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Tuning the electrochemical potential of perfunctionalized dodecaborate clusters through vertex differentiation - SI

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General considerations

Microwave synthesis reactions and all post-microwave work-up and characterization was performed under ambient conditions. The "ambient conditions" for this manuscript refer to room temperature (20 - 25 °C) and uncontrolled laboratory air. The oxidation of **[2c]** to form **[2a]** and the synthesis of **[2c]-ME** describe the use of a nitrogen-filled glovebox for several steps, all other reactions were performed open to air.

Materials

Deuterated solvents were purchased from Cambridge Isotope Laboratories and used as received. MilliQ water described in this manuscript refers to purified potable water with a resistivity at 25 °C of ≤18.2 MΩ·cm. $[NEt_3H]_2[B_{12}H_{12}]$ was purchased from Boron Specialties (USA). Ethanol (200 proof) was purchased from Decon Labs and used as received. Dowex 50W X8 (100-200 mesh, hydrogen form), dimethylformamide (anhydrous, 99.8%), $FeCl_3{\cdot}6H_2O$ (≥97%), $CsOH{\cdot}1H_2O$ (≥99.5%), hydrogen peroxide (30% in H_2O), $[N^nBu_4]OH$ (40% in H_2O), bromoethane (≥99%), acetonitrile (≥99.9%), dichloromethane (≥99.5%), ethyl acetate (≥99.5%), hexanes (≥98.5%), methanol (≥99.8%), 2-mercaptoethanol (≥99%), potassium phosphate tribasic (≥98%), and *N*,*N*-diisopropylethylamine (≥99%) were purchased from Sigma-Aldrich. Tetrabutylammonium hexafluorophosphate (≥98%, recrystallized from ethanol and dried under vacuum at 90 °C), nitrosonium tetrafluoroborate (95%), hydroxylamine-O-sulfonic acid (97%), and 2,3,4,5,6 pentaflurobenzyl bromide (98%) were purchased from Oakwood. NaOH (Certified ACS, 99.2%) was purchased from Fisher. Sodium borohydride (98%) was purchased from Strem. All reagents were used as received unless otherwise indicated.

Instrumentation

A Bruker AV400 spectrometer was used to obtain ^{11}B, ^{1}H, and ^{19}F NMR spectra and Bruker Topspin software was used to process the NMR data. ^{1}H NMR spectra were referenced to residual solvent resonances in deuterated solvents (δ 7.26 for $CDCl_3$, δ 5.32 for CD_2Cl_2, δ 1.94 for CD_3CN, and δ 3.31 for CD_3OD. ^{11}B and ^{19}F NMR spectra were referenced to $BF_3{\cdot}Et_2O$ (δ 0.00 and δ 153.38 for ^{11}B and ^{19}F, respectively). All spectra was obtained at ambient temperature.

A Bruker EMX EPR spectrometer was used to acquire EPR spectra, with all spectra collected in CH_2Cl_2 at ambient temperature.

Mass spectrometry data was acquired using a Thermo Scientific™ Q-Exactive™ Plus instrument with a quadrupole mass filter and Orbitrap mass analyzer.

UV-vis analysis was performed on an Ocean Optics Flame Spectrometer with an Ocean Optics DH-2000-S-DUV-TTL light source and a quartz cuvette.

IR spectroscopy was acquired on solid samples using a PerkinElmer Spectrum One FT-IR spectrometer equipped with a diamond universal ATR probe.

X-ray photoelectron spectroscopy (XPS) data was acquired using an AXIS Ultra DLD instrument (Kratos Analytical Inc., Chestnut Ridge, NY, USA) with a monochromatic Al Kα X-ray source (10 mA for survey and high-resolution scans). A 300 x 700 nm oval spot size and ultrahigh vacuum (10^{-9} Torr) were used, with 160 eV pass energy for survey spectra and 20 eV for high-resolution spectra of B 1s using a 200 ms dwell time and 20 scans. All XPS peaks were externally referenced to the C 1s signal at 284.6 eV.

Elemental analyses were performed by Atlantic Microlab, Inc. (Norcross, GA).

X-ray data collection and processing parameters

For [**2b**] and **[3]**$^{1-}$, a single crystal was mounted on a nylon loop using perfluoropolyether oil and cooled rapidly to 100 K with a stream of cold dinitrogen. Diffraction data were measured using a Bruker APEX-II CCD diffractometer using Mo-K_α radiation. The cell refinement and data reduction were carried out using Bruker SAINT and the structure was solved with SHELXT. All subsequent crystallographic calculations were performed using SHELXT. Olex2 software was used to export the report for **[3]**$^{1-}$.[1]

Cyclic voltammetry

Cyclic voltammetry was performed on [**2b**] using a CH Instruments CHI630D potentiostat with a glassy carbon disc working electrode, platinum wire counter electrode, and Ag/AgCl (in saturated KCl solution) reference electrode. The experiment was conducted in 0.1M $[N^nBu_4]PF_6/CH_3CN$ with 1 mM analyte concentration. The CH_3CN was dried in house with a custom drying system running through two alumina columns prior to use. The solution was degassed by bubbling N_2, and the cyclic voltammetry was performed under N_2 gas. For [**2b**] a scan rate of 100 mV/s was used with Fc/Fc^+ as an internal standard.

Microwave synthesis

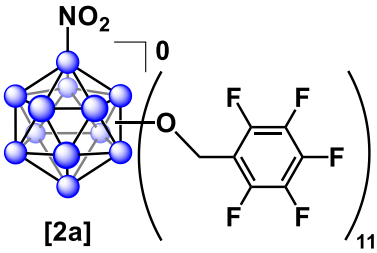
Microwave reactions were performed using a CEM Discover SP microwave synthesis reactor. Except where noted otherwise, all reactions were performed in glass 10 mL microwave reactor vials purchased from the vendor. Reaction vials were sealed with silicone/PTFE caps. Flea micro PTFE-coated stir bars were used in the vials with magnetic stirring set to high and 15 seconds of premixing prior to the temperature ramping. All microwave reactions were carried out at 140 °C

with the pressure release limit set to 250 psi (no reactions exceeded this limit to trigger venting) and the maximum wattage set to 250W (the power applied was dynamically controlled by the microwave instrument and did not exceed this limit for any reactions). Column chromatography was performed using 2.0 - 2.25 cm inner diameter glass fritted chromatography columns with 20-30 cm of slurry-packed silica gel to ensure full separation of reagents and products. Unfiltered pressurized air was used to assist column chromatography.

Synthesis of [1]

Synthesis of $[N^nBu_4]_2B_{12}(OH)_{11}(NO_2)$ **([1])** was performed starting with $Cs_2[B_{12}H_{12}]$ (ion exchanged from $[NEt_3H]_2[B_{12}H_{12}]$ using $CsOH{\cdot}1H_2O$) according to a reported procedure.[2] *Note: the hydroxylation procedure should always be undertaken with caution and careful planning to ensure the $Cs_2[B_{12}H_{12}]$ reagent is pure and contains no organic contaminants. Blast shielding to contain any possible explosions should be utilized. Under no circumstances should the hydrogen peroxide used in the reaction come into contact with any organic material or solvents due to possibility of an explosion.*

Synthesis of [2a]

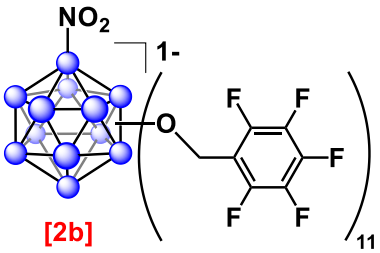


[2a]

$[N^nBu_4]_2B_{12}(OH)_{11}(NO_2)$ (100 mg, 0.12 mmol) was added to a 10 mL glass microwave vial and dissolved in 1 mL of acetonitrile. *N*,*N*-diisopropylethylamine (0.47 mL, 2.7 mmol) and 1-(bromomethyl)-2,3,4,5,6-pentafluorobenzene (2.00 mL, 13.2 mmol) were added along with a flea micro stir bar, the vial was sealed with a PTFE/silicone cap, and the mixture was heated at

140 °C with stirring in the microwave for 1 hour. The excess acetonitrile was evaporated by rotary evaporation and the excess reagents were removed through a slurry-packed silica gel column with 35/65 [v/v] ethyl acetate/hexane, followed by acetone (~20 mL) to elute the yellow-orange product band. The acetone was removed by rotary evaporation, the residue was dried under high vacuum and transferred into the glovebox. 75 mg (0.64 mmol) nitrosonium tetrafluoroborate ($NOBF_4$) was added, 2 mL of acetonitrile was added, and the solution was left to stir at room temperature for ~16 hours. The solution was transferred out of the glovebox, cooled to -15 °C for 1 hour, filtered using a glass fritted funnel, and the orange solid was carefully washed with ~1 mL of cold (-15 °C) acetonitrile 3 times, then dried on the frit for 5 min. The solid product was transferred to a glass vial and dried under high vacuum to obtain 113 mg (41%) of pure, isolated product. Compound [**2a**]^0 is an orange solid. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 5.36 – 5.06 (m, 11H, O-C$\underline{H_2}$-C_6F_5). ^{11}B NMR (128 MHz, CD_2Cl_2): δ 45.22 – 41.32 (m, 10B, $\underline{B}$-OR), 1.99 (s, 1B, $\underline{B}$-NO_2), -9.58 (s, 1B, $\underline{B}$-OR). ^{19}F NMR (376 MHz, CD_2Cl_2): δ -144.34 – -145.48 (m, 22F, *ortho*-$C_6\underline{F_5}$), -152.78 – -154.05 (m, 11F, *para*-$C_6\underline{F_5}$), -162.26 – -162.75 (m, 22F, *meta*-$C_6\underline{F_5}$). HRMS: *m/z* calculated for $C_{77}H_{22}B_{12}F_{55}NO_{13}$ (M^{2-}), 1172.5665 Da; found, 1172.5735 (z = 2) Da. Calc. for $C_{77}H_{22}B_{12}F_{55}NO_{13}$: C, 39.46; H, 0.95; N, 0.60. Found: C, 39.64; H, 0.90; N, 0.62.

