C(14)	1.398(7)		O(7)	-C(36)	1.481(13)
C(13)	-B(3)	1.564(7)		O(8)	-C(40)	1.433(13)
C(14)	-C(15)	1.447(6)		C(36)	-C(37)	1.513(14)
C(15)	-C(16)	1.447(5)		C(36)	-C(40)	1.542(6)
C(16)	-C(17)	1.398(7)		C(37)	-C(38)	1.542(9)
C(16)	-B(4)	1.563(6)		C(38)	-C(39)	1.517(10)
C(17)	-C(18)	1.447(5)		C(39)	-C(40)	1.543(14)
C(18)	-C(19)	1.448(5)		B(5)	-O(10)	1.362(6)
C(19)	-C(20)	1.398(7)		B(5)	-O(9)	1.364(7)
C(19)	-B(5)	1.564(7)		O(9)	-C(41)	1.478(13)
B(1)	-O(2)	1.361(6)		O(10)	-C(45)	1.429(13)
B(1)	-O(1)	1.365(7)		C(41)	-C(42)	1.512(14)
O(1)	-C(21)	1.483(13)		C(41)	-C(45)	1.544(6)
O(2)	-C(25)	1.433(13)		C(42)	-C(43)	1.542(9)
C(21)	-C(22)	1.518(14)		C(43)	-C(44)	1.518(10)
C(21)	-C(25)	1.541(6)		C(44)	-C(45)	1.545(14)
C(22)	-C(23)	1.543(9)		Cl(1)	-C(46)	1.710(6)
C(23)	-C(24)	1.517(9)		Cl(2)	-C(46)	1.783(11)

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C(24) -C(25)    1.545(14)
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TABLE 3. Bond angles (°) with standard uncertainties in parentheses.

C(6) -C(1) -C(2)	122.4(6)	O(2) -C(25) -C(24)	112.7(10)
C(6) -C(1) -C(5)	123.0(5)	C(21) -C(25) -C(24)	102.8(13)
C(2) -C(1) -C(5)	108.4(3)	O(4) -B(2) -O(3)	113.6(4)
C(9) -C(2) -C(1)	124.1(5)	O(4) -B(2) -C(10)	121.3(7)
C(9) -C(2) -C(3)	122.1(5)	O(3) -B(2) -C(10)	125.1(7)
C(1) -C(2) -C(3)	107.9(4)	B(2) -O(3) -C(26)	108.2(6)
C(12) -C(3) -C(2)	123.3(5)	B(2) -O(4) -C(30)	108.4(6)
C(12) -C(3) -C(4)	123.0(5)	O(3) -C(26) -C(27)	109.6(10)
C(2) -C(3) -C(4)	107.6(5)	O(3) -C(26) -C(30)	103.1(10)
C(15) -C(4) -C(5)	123.0(5)	C(27) -C(26) -C(30)	109.0(14)
C(15) -C(4) -C(3)	123.6(5)	C(26) -C(27) -C(28)	101.4(8)
C(5) -C(4) -C(3)	107.9(4)	C(29) -C(28) -C(27)	102.2(5)
C(18) -C(5) -C(4)	122.9(5)	C(28) -C(29) -C(30)	106.4(8)
C(18) -C(5) -C(1)	122.9(5)	O(4) -C(30) -C(26)	105.9(10)
C(4) -C(5) -C(1)	108.3(3)	O(4) -C(30) -C(29)	111.9(10)
C(1) -C(6) -C(7)	116.1(6)	C(26) -C(30) -C(29)	102.7(13)
C(1) -C(6) -C(20)	113.7(6)	O(6) -B(3) -O(5)	113.6(4)