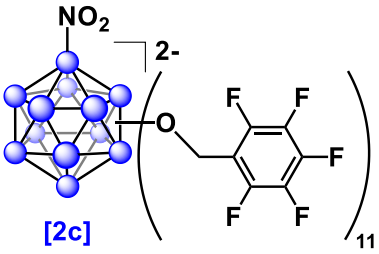
Synthesis of [2b]



$[N^nBu_4]_2B_{12}(OH)_{11}(NO_2)$ (100 mg, 0.12 mmol) was added to a 10 mL glass microwave vial and dissolved in 1 mL of acetonitrile. *N*,*N*-diisopropylethylamine (0.47 mL, 2.7 mmol) and 1-(bromomethyl)-2,3,4,5,6-pentafluorobenzene (2.00 mL, 13.2 mmol) were added along with a flea micro stir bar, the vial was sealed with a PTFE/silicone cap, and the mixture was heated at 140 °C with stirring in the microwave for 1 hour. The excess acetonitrile was evaporated by rotary evaporation and the excess reagents were removed through a slurry-packed silica gel column with 35/65 [v/v] ethyl acetate/hexane, followed by acetone (~20 mL) to elute the yellow-orange product band. The acetone was removed by rotary evaporation, and the residue was dissolved in 5 mL of 9:1 [v/v] ethanol/acetonitrile. 0.3 g (1.11 mmol) iron chloride hexahydrate was added, and the solution was left to stir at room temperature for ~48 hours. The volatiles were removed *via* rotary evaporation followed by high vacuum for 5 minutes, and the residue was dissolved in dichloromethane and loaded onto a slurry-packed silica gel column. The product was eluted with dichloromethane and the dark purple band was collected. The dichloromethane was removed *via* rotary evaporation, and the solid product was dried under high vacuum to obtain 107 mg (35%) isolated product. Compound $[N^nBu_4]$[**2b**] is a purple solid. ^{1}H NMR (400 MHz, CD_3CN): δ 3.11 – 3.04 (m, 8H, $[N^nBu_4]$), 1.65 – 1.55 (m, 8H, $[N^nBu_4]$), 1.40 – 1.30 (m, 8H, $[N^nBu_4]$), 0.97 (t, 12H, $[N^nBu_4]$). *Note: the methylene peak is not visible in ^{1}H NMR due to paramagnetic broadening.* ^{11}B NMR (128 MHz, CD_3CN): No visible signals due to paramagnetic broadening. ^{19}F NMR (376 MHz, CD_3CN): δ -140.13 (br s, *ortho*-$C_6\overline{F_5}$), -157.27 – -158.18 (m, *para*-$C_6\overline{F_5}$), -163.74 – -165.03 (m, *meta*-$C_6\overline{F_5}$). *Note: the ortho fluorine signal is*

extremely broad from the proximity to the paramagnetic core. HRMS: *m/z* calculated for $C_{77}H_{22}B_{12}F_{55}NO_{13}$ (M^{2-}), 1172.5665 Da; found, 1172.5724 (z = 2) Da. Calc. for $C_{93}H_{58}B_{12}F_{55}N_2O_{13}$: C, 43.19; H, 2.26; N, 1.08. Found: C, 43.39; H, 2.21; N, 1.06. Crystallized from $CHCl_3$ and pentane at room temperature for 3 days to obtain a single crystal for X-ray diffraction analysis.

Synthesis of [2c]



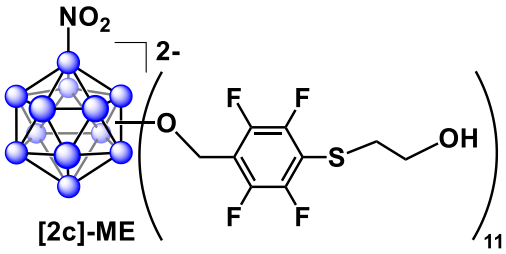
150 mg scale: $[N^nBu_4]_2B_{12}(OH)_{11}(NO_2)$ (150 mg, 0.18 mmol) was added to a 10 mL glass microwave vial and dissolved in 3 mL of acetonitrile. *N*,*N*-diisopropylethylamine (0.71 mL, 4.1 mmol) and 1-(bromomethyl)-2,3,4,5,6-pentafluorobenzene (2.93 mL, 19.4 mmol) were added along with a flea micro stir bar, the vial was sealed with a PTFE/silicone cap, and the mixture was heated at 140 °C with stirring in the microwave for 1 hour. The excess acetonitrile was evaporated by rotary evaporation and the excess reagents were removed through a slurry-packed silica gel column with 35/65 [v/v] ethyl acetate/hexane, followed by acetone to elute the yellow-orange product band. The acetone was removed by rotary evaporation, and the residue was dissolved in 5 mL of acetonitrile. This solution was added to 100 mL of 1:1 [v/v] acetonitrile/water and ion exchanged using Dowex 50W X8 cation exchange resin loaded with Na^+ by eluting the solution through a 1.5 x 40 cm column slurry-packed with ~30 cm of Dowex resin (solution-swelled volume) and washing with an additional 100 mL of 1:1 [v/v] acetonitrile/water. The methanol and water were removed *via* rotary evaporation followed by

high vacuum overnight to obtain 308 mg (71%) isolated product. Compound Na_2[**2c**] is a dark yellow solid.

300 mg scale: $[N^nBu_4]_2B_{12}(OH)_{11}(NO_2)$ (300 mg, 0.36 mmol) was added to a 35 mL glass microwave vial and dissolved in 6 mL of acetonitrile. *N*,*N*-diisopropylethylamine (1.42 mL, 8.2 mmol) and 1-(bromomethyl)-2,3,4,5,6-pentafluorobenzene (5.86 mL, 38.8 mmol) were added along with a flea micro stir bar, the vial was sealed with a PTFE/silicone cap, and the mixture was heated at 140 °C with stirring in the microwave for 1 hour. The excess acetonitrile was evaporated by rotary evaporation and the excess reagents were removed through a slurry-packed silica gel column with 35/65 [v/v] ethyl acetate/hexane, followed by acetone to elute the yellow-orange product band. The acetone was removed by rotary evaporation, and the residue was dissolved in 5 mL of acetonitrile. This solution was added to 200 mL of 1:1 [v/v] acetonitrile/water and ion exchanged using Dowex 50W X8 cation exchange resin loaded with Na^+ by eluting the solution through a 6 x 30 cm column slurry-packed with ~25 cm of Dowex resin (solution-swelled volume) and washing with an additional 250 mL of 1:1 [v/v] acetonitrile/water. *Note: if residual $[N^nBu_4]^+$ remains after the ion exchange, repeating the exchange procedure using freshly Na^+-loaded Dowex with the partially-exchanged product will remove any traces of $[N^nBu_4]^+$.* The methanol and water were removed *via* rotary evaporation followed by high vacuum overnight to obtain 610 mg (70%) isolated product. Compound Na_2[**2c**] is a yellow solid. ^{1}H NMR (400 MHz, CD_3CN): δ 5.54 – 5.21 (m, 22H, methylene). ^{11}B NMR (128 MHz, CD_3CN): δ -10.16 (s, 1B, B-NO_2), -11.87 – -18.32 (m, 10B, B-OR), -21.53 (br s, 1B, B-OR). ^{19}F NMR (376 MHz, CD_3CN): δ -144.39 (m, 22F, *ortho*-C_6F_5), -157.85 – -158.97 (m, 11F, *para*-C_6F_5), -164.86 – -165.77 (m, 22F, *meta*-C_6F_5). HRMS: *m/z* calculated for

$C_{77}H_{22}B_{12}F_{55}NO_{13}$ (M^{2-}), 1172.5665 Da; found, 1172.5734 (z = 2) Da. Calc. for $C_{77}H_{22}B_{12}F_{55}NNa_2O_{13}$: C, 38.70; H, 0.93; N, 0.59. Found: C, 38.67; H, 1.06; N, 1.45.

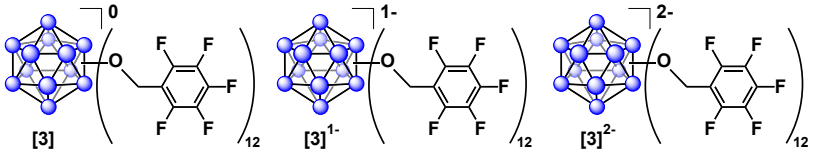
Synthesis of [2c]-ME



[2c] (7.5 mg, 0.0031 mmol) and K_3PO_4 (22.3 mg, 0.105 mmol) were added along with a flea micro stir bar to a 4-mL glass vial, which was then sealed with a PTFE/silicone cap under ambient conditions. The vial was then purged and backfilled with N_2 three times before being transferred into the glovebox. In the glovebox, the vial was opened and 150 µL anhydrous DMF was added, followed by 2-mercaptoethanol (2.54 µL, 0.036 mmol). The vial was sealed again and set to stir at 400 rpm for 22 hours. The vial was transferred out of the glovebox, and its contents were transferred into an NMR tube for *in situ* ^{19}F NMR spectroscopy to ensure nearly quantitative conversion and *in situ* ^{11}B NMR spectroscopy to ensure structural integrity of the cluster. The crude mixture was filtered through a 0.45 µm pore size syringe filter unit, then transferred into a 15-mL conical centrifuge tube and lyophilized for solvent removal. The dried sample was redissolved in MeOD and subjected to characterization *via* ^{1}H, ^{11}B, and ^{19}F NMR spectroscopy. Compound K_2[**2c**] is a dark yellow solid. ^{1}H NMR (400 MHz, CD_3OD): δ 5.58 – 5.35 (m, 22H, methylene), 3.70 – 3.58 (m, 22H, S-CH_2CH_2-OH), 3.05 – 2.96 (m, 22H, S-CH_2CH_2-OH). ^{11}B NMR (128 MHz, CD_3OD): δ -9.61 (br s, 1B, B-NO_2), -14.71 (br s, 11B, B-OR). ^{19}F NMR (376 MHz, CD_3OD): δ -136.40 – -137.35 (m, 22F, *ortho*-C_6F_5), -143.99 –

-145.38 (m, 22F, *meta*-$C_6\underline{F}_5$). HRMS: *m/z* calculated for $C_{77}H_{22}B_{12}F_{55}NO_{13}$ (M^{2-}), 1491.6089 Da; found, 1491.6154 (z = 2) Da.

Synthesis of [3], $[3]^{1-}$, and $[3]^{2-}$



Synthesis of **[3]** was performed according to a previously reported procedure.[3] *Note: the procedure below was not optimized, and was only suitable to produce enough of the radical salt to crystallize for X-ray diffraction analysis for comparison with **[2b]***. $\mathbf{[3]}^{1-}$ was synthesized by performing an extraction on the crude 2-/1- mixture of **[3]** with 25 mL dichloromethane and a solution of 0.65 g disodium EDTA in 150 mL MilliQ H_2O in lieu of the reported post-oxidation column chromatography with dichloromethane, vigorously stirring and shaking the mixture before draining off the organic layer and drying with sodium sulfate. The volatiles were removed *via* rotary evaporation, the residue was re-dissolved in dichloromethane and eluted through a plug of silica, and the dichloromethane was removed *via* rotary evaporation followed by high vacuum. The red-purple solid residue was taken up in chloroform and pentane was layered on top, resulting in formation of single crystals suitable for X-ray analysis after 5 days at room temperature. $\mathbf{[3]}^{2-}$ was generated by treatment of $\mathbf{[3]}^{0}$ (2.3 mg, 0.9 µmol) with $NaBH_4$ (2.0 mg, 53 mmol) in 9:1 [v/v] ethanol/acetonitrile and shaking for 5 min at room temperature. The resulting, unpurified solution of $\mathbf{[3]}^{2-}$ was used for UV-vis analysis.

Table 1. Crystal data and structure refinement for $[2b]^{1-}$

Identification code	**$[2b]^{1-}$**	
Empirical formula	C93 H58 B12 F55 N2 O13	
Formula weight	2586.13	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.1250(3) Å	α= 110.4400(10)°.
	b = 27.2616(5) Å	β= 91.6990(10)°.
	c = 29.4644(6) Å	γ = 97.1390(10)°.
Volume	10516.5(4) $Å^3$	
Z	4	
Density (calculated)	1.633 Mg/m^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	5156	
Crystal size	0.32 x 0.28 x 0.2 mm^3	
Theta range for data collection	1.273 to 25.292°.	
Index ranges	-16<=h<=16, -32<=k<=32, -30<=l<=35	
Reflections collected	79433	
Independent reflections	38080 [R(int) = 0.0454]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6462 and 0.6188	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	38080 / 3236 / 3184	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0857, wR2 = 0.2226	
R indices (all data)	R1 = 0.1376, wR2 = 0.2595	
Largest diff. peak and hole	1.257 and -0.520 e.$Å^{-3}$	
SQUEEZE	Found 129e/uc. Calc'ed for 2 $CHCl_3$, 116e/uc	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[2b]^{1-}$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	7569(2)	4922(2)	8571(2)	51(1)
F(2)	7883(3)	4089(2)	7797(2)	73(1)
F(3)	9562(4)	4127(2)	7362(2)	91(2)
F(4)	10889(3)	4990(2)	7713(2)	79(2)
F(5)	10564(3)	5826(1)	8482(2)	56(1)
F(6)	5603(2)	4847(1)	8639(1)	30(1)
F(7)	5918(3)	3891(1)	8624(1)	41(1)
F(8)	6340(3)	3740(1)	9470(1)	45(1)
F(9)	6476(2)	4570(1)	10330(1)	39(1)
F(10)	6211(2)	5531(1)	10342(1)	25(1)
F(11)	8538(2)	5420(1)	10225(1)	44(1)
F(12)	10004(3)	5026(2)	10510(2)	67(1)
F(13)	11614(3)	5686(2)	10989(2)	79(2)
F(14)	11709(3)	6745(2)	11216(2)	66(1)
F(15)	10232(2)	7142(1)	10941(1)	42(1)
F(16)	8425(3)	7687(2)	11445(1)	57(1)
F(17)	9920(4)	7839(2)	12093(2)	92(2)
F(18)	11422(3)	8610(2)	12193(2)	92(2)
F(19)	11430(3)	9214(2)	11639(2)	78(1)
F(20)	9938(3)	9062(2)	10987(2)	62(1)
F(21)	6230(3)	8269(1)	11351(1)	39(1)
F(22)	6344(3)	8493(1)	12316(1)	48(1)
F(23)	6236(3)	7701(2)	12679(1)	51(1)
F(24)	6022(3)	6680(1)	12068(1)	52(1)
F(25)	5908(2)	6451(1)	11093(1)	36(1)
F(26)	11287(2)	8389(1)	10344(1)	43(1)
F(27)	12911(3)	8888(1)	10146(2)	58(1)

F(28)	13787(2)	8410(2)	9326(2)	52(1)
F(29)	13031(2)	7429(2)	8713(1)	38(1)
F(30)	11394(2)	6938(1)	8901(1)	27(1)
F(31)	8731(3)	9416(2)	10424(1)	64(1)
F(32)	8575(3)	10383(2)	10411(2)	75(1)
F(33)	8711(4)	10577(2)	9582(2)	86(2)
F(34)	9004(4)	9794(2)	8750(2)	84(2)
F(35)	9179(3)	8824(1)	8755(1)	54(1)
F(36)	8768(2)	7914(1)	7937(1)	33(1)
F(37)	8853(2)	7779(1)	6990(1)	34(1)
F(38)	9232(2)	6844(1)	6355(1)	40(1)
F(39)	9582(3)	6065(1)	6677(1)	48(1)
F(40)	9487(3)	6193(1)	7629(1)	45(1)
F(41)	3538(2)	5864(1)	8715(1)	38(1)
F(42)	1886(2)	5449(1)	8962(1)	46(1)
F(43)	1057(2)	6028(1)	9757(1)	43(1)
F(44)	1902(2)	7021(1)	10311(1)	33(1)
F(45)	3546(2)	7437(1)	10059(1)	24(1)
F(46)	6465(2)	8846(1)	8616(1)	39(1)
F(47)	4988(3)	9234(1)	8322(1)	45(1)
F(48)	3345(2)	8595(1)	7896(1)	41(1)
F(49)	3187(2)	7544(1)	7744(1)	34(1)
F(50)	4642(2)	7151(1)	8032(1)	24(1)
F(51)	6691(3)	8974(1)	9638(1)	44(1)
F(52)	6552(3)	10016(1)	9974(2)	52(1)
F(53)	5367(3)	10406(1)	10678(1)	46(1)
F(54)	4296(3)	9735(1)	11037(1)	44(1)
F(55)	4479(3)	8706(1)	10724(1)	40(1)
O(1)	5849(3)	5864(2)	8491(1)	43(1)
O(2)	6052(3)	6439(1)	8151(1)	28(1)
O(3)	8038(2)	7094(1)	8430(1)	16(1)
O(4)	8340(2)	6162(1)	8803(1)	16(1)
O(5)	6759(2)	6039(1)	9556(1)	15(1)
O(6)	8814(2)	6661(1)	10008(1)	15(1)
O(7)	9645(2)	7356(1)	9352(1)	17(1)
O(8)	6892(2)	7148(1)	10482(1)	15(1)