C(7)	–C(6)	–C(20)	129.1(7)	O(6)	–B(3)	–C(13)
			121.3(6)			
C(8)	–C(7)	–C(6)	118.8(5)	O(5)	–B(3)	–C(13)
			125.1(7)			
C(8)	–C(7)	–B(1)	118.8(6)	B(3)	–O(5)	–C(31)
			108.1(6)			
C(6)	–C(7)	–B(1)	122.3(6)	B(3)	–O(6)	–C(35)
			108.7(6)			
C(7)	–C(8)	–C(9)	124.5(6)	O(5)	–C(31)	–C(32)
			110.5(10)			
C(2)	–C(9)	–C(8)	112.6(6)	O(5)	–C(31)	–C(35)
			103.3(9)			
C(2)	–C(9)	–C(10)	115.8(5)	C(32)	–C(31)	–C(35)
			109.6(14)			
C(8)	–C(9)	–C(10)	130.2(6)	C(31)	–C(32)	–C(33)
			102.7(8)			
C(11)	–C(10)	–C(9)	120.5(6)	C(34)	–C(33)	–C(32)
			102.5(5)			
C(11)	–C(10)	–B(2)	115.5(6)	C(33)	–C(34)	–C(35)
			106.3(8)			
C(9)	–C(10)	–B(2)	123.9(6)	O(6)	–C(35)	–C(31)
			106.1(10)			
C(10)	–C(11)	–C(12)	122.7(7)	O(6)	–C(35)	–C(34)
			112.6(10)			
C(3)	–C(12)	–C(11)	114.3(6)	C(31)	–C(35)	–C(34)
			102.6(13)			
C(3)	–C(12)	–C(13)	115.0(5)	O(8)	–B(4)	–O(7)
			113.7(4)			
C(11)	–C(12)	–C(13)	129.2(7)	O(8)	–B(4)	–C(16)
			121.9(6)			
C(14)	–C(13)	–C(12)	120.8(6)	O(7)	–B(4)	–C(16)
			124.4(6)			
C(14)	–C(13)	–B(3)	115.8(6)	B(4)	–O(7)	–C(36)
			108.1(6)			
C(12)	–C(13)	–B(3)	123.3(6)	B(4)	–O(8)	–C(40)
			108.6(6)			
C(13)	–C(14)	–C(15)	123.4(8)	O(7)	–C(36)	–C(37)
			110.4(10)			

C(4) –C(15) –C(14)	113.3(6)	O(7) –C(36) –C(40)	103.2(9)
C(4) –C(15) –C(16)	115.8(5)	C(37) –C(36) –C(40)	109.4(14)
C(14) –C(15) –C(16)	129.7(7)	C(36) –C(37) –C(38)	102.5(8)
C(17) –C(16) –C(15)	119.0(5)	C(39) –C(38) –C(37)	102.6(4)
C(17) –C(16) –B(4)	118.0(5)	C(38) –C(39) –C(40)	106.8(8)
C(15) –C(16) –B(4)	123.0(5)	O(8) –C(40) –C(36)	106.1(10)
C(16) –C(17) –C(18)	123.9(7)	O(8) –C(40) –C(39)	112.7(10)
C(5) –C(18) –C(17)	113.6(7)	C(36) –C(40) –C(39)	102.6(13)
C(5) –C(18) –C(19)	115.4(5)	O(10) –B(5) –O(9)	113.6(4)
C(17) –C(18) –C(19)	130.2(7)	O(10) –B(5) –C(19)	122.1(6)
C(20) –C(19) –C(18)	119.6(6)	O(9) –B(5) –C(19)	124.3(6)
C(20) –C(19) –B(5)	117.1(6)	B(5) –O(9) –C(41)	108.2(6)
C(18) –C(19) –B(5)	123.0(6)	B(5) –O(10) –C(45)	108.6(6)
C(19) –C(20) –C(6)	123.7(7)	O(9) –C(41) –C(42)	110.4(10)
O(2) –B(1) –O(1)	113.6(4)	O(9) –C(41) –C(45)	103.1(9)
O(2) –B(1) –C(7)	125.1(7)	C(42) –C(41) –C(45)	109.6(14)
O(1) –B(1) –C(7)	121.1(7)	C(41) –C(42) –C(43)	102.5(8)
B(1) –O(1) –C(21)	108.1(6)	C(44) –C(43) –C(42)	102.5(5)
B(1) –O(2) –C(25)	108.5(6)	C(43) –C(44) –C(45)	106.5(8)

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O(1)  -C(21) -C(22)    109.5(10)              O(10) -C(45) -C(41)
106.2(10)

O(1)  -C(21) -C(25)    103.1(10)              O(10) -C(45) -C(44)
112.7(10)

C(22) -C(21) -C(25)    109.2(14)              C(41) -C(45) -C(44)
102.5(13)

C(21) -C(22) -C(23)    101.9(8)               Cl(1) -C(46) -Cl(1')
116.6(6)

C(24) -C(23) -C(22)    102.6(4)               Cl(1) -C(46) -Cl(2)
110.1(3)

C(23) -C(24) -C(25)    106.7(8)

O(2)  -C(25) -C(21)    106.0(10)
```

Primed atoms refer to the molecule in the following symmetry related position:

' 1-*x*, *y*, *z*

```
C(6)  -C(1)  -C(2)  -C(9)      -0(1)          B(1)  -O(2)  -C(25) -C(24)
104(1)
C(5)  -C(1)  -C(2)  -C(9)    153.0(7)         O(1)  -C(21) -C(25) -O(2)
8(2)
C(6)  -C(1)  -C(2)  -C(3)   -153.4(7)         C(22) -C(21) -C(25) -O(2)
124(1)
C(5)  -C(1)  -C(2)  -C(3)      -0(1)          O(1)  -C(21) -C(25) -C(24)
-111(1)
C(9)  -C(2)  -C(3)  -C(12)     -1(1)          C(22) -C(21) -C(25) -C(24)
6(2)
C(1)  -C(2)  -C(3)  -C(12)   153.3(7)         C(23) -C(24) -C(25) -O(2)
-94(1)
C(9)  -C(2)  -C(3)  -C(4)   -153.5(7)         C(23) -C(24) -C(25) -C(21)
20(1)
C(1)  -C(2)  -C(3)  -C(4)      0.4(9)         C(11) -C(10) -B(2)  -O(4)
-4(2)
C(12) -C(3)  -C(4)  -C(15)     1(1)           C(9)  -C(10) -B(2)  -O(4)
179(1)
C(2)  -C(3)  -C(4)  -C(15)   153.9(7)         C(11) -C(10) -B(2)  -O(3)
178(1)
C(12) -C(3)  -C(4)  -C(5)   -153.3(8)         C(9)  -C(10) -B(2)  -O(3)
1(2)
C(2)  -C(3)  -C(4)  -C(5)     -0.3(8)         O(4)  -B(2)  -O(3)  -C(26)
-1(2)
```

C(15)	−C(4)	−C(5)	−C(18)	−1(1)	C(10)	−B(2)	−O(3)	−C(26)	176(1)
C(3)	−C(4)	−C(5)	−C(18)	153.8(8)	O(3)	−B(2)	−O(4)	−C(30)	7(2)
C(15)	−C(4)	−C(5)	−C(1)	−154.2(7)	C(10)	−B(2)	−O(4)	−C(30)	−171(1)
C(3)	−C(4)	−C(5)	−C(1)	0.1(8)	B(2)	−O(3)	−C(26)	−C(27)	−120(1)
C(6)	−C(1)	−C(5)	−C(18)	−1(1)	B(2)	−O(3)	−C(26)	−C(30)	−4(2)
C(2)	−C(1)	−C(5)	−C(18)	−153.5(8)	O(3)	−C(26)	−C(27)	−C(28)	82(1)
C(6)	−C(1)	−C(5)	−C(4)	153.1(7)	C(30)	−C(26)	−C(27)	−C(28)	−30(1)
C(2)	−C(1)	−C(5)	−C(4)	0.1(9)	C(26)	−C(27)	−C(28)	−C(29)	41.8(9)
C(2)	−C(1)	−C(6)	−C(7)	−10(1)	C(27)	−C(28)	−C(29)	−C(30)	−39.1(9)
C(5)	−C(1)	−C(6)	−C(7)	−158.8(7)	B(2)	−O(4)	−C(30)	−C(26)	−9(2)
C(2)	−C(1)	−C(6)	−C(20)	159.6(9)	B(2)	−O(4)	−C(30)	−C(29)	102(1)
C(5)	−C(1)	−C(6)	−C(20)	10(1)	O(3)	−C(26)	−C(30)	−O(4)	8(2)
C(1)	−C(6)	−C(7)	−C(8)	10(1)	C(27)	−C(26)	−C(30)	−O(4)	124(1)
C(20)	−C(6)	−C(7)	−C(8)	−158(1)	O(3)	−C(26)	−C(30)	−C(29)	−110(1)
C(1)	−C(6)	−C(7)	−B(1)	−173.7(9)	C(27)	−C(26)	−C(30)	−C(29)	7(2)
C(20)	−C(6)	−C(7)	−B(1)	19(2)	C(28)	−C(29)	−C(30)	−O(4)	−93(1)
C(6)	−C(7)	−C(8)	−C(9)	−0(1)	C(28)	−C(29)	−C(30)	−C(26)	20(1)