O(9)	8735(2)	7944(1)	10354(1)	19(1)
O(10)	8183(2)	8215(1)	9357(1)	19(1)
O(11)	6542(2)	8110(1)	10099(1)	16(1)
O(12)	6076(2)	7603(1)	8900(1)	14(1)
O(13)	5247(2)	6915(1)	9585(1)	13(1)
N(1)	6191(3)	6305(2)	8501(1)	16(1)
C(1)	8873(5)	5855(2)	8987(2)	37(1)
C(2)	9070(4)	5388(2)	8557(2)	23(1)
C(3)	8410(4)	4941(2)	8368(2)	31(1)
C(4)	8552(5)	4514(2)	7972(2)	43(2)
C(5)	9405(5)	4539(2)	7756(2)	48(2)
C(6)	10068(5)	4976(3)	7927(3)	49(2)
C(7)	9900(4)	5397(2)	8326(2)	32(1)
C(8)	5798(3)	5770(2)	9503(2)	17(1)
C(9)	5899(3)	5220(2)	9490(2)	16(1)
C(10)	6128(3)	5131(2)	9912(2)	18(1)
C(11)	6270(4)	4640(2)	9911(2)	24(1)
C(12)	6200(4)	4222(2)	9476(2)	28(1)
C(13)	5978(4)	4293(2)	9047(2)	26(1)
C(14)	5827(3)	4791(2)	9064(2)	19(1)
C(15)	8528(4)	6525(2)	10415(2)	24(1)
C(16)	9335(4)	6292(2)	10572(2)	22(1)
C(17)	9314(4)	5760(2)	10468(2)	32(1)
C(18)	10073(4)	5548(3)	10615(3)	44(2)
C(19)	10867(4)	5882(3)	10855(3)	47(2)
C(20)	10917(4)	6417(3)	10971(2)	42(2)
C(21)	10167(4)	6615(2)	10826(2)	30(1)
C(22)	6017(4)	6958(2)	11387(2)	24(1)
C(23)	6078(4)	7072(2)	11889(2)	29(1)
C(24)	6181(4)	7586(2)	12194(2)	30(1)
C(25)	6244(4)	7985(2)	12015(2)	29(1)
C(26)	6176(4)	7864(2)	11520(2)	24(1)
C(27)	6056(3)	7349(2)	11193(2)	18(1)
C(28)	8363(4)	8249(2)	10796(2)	33(1)
C(29)	9150(4)	8379(2)	11189(2)	34(1)
C(30)	9165(4)	8072(3)	11482(2)	40(1)

C(31)	9923(5)	8134(3)	11810(2)	54(2)
C(32)	10693(5)	8527(3)	11862(2)	57(2)
C(33)	10685(5)	8853(3)	11575(2)	54(2)
C(34)	9921(4)	8748(3)	11257(2)	40(1)
C(35)	5972(3)	7223(2)	10649(2)	23(1)
C(36)	10358(3)	7371(2)	9713(2)	16(1)
C(37)	11282(3)	7656(2)	9621(2)	18(1)
C(38)	11696(4)	8149(2)	9934(2)	28(1)
C(39)	12530(4)	8410(2)	9837(2)	35(1)
C(40)	12972(4)	8165(2)	9421(2)	31(1)
C(41)	12588(4)	7670(2)	9107(2)	27(1)
C(42)	11748(3)	7421(2)	9209(2)	19(1)
C(43)	9069(4)	8542(2)	9587(2)	24(1)
C(44)	8986(4)	9086(2)	9591(2)	25(1)
C(45)	8823(4)	9500(2)	10004(2)	37(1)
C(46)	8736(4)	9993(2)	10001(3)	44(2)
C(47)	8790(5)	10088(2)	9586(3)	49(2)
C(48)	8951(5)	9701(3)	9163(3)	49(2)
C(49)	9041(4)	9202(2)	9169(2)	33(1)
C(50)	9028(3)	7137(2)	8336(2)	25(1)
C(51)	9094(3)	7053(2)	7810(2)	23(1)
C(52)	8934(3)	7452(2)	7630(2)	21(1)
C(53)	8988(3)	7384(2)	7149(2)	23(1)
C(54)	9179(4)	6913(2)	6829(2)	26(1)
C(55)	9351(4)	6514(2)	6991(2)	30(1)
C(56)	9298(4)	6588(2)	7480(2)	27(1)
C(57)	6396(3)	7746(2)	8501(2)	18(1)
C(58)	5604(3)	7988(2)	8340(2)	15(1)
C(59)	5671(4)	8516(2)	8407(2)	22(1)
C(60)	4906(4)	8720(2)	8259(2)	30(1)
C(61)	4082(4)	8395(2)	8041(2)	25(1)
C(62)	3997(4)	7871(2)	7970(2)	22(1)
C(63)	4748(3)	7673(2)	8115(2)	18(1)
C(64)	4503(3)	6905(2)	9241(2)	16(1)
C(65)	3590(3)	6670(2)	9373(2)	16(1)
C(66)	3147(3)	6943(2)	9780(2)	15(1)

C(67)	2305(3)	6735(2)	9915(2)	21(1)
C(68)	1877(3)	6236(2)	9635(2)	24(1)
C(69)	2292(4)	5947(2)	9230(2)	26(1)
C(70)	3128(4)	6162(2)	9107(2)	22(1)
C(71)	5650(4)	8234(2)	9959(2)	24(1)
C(72)	5620(4)	8810(2)	10173(2)	24(1)
C(73)	5013(4)	9022(2)	10532(2)	31(1)
C(74)	4914(4)	9548(2)	10701(2)	34(1)
C(75)	5452(4)	9888(2)	10519(2)	34(1)
C(76)	6060(4)	9693(2)	10158(2)	33(1)
C(77)	6123(4)	9161(2)	9991(2)	28(1)
B(1)	8165(4)	6874(2)	9772(2)	13(1)
B(2)	8128(4)	7583(2)	9959(2)	15(1)
B(3)	7119(4)	7144(2)	10018(2)	12(1)
B(4)	6995(4)	6522(2)	9495(2)	13(1)
B(5)	7976(4)	6594(2)	9118(2)	13(1)
B(6)	8664(4)	7253(2)	9422(2)	14(1)
B(7)	7903(4)	7733(2)	9414(2)	14(1)
B(8)	6715(4)	7389(2)	9136(2)	13(1)
B(9)	7786(4)	7117(2)	8891(2)	13(1)
B(10)	6913(4)	7671(2)	9795(2)	13(1)
B(11)	6784(4)	6699(2)	8965(2)	14(1)
B(12)	6219(4)	7012(2)	9498(2)	12(1)
F(1')	7712(2)	62(1)	3797(1)	47(1)
F(2')	7715(4)	-893(2)	3114(2)	106(2)
F(3')	9197(8)	-1057(2)	2547(4)	240(6)
F(4')	10637(5)	-264(2)	2642(3)	158(4)
F(5')	10578(3)	706(2)	3308(2)	65(1)
F(6')	5686(2)	-232(1)	3654(1)	30(1)
F(7')	6028(2)	-1155(1)	3714(1)	36(1)
F(8')	6416(2)	-1226(1)	4598(1)	40(1)
F(9')	6484(2)	-356(1)	5416(1)	35(1)
F(10')	6181(2)	570(1)	5356(1)	25(1)
F(11')	8437(2)	477(1)	5239(1)	40(1)
F(12')	9914(3)	66(1)	5495(2)	55(1)
F(13')	11589(3)	691(2)	5882(2)	73(1)

F(14')	11749(3)	1747(2)	6086(2)	70(1)
F(15')	10257(2)	2172(1)	5852(1)	39(1)
F(16')	10156(3)	3343(1)	6148(1)	51(1)
F(17')	11145(3)	4309(1)	6632(1)	53(1)
F(18')	10299(3)	5185(1)	6739(2)	56(1)
F(19')	8488(3)	5084(1)	6328(2)	56(1)
F(20')	7511(3)	4119(1)	5856(1)	53(1)
F(21')	5907(3)	3304(1)	6234(1)	50(1)
F(22')	5922(3)	3564(1)	7202(1)	59(1)
F(23')	5863(3)	2802(2)	7600(1)	53(1)
F(24')	5809(3)	1775(1)	7022(1)	50(1)
F(25')	5821(2)	1512(1)	6047(1)	36(1)
F(26')	11175(2)	3458(1)	5125(1)	39(1)
F(27')	12823(2)	3867(1)	4866(1)	46(1)
F(28')	13693(2)	3268(1)	4099(1)	41(1)
F(29')	12904(2)	2256(1)	3591(1)	31(1)
F(30')	11257(2)	1842(1)	3844(1)	22(1)
F(31')	9179(3)	4444(1)	5208(1)	39(1)
F(32')	8844(3)	5384(1)	5179(1)	45(1)
F(33')	8189(3)	5453(1)	4327(1)	50(1)
F(34')	7860(3)	4585(1)	3517(1)	47(1)
F(35')	8301(3)	3651(1)	3527(1)	38(1)
F(36')	8671(2)	2685(1)	2731(1)	24(1)
F(37')	8704(2)	2448(1)	1765(1)	34(1)
F(38')	8864(3)	1452(2)	1177(1)	51(1)
F(39')	9031(3)	690(2)	1563(1)	65(1)
F(40')	9032(3)	927(1)	2533(1)	49(1)
F(41')	3459(2)	750(1)	3666(1)	41(1)
F(42')	1792(2)	364(1)	3918(2)	48(1)
F(43')	925(2)	987(1)	4676(1)	43(1)
F(44')	1762(2)	1991(1)	5191(1)	35(1)
F(45')	3418(2)	2385(1)	4938(1)	27(1)
F(46')	6177(2)	3721(1)	3526(1)	40(1)
F(47')	4682(3)	4096(1)	3241(1)	46(1)
F(48')	3080(2)	3422(1)	2778(1)	40(1)
F(49')	3009(2)	2367(1)	2588(1)	32(1)