B(1)	−C(7)	−C(8)	−C(9)	−177.3(9)	C(14)	−C(13)	−B(3)	−O(6)	−4(2)
C(1)	−C(2)	−C(9)	−C(8)	9(1)	C(12)	−C(13)	−B(3)	−O(6)	179(1)
C(3)	−C(2)	−C(9)	−C(8)	158.7(7)	C(14)	−C(13)	−B(3)	−O(5)	177(1)
C(1)	−C(2)	−C(9)	−C(10)	−158.7(7)	C(12)	−C(13)	−B(3)	−O(5)	−0(2)
C(3)	−C(2)	−C(9)	−C(10)	−9(1)	O(6)	−B(3)	−O(5)	−C(31)	5(1)
C(7)	−C(8)	−C(9)	−C(2)	−9(1)	C(13)	−B(3)	−O(5)	−C(31)	−176(1)
C(7)	−C(8)	−C(9)	−C(10)	156.8(8)	O(5)	−B(3)	−O(6)	−C(35)	−4(1)
C(2)	−C(9)	−C(10)	−C(11)	9(1)	C(13)	−B(3)	−O(6)	−C(35)	177(1)

C(8)	−C(9)	−C(10)	−C(11)	−156(1)	B(3) −O(5) −C(31) −C(32)			−121(1)
C(2)	−C(9)	−C(10)	−B(2)	−173.8(8)	B(3) −O(5) −C(31) −C(35)			−4(2)
C(8)	−C(9)	−C(10)	−B(2)	21(1)	O(5) −C(31) −C(32) −C(33)			88(1)
C(9)	−C(10)	−C(11)	−C(12)	−0(2)	C(35) −C(31) −C(32) −C(33)			−25(2)
B(2)	−C(10)	−C(11)	−C(12)	−177(1)	C(31) −C(32) −C(33) −C(34)			39(1)
C(2)	−C(3)	−C(12)	−C(11)	10(1)	C(32) −C(33) −C(34) −C(35)			−39(1)
C(4)	−C(3)	−C(12)	−C(11)	158.4(9)	B(3) −O(6) −C(35) −C(31)			1(2)
C(2)	−C(3)	−C(12)	−C(13)	−157.3(7)	B(3) −O(6) −C(35) −C(34)			112(1)
C(4)	−C(3)	−C(12)	−C(13)	−9(1)	O(5) −C(31) −C(35) −O(6)			2(2)
C(10)	−C(11)	−C(12)	−C(3)	−9(2)	C(32) −C(31) −C(35) −O(6)			120(1)
C(10)	−C(11)	−C(12)	−C(13)	156(1)	O(5) −C(31) −C(35) −C(34)			−116(1)
C(3)	−C(12)	−C(13)	−C(14)	8(1)	C(32) −C(31) −C(35) −C(34)			2(2)
C(11)	−C(12)	−C(13)	−C(14)	−157(1)	C(33) −C(34) −C(35) −O(6)			−90(1)
C(3)	−C(12)	−C(13)	−B(3)	−175.6(8)	C(33) −C(34) −C(35) −C(31)			23(2)
C(11)	−C(12)	−C(13)	−B(3)	20(1)	C(17) −C(16) −B(4) −O(8)			−7(2)
C(12)	−C(13)	−C(14)	−C(15)	1(2)	C(15) −C(16) −B(4) −O(8)			173(1)
B(3)	−C(13)	−C(14)	−C(15)	−176(1)	C(17) −C(16) −B(4) −O(7)			175(1)
C(5)	−C(4)	−C(15)	−C(14)	158(1)	C(15) −C(16) −B(4) −O(7)			−5(1)
C(3)	−C(4)	−C(15)	−C(14)	7(1)	O(8) −B(4) −O(7) −C(36)			3(1)
C(5)	−C(4)	−C(15)	−C(16)	−11(1)	C(16) −B(4) −O(7) −C(36)			−180(1)
C(3)	−C(4)	−C(15)	−C(16)	−161.4(7)	O(7) −B(4) −O(8) −C(40)			1(1)
C(13)	−C(14)	−C(15)	−C(4)	−8(2)	C(16) −B(4) −O(8) −C(40)			−177.1(9)
C(13)	−C(14)	−C(15)	−C(16)	159(1)	B(4) −O(7) −C(36) −C(37)			−122(1)
C(4)	−C(15)	−C(16)	−C(17)	12(1)	B(4) −O(7) −C(36) −C(40)			−5(2)
C(14)	−C(15)	−C(16)	−C(17)	−154.6(8)	O(7) −C(36) −C(37) −C(38)			86(1)