F(50')	4501(2)	1997(1)	2876(1)	26(1)
F(51')	6645(3)	3997(2)	4599(2)	56(1)
F(52')	6588(3)	5036(2)	5026(2)	75(1)
F(53')	5354(3)	5382(1)	5711(2)	68(1)
F(54')	4163(3)	4675(2)	5970(2)	66(1)
F(55')	4257(3)	3633(2)	5561(2)	60(1)
O(1')	5963(3)	735(1)	3426(1)	40(1)
O(2')	5895(3)	1317(1)	3096(1)	31(1)
O(3')	7891(2)	1995(1)	3335(1)	15(1)
O(4')	8298(2)	1132(1)	3770(1)	16(1)
O(5')	6730(2)	1028(1)	4548(1)	16(1)
O(6')	8757(2)	1698(1)	4977(1)	15(1)
O(7')	9517(2)	2339(1)	4259(1)	16(1)
O(8')	6777(2)	2163(1)	5422(1)	16(1)
O(9')	8570(2)	2987(1)	5248(1)	20(1)
O(10')	7975(2)	3154(1)	4225(1)	18(1)
O(11')	6365(2)	3062(1)	4979(1)	19(1)
O(12')	5914(2)	2488(1)	3781(1)	17(1)
O(13')	5144(2)	1841(1)	4505(1)	17(1)
N(1')	6148(3)	1197(2)	3443(1)	17(1)
C(1')	9061(4)	940(2)	3943(2)	31(1)
C(2')	9136(4)	401(2)	3572(2)	26(1)
C(3')	8437(4)	-16(2)	3506(2)	34(1)
C(4')	8444(6)	-497(3)	3162(3)	67(2)
C(5')	9175(8)	-576(3)	2887(4)	101(4)
C(6')	9929(7)	-182(3)	2935(4)	87(3)
C(7')	9876(5)	315(2)	3283(3)	44(2)
C(8')	5793(3)	731(2)	4475(2)	20(1)
C(9')	5920(3)	200(2)	4500(2)	16(1)
C(10')	6139(3)	149(2)	4942(2)	19(1)
C(11')	6304(3)	-322(2)	4980(2)	22(1)
C(12')	6261(4)	-763(2)	4566(2)	26(1)
C(13')	6055(4)	-733(2)	4119(2)	24(1)
C(14')	5884(3)	-248(2)	4096(2)	21(1)
C(15')	8486(3)	1579(2)	5395(2)	20(1)
C(16')	9293(3)	1335(2)	5540(2)	18(1)

C(17')	9236(4)	806(2)	5455(2)	25(1)
C(18')	9994(4)	589(2)	5581(2)	34(1)
C(19')	10839(4)	902(3)	5781(2)	39(1)
C(20')	10917(4)	1437(3)	5878(2)	40(1)
C(21')	10158(4)	1649(2)	5761(2)	26(1)
C(22')	5844(4)	2022(2)	6329(2)	23(1)
C(23')	5842(4)	2152(2)	6826(2)	32(1)
C(24')	5866(4)	2672(2)	7119(2)	34(1)
C(25')	5894(5)	3055(2)	6916(2)	38(1)
C(26')	5891(4)	2915(2)	6417(2)	30(1)
C(27')	5862(4)	2396(2)	6111(2)	21(1)
C(28')	8254(4)	3163(2)	5725(2)	32(1)
C(29')	8803(4)	3698(2)	5998(2)	34(1)
C(30')	9733(4)	3767(2)	6189(2)	35(1)
C(31')	10238(4)	4257(2)	6435(2)	40(1)
C(32')	9812(4)	4700(2)	6491(2)	39(1)
C(33')	8899(5)	4653(2)	6293(2)	40(1)
C(34')	8403(4)	4157(2)	6053(2)	37(1)
C(35')	5834(4)	2241(2)	5565(2)	23(1)
C(36')	10246(3)	2401(2)	4628(2)	17(1)
C(37')	11164(3)	2637(2)	4494(2)	16(1)
C(38')	11584(4)	3153(2)	4742(2)	24(1)
C(39')	12422(4)	3366(2)	4618(2)	29(1)
C(40')	12863(4)	3062(2)	4226(2)	26(1)
C(41')	12464(3)	2550(2)	3966(2)	20(1)
C(42')	11625(3)	2347(2)	4102(2)	16(1)
C(43')	8881(4)	3480(2)	4390(2)	25(1)
C(44')	8760(3)	4018(2)	4376(2)	22(1)
C(45')	8878(4)	4468(2)	4778(2)	26(1)
C(46')	8713(4)	4955(2)	4772(2)	29(1)
C(47')	8378(4)	4987(2)	4340(2)	32(1)
C(48')	8228(4)	4548(2)	3931(2)	31(1)
C(49')	8438(4)	4071(2)	3939(2)	27(1)
C(50')	8853(3)	1968(2)	3209(2)	21(1)
C(51')	8859(3)	1816(2)	2667(2)	20(1)
C(52')	8765(3)	2188(2)	2451(2)	20(1)

C(53')	8781(4)	2066(2)	1956(2)	24(1)
C(54')	8867(4)	1564(2)	1658(2)	33(1)
C(55')	8954(5)	1184(2)	1853(2)	37(1)
C(56')	8941(4)	1314(2)	2354(2)	31(1)
C(57')	6210(3)	2618(2)	3372(2)	20(1)
C(58')	5397(4)	2845(2)	3209(2)	19(1)
C(59')	5405(4)	3375(2)	3295(2)	24(1)
C(60')	4639(4)	3570(2)	3147(2)	31(1)
C(61')	3836(4)	3235(2)	2914(2)	26(1)
C(62')	3783(4)	2704(2)	2822(2)	24(1)
C(63')	4567(3)	2519(2)	2972(2)	18(1)
C(64')	4406(3)	1812(2)	4149(2)	22(1)
C(65')	3483(3)	1588(2)	4288(2)	20(1)
C(66')	3030(4)	1881(2)	4677(2)	20(1)
C(67')	2181(4)	1685(2)	4814(2)	23(1)
C(68')	1759(4)	1178(2)	4553(2)	28(1)
C(69')	2188(4)	869(2)	4163(2)	31(1)
C(70')	3041(4)	1072(2)	4039(2)	26(1)
C(71')	5516(4)	3207(2)	4815(2)	33(1)
C(72')	5486(4)	3785(2)	5071(2)	24(1)
C(73')	4847(4)	3965(2)	5418(2)	33(1)
C(74')	4787(5)	4503(3)	5638(2)	40(1)
C(75')	5403(5)	4861(2)	5509(2)	42(1)
C(76')	6021(5)	4685(2)	5157(3)	44(2)
C(77')	6058(4)	4161(2)	4949(2)	33(1)
B(1')	8088(4)	1880(2)	4722(2)	14(1)
B(2')	7994(4)	2576(2)	4872(2)	14(1)
B(3')	7017(4)	2139(2)	4952(2)	13(1)
B(4')	6933(4)	1496(2)	4452(2)	13(1)
B(5')	7897(4)	1561(2)	4068(2)	15(1)
B(6')	8546(4)	2232(2)	4341(2)	13(1)
B(7')	7749(4)	2685(2)	4307(2)	16(1)
B(8')	6573(4)	2306(2)	4037(2)	14(1)
B(9')	7658(4)	2048(2)	3804(2)	15(1)
B(10')	6767(4)	2623(2)	4694(2)	15(1)
B(11')	6691(4)	1626(2)	3903(2)	15(1)

B(12')	6116(4)	1950(2)	4423(2)	14(1)
N(2)	4329(3)	-373(2)	2373(2)	29(1)
C(78)	4116(4)	151(2)	2376(2)	38(1)
C(79)	3118(4)	275(2)	2450(2)	39(1)
C(80)	2990(6)	785(3)	2386(3)	63(2)
C(81)	2062(6)	978(3)	2503(4)	81(3)
C(82)	4142(4)	-435(2)	2860(2)	30(1)
C(83)	3160(4)	-665(2)	2924(2)	35(1)
C(84)	3128(5)	-668(2)	3442(2)	40(2)
C(85)	2206(6)	-955(3)	3521(3)	59(2)
C(86)	5441(4)	-366(2)	2353(2)	39(1)
C(87)	5848(4)	-328(3)	1902(2)	44(2)
C(88)	6944(5)	-326(3)	1933(3)	58(2)
C(89)	7364(6)	-355(4)	1434(3)	77(3)
C(90)	3807(4)	-824(2)	1954(2)	30(1)
C(91)	4058(4)	-1370(2)	1863(2)	38(1)
C(92)	3321(5)	-1794(2)	1495(2)	42(2)
C(93)	3616(5)	-2340(3)	1344(3)	55(2)
N(3)	4138(3)	4776(2)	7360(2)	36(1)
C(94)	4027(5)	4673(2)	7829(2)	47(2)
C(95)	3068(5)	4459(3)	7924(2)	48(2)
C(96)	3092(9)	4428(3)	8427(3)	89(3)
C(97)	2208(9)	4165(4)	8536(4)	109(4)
C(98)	3976(4)	5341(2)	7426(2)	38(1)
C(99)	2992(4)	5489(2)	7537(2)	30(1)
C(100)	2987(4)	6059(2)	7585(2)	37(1)
C(101)	2020(5)	6241(2)	7686(2)	44(2)
C(102)	3488(5)	4382(2)	6951(2)	40(2)
C(103)	3689(5)	3816(2)	6791(3)	56(2)
C(104)	2891(6)	3439(3)	6447(3)	70(2)
C(105)	3142(7)	2875(3)	6238(3)	88(3)
C(106)	5247(8)	4737(4)	7407(5)	30(2)
C(107)	5688(9)	4798(5)	6955(5)	39(2)
C(108)	7298(12)	5279(5)	7376(6)	60(5)
C(109)	6764(10)	4782(5)	6976(5)	39(2)
C(110)	5113(8)	4728(5)	7108(5)	31(2)

C(111)	5930(8)	5117(4)	7400(4)	31(2)
C(112)	6871(8)	4970(5)	7173(5)	38(3)
C(113)	7693(8)	5418(5)	7436(5)	31(2)

Table 3. Bond lengths [Å] and angles [°] for [2b]$^{1-}$

F(1)-C(3)	1.349(6)
F(2)-C(4)	1.335(7)
F(3)-C(5)	1.352(7)
F(4)-C(6)	1.338(7)
F(5)-C(7)	1.336(7)
F(6)-C(14)	1.346(5)
F(7)-C(13)	1.334(6)
F(8)-C(12)	1.347(6)
F(9)-C(11)	1.343(6)
F(10)-C(10)	1.343(6)
F(11)-C(17)	1.346(7)
F(12)-C(18)	1.335(7)
F(13)-C(19)	1.346(7)
F(14)-C(20)	1.350(7)
F(15)-C(21)	1.345(7)
F(16)-C(30)	1.358(7)
F(17)-C(31)	1.344(9)
F(18)-C(32)	1.337(8)
F(19)-C(33)	1.308(8)
F(20)-C(34)	1.357(8)
F(21)-C(26)	1.357(6)
F(22)-C(25)	1.345(6)
F(23)-C(24)	1.350(6)
F(24)-C(23)	1.345(6)
F(25)-C(22)	1.336(6)
F(26)-C(38)	1.344(6)
F(27)-C(39)	1.336(7)
F(28)-C(40)	1.345(6)
F(29)-C(41)	1.336(6)

F(30)-C(42)	1.335(6)
F(31)-C(45)	1.341(7)
F(32)-C(46)	1.350(7)
F(33)-C(47)	1.356(7)
F(34)-C(48)	1.330(8)
F(35)-C(49)	1.333(7)
F(36)-C(52)	1.322(6)
F(37)-C(53)	1.348(6)
F(38)-C(54)	1.348(6)
F(39)-C(55)	1.338(6)
F(40)-C(56)	1.347(6)
F(41)-C(70)	1.355(6)
F(42)-C(69)	1.350(6)
F(43)-C(68)	1.341(6)
F(44)-C(67)	1.344(6)
F(45)-C(66)	1.347(5)
F(46)-C(59)	1.330(6)
F(47)-C(60)	1.338(6)
F(48)-C(61)	1.355(6)
F(49)-C(62)	1.354(6)
F(50)-C(63)	1.347(5)
F(51)-C(77)	1.329(6)
F(52)-C(76)	1.325(6)
F(53)-C(75)	1.344(6)
F(54)-C(74)	1.347(6)
F(55)-C(73)	1.355(6)
O(1)-N(1)	1.229(5)
O(2)-N(1)	1.227(5)
O(3)-C(50)	1.433(6)
O(3)-B(9)	1.397(6)
O(4)-C(1)	1.419(6)
O(4)-B(5)	1.390(6)
O(5)-C(8)	1.436(5)
O(5)-B(4)	1.393(6)
O(6)-C(15)	1.430(5)
O(6)-B(1)	1.427(6)

O(7)-C(36)	1.429(5)
O(7)-B(6)	1.415(6)
O(8)-C(35)	1.417(6)
O(8)-B(3)	1.410(6)
O(9)-C(28)	1.432(6)
O(9)-B(2)	1.410(6)
O(10)-C(43)	1.440(6)
O(10)-B(7)	1.392(6)
O(11)-C(71)	1.431(6)
O(11)-B(10)	1.393(6)
O(12)-C(57)	1.431(5)
O(12)-B(8)	1.419(6)
O(13)-C(64)	1.429(5)
O(13)-B(12)	1.414(6)
N(1)-B(11)	1.550(6)
C(1)-C(2)	1.512(7)
C(2)-C(3)	1.371(8)
C(2)-C(7)	1.374(8)
C(3)-C(4)	1.371(8)
C(4)-C(5)	1.385(9)
C(5)-C(6)	1.351(10)
C(6)-C(7)	1.378(9)
C(8)-C(9)	1.511(6)
C(9)-C(10)	1.384(6)
C(9)-C(14)	1.373(7)
C(10)-C(11)	1.376(7)
C(11)-C(12)	1.377(8)
C(12)-C(13)	1.377(8)
C(13)-C(14)	1.384(7)
C(15)-C(16)	1.508(7)
C(16)-C(17)	1.369(8)
C(16)-C(21)	1.395(7)
C(17)-C(18)	1.404(8)
C(18)-C(19)	1.355(10)
C(19)-C(20)	1.371(10)
C(20)-C(21)	1.368(8)

C(22)-C(23)	1.397(7)
C(22)-C(27)	1.374(7)
C(23)-C(24)	1.361(8)
C(24)-C(25)	1.358(8)
C(25)-C(26)	1.375(7)
C(26)-C(27)	1.384(7)
C(27)-C(35)	1.512(6)
C(28)-C(29)	1.498(8)
C(29)-C(30)	1.398(9)
C(29)-C(34)	1.344(8)
C(30)-C(31)	1.374(9)
C(31)-C(32)	1.393(11)
C(32)-C(33)	1.425(11)
C(33)-C(34)	1.342(9)
C(36)-C(37)	1.514(6)
C(37)-C(38)	1.379(7)
C(37)-C(42)	1.389(7)
C(38)-C(39)	1.389(8)
C(39)-C(40)	1.383(9)
C(40)-C(41)	1.372(8)
C(41)-C(42)	1.386(7)
C(43)-C(44)	1.501(7)
C(44)-C(45)	1.389(8)
C(44)-C(49)	1.387(8)
C(45)-C(46)	1.368(9)
C(46)-C(47)	1.338(10)
C(47)-C(48)	1.368(10)
C(48)-C(49)	1.388(8)
C(50)-C(51)	1.493(7)
C(51)-C(52)	1.407(7)
C(51)-C(56)	1.372(8)
C(52)-C(53)	1.368(7)
C(53)-C(54)	1.365(8)
C(54)-C(55)	1.373(8)
C(55)-C(56)	1.390(7)
C(57)-C(58)	1.511(6)

C(58)-C(59)	1.372(7)
C(58)-C(63)	1.391(7)
C(59)-C(60)	1.400(7)
C(60)-C(61)	1.362(8)
C(61)-C(62)	1.359(7)
C(62)-C(63)	1.369(7)
C(64)-C(65)	1.490(6)
C(65)-C(66)	1.387(7)
C(65)-C(70)	1.395(7)
C(66)-C(67)	1.382(7)
C(67)-C(68)	1.372(7)
C(68)-C(69)	1.374(8)
C(69)-C(70)	1.367(7)
C(71)-C(72)	1.480(7)
C(72)-C(73)	1.394(8)
C(72)-C(77)	1.382(8)
C(73)-C(74)	1.371(8)
C(74)-C(75)	1.386(8)
C(75)-C(76)	1.388(8)
C(76)-C(77)	1.377(8)
B(1)-B(2)	1.823(8)
B(1)-B(3)	1.790(7)
B(1)-B(4)	1.815(7)
B(1)-B(5)	1.806(7)
B(1)-B(6)	1.799(7)
B(2)-B(3)	1.796(7)
B(2)-B(6)	1.771(7)
B(2)-B(7)	1.821(7)
B(2)-B(10)	1.837(7)
B(3)-B(4)	1.834(7)
B(3)-B(10)	1.826(7)
B(3)-B(12)	1.864(7)
B(4)-B(5)	1.834(7)
B(4)-B(11)	1.814(7)
B(4)-B(12)	1.828(7)
B(5)-B(6)	1.834(7)

B(5)-B(9)	1.816(7)
B(5)-B(11)	1.812(7)
B(6)-B(7)	1.800(7)
B(6)-B(9)	1.867(7)
B(7)-B(8)	1.832(7)
B(7)-B(9)	1.825(8)
B(7)-B(10)	1.847(7)
B(8)-B(9)	1.827(7)
B(8)-B(10)	1.819(7)
B(8)-B(11)	1.788(7)
B(8)-B(12)	1.821(7)
B(9)-B(11)	1.773(7)
B(10)-B(12)	1.835(7)
B(11)-B(12)	1.773(7)
F(1')-C(3')	1.346(7)
F(2')-C(4')	1.361(8)
F(3')-C(5')	1.348(9)
F(4')-C(6')	1.330(9)
F(5')-C(7')	1.342(7)
F(6')-C(14')	1.341(6)
F(7')-C(13')	1.332(6)
F(8')-C(12')	1.341(6)
F(9')-C(11')	1.339(6)
F(10')-C(10')	1.345(6)
F(11')-C(17')	1.338(6)
F(12')-C(18')	1.347(6)
F(13')-C(19')	1.341(7)
F(14')-C(20')	1.349(7)
F(15')-C(21')	1.342(6)
F(16')-C(30')	1.336(7)
F(17')-C(31')	1.360(7)
F(18')-C(32')	1.351(6)
F(19')-C(33')	1.347(7)
F(20')-C(34')	1.347(7)
F(21')-C(26')	1.347(6)
F(22')-C(25')	1.343(7)