C(4) -C(15) -C(16) -B(4)   -168.0(8)
C(14) -C(15) -C(16) -B(4)   25(2)
C(15) -C(16) -C(17) -C(18) -2(2)
B(4) -C(16) -C(17) -C(18) 178(1)
C(4) -C(5) -C(18) -C(17) 11(1)
C(1) -C(5) -C(18) -C(17) 160(1)
C(4) -C(5) -C(18) -C(19) -160.1(7)
C(1) -C(5) -C(18) -C(19) -10(1)
C(16) -C(17) -C(18) -C(5)   -9(2)
C(16) -C(17) -C(18) -C(19) 160(1)
C(5) -C(18) -C(19) -C(20) 11(1)
C(17) -C(18) -C(19) -C(20) -158(1)
C(5) -C(18) -C(19) -B(5)   -176.2(8)
C(17) -C(18) -C(19) -B(5)   15(2)
C(18) -C(19) -C(20) -C(6)   -1(2)
B(5) -C(19) -C(20) -C(6)   -174(1)
C(1) -C(6) -C(20) -C(19) -10(2)
C(7) -C(6) -C(20) -C(19) 158(1)
C(8) -C(7) -B(1) -O(2)   -9(2)
C(6) -C(7) -B(1) -O(2)   174(1)
C(8) -C(7) -B(1) -O(1)   175(1)
C(6) -C(7) -B(1) -O(1)   -2(2)
O(2) -B(1) -O(1) -C(21) 0(2)
C(7) -B(1) -O(1) -C(21) 177(1)
O(1) -B(1) -O(2) -C(25) 5(2)

C(40) -C(36) -C(37) -C(38) -27(2)
C(36) -C(37) -C(38) -C(39) 38.9(8)
C(37) -C(38) -C(39) -C(40) -37.8(9)
B(4) -O(8) -C(40) -C(36) -4(2)
B(4) -O(8) -C(40) -C(39) 108(1)
O(7) -C(36) -C(40) -O(8)   5(2)
C(37) -C(36) -C(40) -O(8)   123(1)
O(7) -C(36) -C(40) -C(39) -113(1)
C(37) -C(36) -C(40) -C(39) 4(2)
C(38) -C(39) -C(40) -O(8)   -93(1)
C(38) -C(39) -C(40) -C(36) 21(2)
C(20) -C(19) -B(5) -O(10) -12(2)
C(18) -C(19) -B(5) -O(10) 174(1)
C(20) -C(19) -B(5) -O(9)   168(1)
C(18) -C(19) -B(5) -O(9)   -5(2)
O(10) -B(5) -O(9) -C(41) 6(1)
C(19) -B(5) -O(9) -C(41) -175(1)
O(9) -B(5) -O(10) -C(45) -3(1)
C(19) -B(5) -O(10) -C(45) -122(1)
B(5) -O(9) -C(41) -C(42) -5(2)
B(5) -O(9) -C(41) -C(45) 87(1)
O(9) -C(41) -C(42) -C(43) -26(2)
C(45) -C(41) -C(42) -C(43) 39(1)
C(41) -C(42) -C(43) -C(44) -39(1)
C(42) -C(43) -C(44) -C(45)

C(7)	–B(1)	–O(2)	–C(25)	–171(1)	B(5)	–O(10)	–C(45)	–C(41) –0(2)
B(1)	–O(1)	–C(21)	–C(22)	–121(1)	B(5)	–O(10)	–C(45)	–C(44) 111(1)
B(1)	–O(1)	–C(21)	–C(25)	–5(2)	O(9)	–C(41)	–C(45)	–O(10) 3(2)
O(1)	–C(21)	–C(22)	–C(23)	84(1)	C(42)	–C(41)	–C(45)	–O(10) 121(1)
C(25)	–C(21)	–C(22)	–C(23)	–29(1)	O(9)	–C(41)	–C(45)	–C(44) –115(1)
C(21)	–C(22)	–C(23)	–C(24)	40.0(9)	C(42)	–C(41)	–C(45)	–C(44) 2(2)
C(22)	–C(23)	–C(24)	–C(25)	–38(1)	C(43)	–C(44)	–C(45)	–O(10) –91(1)
B(1)	–O(2)	–C(25)	–C(21)	–8(2)	C(43)	–C(44)	–C(45)	–C(41) 23(2)