F(23')-C(24')	1.334(6)
F(24')-C(23')	1.340(6)
F(25')-C(22')	1.344(6)
F(26')-C(38')	1.342(6)
F(27')-C(39')	1.343(6)
F(28')-C(40')	1.354(6)
F(29')-C(41')	1.341(6)
F(30')-C(42')	1.344(5)
F(31')-C(45')	1.349(6)
F(32')-C(46')	1.339(6)
F(33')-C(47')	1.342(6)
F(34')-C(48')	1.355(6)
F(35')-C(49')	1.335(6)
F(36')-C(52')	1.343(6)
F(37')-C(53')	1.359(6)
F(38')-C(54')	1.340(6)
F(39')-C(55')	1.340(7)
F(40')-C(56')	1.354(6)
F(41')-C(70')	1.350(6)
F(42')-C(69')	1.349(6)
F(43')-C(68')	1.340(6)
F(44')-C(67')	1.340(6)
F(45')-C(66')	1.352(6)
F(46')-C(59')	1.340(6)
F(47')-C(60')	1.354(6)
F(48')-C(61')	1.348(6)
F(49')-C(62')	1.333(6)
F(50')-C(63')	1.341(6)
F(51')-C(77')	1.331(7)
F(52')-C(76')	1.340(7)
F(53')-C(75')	1.346(7)
F(54')-C(74')	1.336(7)
F(55')-C(73')	1.336(6)
O(1')-N(1')	1.236(5)
O(2')-N(1')	1.235(5)
O(3')-C(50')	1.423(6)

O(3')-B(9')	1.393(6)
O(4')-C(1')	1.413(6)
O(4')-B(5')	1.391(6)
O(5')-C(8')	1.432(5)
O(5')-B(4')	1.397(6)
O(6')-C(15')	1.431(5)
O(6')-B(1')	1.428(6)
O(7')-C(36')	1.427(5)
O(7')-B(6')	1.412(6)
O(8')-C(35')	1.427(6)
O(8')-B(3')	1.417(6)
O(9')-C(28')	1.422(6)
O(9')-B(2')	1.415(6)
O(10')-C(43')	1.429(6)
O(10')-B(7')	1.382(6)
O(11')-C(71')	1.431(6)
O(11')-B(10')	1.399(6)
O(12')-C(57')	1.431(5)
O(12')-B(8')	1.421(6)
O(13')-C(64')	1.433(6)
O(13')-B(12')	1.415(6)
N(1')-B(11')	1.549(6)
C(1')-C(2')	1.511(7)
C(2')-C(3')	1.364(8)
C(2')-C(7')	1.358(8)
C(3')-C(4')	1.348(9)
C(4')-C(5')	1.325(12)
C(5')-C(6')	1.381(12)
C(6')-C(7')	1.398(10)
C(8')-C(9')	1.508(6)
C(9')-C(10')	1.385(7)
C(9')-C(14')	1.370(7)
C(10')-C(11')	1.377(7)
C(11')-C(12')	1.375(7)
C(12')-C(13')	1.373(7)
C(13')-C(14')	1.399(7)

C(15')-C(16')	1.510(7)
C(16')-C(17')	1.367(7)
C(16')-C(21')	1.396(7)
C(17')-C(18')	1.387(8)
C(18')-C(19')	1.361(9)
C(19')-C(20')	1.373(9)
C(20')-C(21')	1.369(8)
C(22')-C(23')	1.381(7)
C(22')-C(27')	1.382(7)
C(23')-C(24')	1.375(8)
C(24')-C(25')	1.370(8)
C(25')-C(26')	1.384(8)
C(26')-C(27')	1.381(7)
C(27')-C(35')	1.510(7)
C(28')-C(29')	1.495(7)
C(29')-C(30')	1.378(9)
C(29')-C(34')	1.396(9)
C(30')-C(31')	1.368(8)
C(31')-C(32')	1.377(9)
C(32')-C(33')	1.371(9)
C(33')-C(34')	1.374(8)
C(36')-C(37')	1.501(6)
C(37')-C(38')	1.384(7)
C(37')-C(42')	1.386(7)
C(38')-C(39')	1.369(7)
C(39')-C(40')	1.383(8)
C(40')-C(41')	1.372(7)
C(41')-C(42')	1.376(6)
C(43')-C(44')	1.512(7)
C(44')-C(45')	1.364(7)
C(44')-C(49')	1.414(7)
C(45')-C(46')	1.383(8)
C(46')-C(47')	1.381(8)
C(47')-C(48')	1.358(8)
C(48')-C(49')	1.376(8)
C(50')-C(51')	1.504(7)

C(51')-C(52')	1.389(7)
C(51')-C(56')	1.378(7)
C(52')-C(53')	1.378(7)
C(53')-C(54')	1.369(8)
C(54')-C(55')	1.365(8)
C(55')-C(56')	1.393(8)
C(57')-C(58')	1.513(7)
C(58')-C(59')	1.375(7)
C(58')-C(63')	1.382(7)
C(59')-C(60')	1.386(8)
C(60')-C(61')	1.361(8)
C(61')-C(62')	1.370(7)
C(62')-C(63')	1.393(7)
C(64')-C(65')	1.499(7)
C(65')-C(66')	1.376(7)
C(65')-C(70')	1.393(7)
C(66')-C(67')	1.380(7)
C(67')-C(68')	1.372(8)
C(68')-C(69')	1.373(8)
C(69')-C(70')	1.376(8)
C(71')-C(72')	1.498(8)
C(72')-C(73')	1.385(8)
C(72')-C(77')	1.377(7)
C(73')-C(74')	1.395(8)
C(74')-C(75')	1.389(9)
C(75')-C(76')	1.370(9)
C(76')-C(77')	1.351(8)
B(1')-B(2')	1.816(7)
B(1')-B(3')	1.800(7)
B(1')-B(4')	1.817(7)
B(1')-B(5')	1.811(7)
B(1')-B(6')	1.800(7)
B(2')-B(3')	1.785(7)
B(2')-B(6')	1.778(7)
B(2')-B(7')	1.821(7)
B(2')-B(10')	1.828(8)

B(3')-B(4')	1.842(7)
B(3')-B(10')	1.802(7)
B(3')-B(12')	1.864(7)
B(4')-B(5')	1.827(7)
B(4')-B(11')	1.806(7)
B(4')-B(12')	1.815(7)
B(5')-B(6')	1.830(7)
B(5')-B(9')	1.816(7)
B(5')-B(11')	1.804(7)
B(6')-B(7')	1.798(8)
B(6')-B(9')	1.870(7)
B(7')-B(8')	1.838(8)
B(7')-B(9')	1.834(8)
B(7')-B(10')	1.850(7)
B(8')-B(9')	1.818(8)
B(8')-B(10')	1.817(7)
B(8')-B(11')	1.786(7)
B(8')-B(12')	1.819(7)
B(9')-B(11')	1.771(7)
B(10')-B(12')	1.834(7)
B(11')-B(12')	1.760(8)
N(2)-C(78)	1.491(7)
N(2)-C(82)	1.530(7)
N(2)-C(86)	1.573(8)
N(2)-C(90)	1.497(6)
C(78)-C(79)	1.496(9)
C(79)-C(80)	1.497(9)
C(80)-C(81)	1.478(10)
C(82)-C(83)	1.494(8)
C(83)-C(84)	1.534(8)
C(84)-C(85)	1.501(9)
C(86)-C(87)	1.493(9)
C(87)-C(88)	1.548(9)
C(88)-C(89)	1.579(11)
C(90)-C(91)	1.507(8)
C(91)-C(92)	1.534(8)

C(92)-C(93)	1.512(9)
N(3)-C(94)	1.512(8)
N(3)-C(98)	1.531(8)
N(3)-C(102)	1.496(7)
N(3)-C(106)	1.588(13)
N(3)-C(110)	1.583(13)
C(94)-C(95)	1.480(10)
C(95)-C(96)	1.514(9)
C(96)-C(97)	1.463(14)
C(98)-C(99)	1.509(8)
C(99)-C(100)	1.512(8)
C(100)-C(101)	1.514(9)
C(102)-C(103)	1.514(9)
C(103)-C(104)	1.507(10)
C(104)-C(105)	1.534(11)
C(106)-C(107)	1.540(18)
C(107)-C(109)	1.526(19)
C(108)-C(109)	1.5399(11)
C(110)-C(111)	1.482(15)
C(111)-C(112)	1.540(17)
C(112)-C(113)	1.5399(11)

B(9)-O(3)-C(50)	119.3(4)
B(5)-O(4)-C(1)	120.4(4)
B(4)-O(5)-C(8)	124.0(4)
B(1)-O(6)-C(15)	119.3(4)
B(6)-O(7)-C(36)	119.8(3)
B(3)-O(8)-C(35)	122.1(4)
B(2)-O(9)-C(28)	121.6(4)
B(7)-O(10)-C(43)	121.3(4)
B(10)-O(11)-C(71)	120.1(4)
B(8)-O(12)-C(57)	118.3(3)
B(12)-O(13)-C(64)	120.6(3)
O(1)-N(1)-B(11)	119.6(4)
O(2)-N(1)-O(1)	120.6(4)
O(2)-N(1)-B(11)	119.9(4)

O(4)-C(1)-C(2)	107.0(4)
C(3)-C(2)-C(1)	121.2(5)
C(3)-C(2)-C(7)	116.8(5)
C(7)-C(2)-C(1)	122.0(5)
F(1)-C(3)-C(2)	118.9(5)
F(1)-C(3)-C(4)	118.1(5)
C(4)-C(3)-C(2)	123.1(5)
F(2)-C(4)-C(3)	121.0(6)
F(2)-C(4)-C(5)	121.0(6)
C(3)-C(4)-C(5)	118.0(6)
F(3)-C(5)-C(4)	119.4(6)
C(6)-C(5)-F(3)	119.7(6)
C(6)-C(5)-C(4)	120.8(6)
F(4)-C(6)-C(5)	119.7(6)
F(4)-C(6)-C(7)	120.8(6)
C(5)-C(6)-C(7)	119.4(6)
F(5)-C(7)-C(2)	120.1(5)
F(5)-C(7)-C(6)	118.0(5)
C(2)-C(7)-C(6)	121.9(6)
O(5)-C(8)-C(9)	105.5(4)
C(10)-C(9)-C(8)	120.7(4)
C(14)-C(9)-C(8)	122.6(4)
C(14)-C(9)-C(10)	116.6(4)
F(10)-C(10)-C(9)	119.9(4)
F(10)-C(10)-C(11)	117.8(4)
C(11)-C(10)-C(9)	122.2(5)
F(9)-C(11)-C(10)	120.3(5)
F(9)-C(11)-C(12)	120.3(5)
C(10)-C(11)-C(12)	119.4(5)
F(8)-C(12)-C(11)	119.9(5)
F(8)-C(12)-C(13)	119.9(5)
C(11)-C(12)-C(13)	120.2(5)
F(7)-C(13)-C(12)	120.5(5)
F(7)-C(13)-C(14)	120.8(5)
C(12)-C(13)-C(14)	118.6(5)
F(6)-C(14)-C(9)	119.9(4)

F(6)-C(14)-C(13)	117.2(4)
C(9)-C(14)-C(13)	122.9(5)
O(6)-C(15)-C(16)	107.3(4)
C(17)-C(16)-C(15)	123.0(5)
C(17)-C(16)-C(21)	116.2(5)
C(21)-C(16)-C(15)	120.8(5)
F(11)-C(17)-C(16)	120.1(5)
F(11)-C(17)-C(18)	117.4(5)
C(16)-C(17)-C(18)	122.4(6)
F(12)-C(18)-C(17)	119.7(6)
F(12)-C(18)-C(19)	121.7(6)
C(19)-C(18)-C(17)	118.6(6)
F(13)-C(19)-C(18)	119.7(6)
F(13)-C(19)-C(20)	119.3(6)
C(18)-C(19)-C(20)	121.0(5)
F(14)-C(20)-C(19)	120.3(5)
F(14)-C(20)-C(21)	120.4(6)
C(21)-C(20)-C(19)	119.3(6)
F(15)-C(21)-C(16)	119.1(5)
F(15)-C(21)-C(20)	118.5(5)
C(20)-C(21)-C(16)	122.4(6)
F(25)-C(22)-C(23)	118.4(4)
F(25)-C(22)-C(27)	119.7(4)
C(27)-C(22)-C(23)	121.8(5)
F(24)-C(23)-C(22)	120.4(5)
F(24)-C(23)-C(24)	120.4(5)
C(24)-C(23)-C(22)	119.2(5)
F(23)-C(24)-C(23)	119.6(5)
F(23)-C(24)-C(25)	119.6(5)
C(25)-C(24)-C(23)	120.8(5)
F(22)-C(25)-C(24)	120.7(5)
F(22)-C(25)-C(26)	120.1(5)
C(24)-C(25)-C(26)	119.2(5)
F(21)-C(26)-C(25)	118.1(5)
F(21)-C(26)-C(27)	119.3(5)
C(25)-C(26)-C(27)	122.7(5)

C(22)-C(27)-C(26)	116.3(5)
C(22)-C(27)-C(35)	121.7(5)
C(26)-C(27)-C(35)	122.0(4)
O(9)-C(28)-C(29)	106.5(5)
C(30)-C(29)-C(28)	119.9(5)
C(34)-C(29)-C(28)	124.3(6)
C(34)-C(29)-C(30)	115.5(6)
F(16)-C(30)-C(29)	120.7(5)
F(16)-C(30)-C(31)	117.0(6)
C(31)-C(30)-C(29)	122.4(6)
F(17)-C(31)-C(30)	121.5(7)
F(17)-C(31)-C(32)	119.6(6)
C(30)-C(31)-C(32)	118.8(7)
F(18)-C(32)-C(31)	120.0(8)
F(18)-C(32)-C(33)	120.1(7)
C(31)-C(32)-C(33)	119.8(6)
F(19)-C(33)-C(32)	117.0(6)
F(19)-C(33)-C(34)	126.7(8)
C(34)-C(33)-C(32)	116.3(7)
C(29)-C(34)-F(20)	118.0(5)
C(33)-C(34)-F(20)	114.8(6)
C(33)-C(34)-C(29)	127.2(7)
O(8)-C(35)-C(27)	107.5(4)
O(7)-C(36)-C(37)	107.1(4)
C(38)-C(37)-C(36)	122.7(5)
C(38)-C(37)-C(42)	117.3(4)
C(42)-C(37)-C(36)	120.0(4)
F(26)-C(38)-C(37)	119.8(5)
F(26)-C(38)-C(39)	118.4(5)
C(37)-C(38)-C(39)	121.8(5)
F(27)-C(39)-C(38)	120.4(6)
F(27)-C(39)-C(40)	120.3(5)
C(40)-C(39)-C(38)	119.2(5)
F(28)-C(40)-C(39)	119.9(5)
F(28)-C(40)-C(41)	119.7(5)
C(41)-C(40)-C(39)	120.4(5)

F(29)-C(41)-C(40)	120.2(5)
F(29)-C(41)-C(42)	120.5(5)
C(40)-C(41)-C(42)	119.3(5)
F(30)-C(42)-C(37)	119.8(4)
F(30)-C(42)-C(41)	118.2(5)
C(41)-C(42)-C(37)	122.0(5)
O(10)-C(43)-C(44)	106.4(4)
C(45)-C(44)-C(43)	123.2(5)
C(49)-C(44)-C(43)	121.1(5)
C(49)-C(44)-C(45)	115.6(5)
F(31)-C(45)-C(44)	119.3(5)
F(31)-C(45)-C(46)	118.1(6)
C(46)-C(45)-C(44)	122.6(6)
F(32)-C(46)-C(45)	120.6(7)
C(47)-C(46)-F(32)	119.5(6)
C(47)-C(46)-C(45)	119.9(6)
F(33)-C(47)-C(48)	118.9(7)
C(46)-C(47)-F(33)	120.1(6)
C(46)-C(47)-C(48)	121.0(6)
F(34)-C(48)-C(47)	121.2(6)
F(34)-C(48)-C(49)	120.0(6)
C(47)-C(48)-C(49)	118.8(6)
F(35)-C(49)-C(44)	119.3(5)
F(35)-C(49)-C(48)	118.7(5)
C(44)-C(49)-C(48)	122.0(6)
O(3)-C(50)-C(51)	108.4(4)
C(52)-C(51)-C(50)	120.8(5)
C(56)-C(51)-C(50)	122.5(5)
C(56)-C(51)-C(52)	116.7(5)
F(36)-C(52)-C(51)	119.0(4)
F(36)-C(52)-C(53)	119.2(5)
C(53)-C(52)-C(51)	121.8(5)
F(37)-C(53)-C(52)	120.2(5)
F(37)-C(53)-C(54)	119.9(4)
C(54)-C(53)-C(52)	119.9(5)
F(38)-C(54)-C(53)	120.0(5)

F(38)-C(54)-C(55)	119.6(5)
C(53)-C(54)-C(55)	120.3(5)
F(39)-C(55)-C(54)	119.6(5)
F(39)-C(55)-C(56)	121.0(5)
C(54)-C(55)-C(56)	119.4(5)
F(40)-C(56)-C(51)	120.1(5)
F(40)-C(56)-C(55)	118.0(5)
C(51)-C(56)-C(55)	121.9(5)
O(12)-C(57)-C(58)	106.9(4)
C(59)-C(58)-C(57)	123.5(4)
C(59)-C(58)-C(63)	116.5(4)
C(63)-C(58)-C(57)	120.0(4)
F(46)-C(59)-C(58)	120.7(4)
F(46)-C(59)-C(60)	118.3(4)
C(58)-C(59)-C(60)	121.0(5)
F(47)-C(60)-C(59)	120.2(5)
F(47)-C(60)-C(61)	119.6(5)
C(61)-C(60)-C(59)	120.2(5)
F(48)-C(61)-C(60)	120.0(5)
F(48)-C(61)-C(62)	120.0(5)
C(62)-C(61)-C(60)	120.0(5)
F(49)-C(62)-C(61)	120.3(4)
F(49)-C(62)-C(63)	120.2(5)
C(61)-C(62)-C(63)	119.5(5)
F(50)-C(63)-C(58)	119.4(4)
F(50)-C(63)-C(62)	117.7(4)
C(62)-C(63)-C(58)	122.8(5)
O(13)-C(64)-C(65)	107.6(4)
C(66)-C(65)-C(64)	121.7(4)
C(66)-C(65)-C(70)	115.0(4)
C(70)-C(65)-C(64)	123.3(4)
F(45)-C(66)-C(65)	119.0(4)
F(45)-C(66)-C(67)	117.9(4)
C(67)-C(66)-C(65)	123.1(4)
F(44)-C(67)-C(66)	120.5(5)
F(44)-C(67)-C(68)	120.3(4)

C(68)-C(67)-C(66)	119.2(5)
F(43)-C(68)-C(67)	120.1(5)
F(43)-C(68)-C(69)	119.9(5)
C(67)-C(68)-C(69)	120.0(5)
F(42)-C(69)-C(68)	120.0(5)
F(42)-C(69)-C(70)	120.5(5)
C(70)-C(69)-C(68)	119.5(5)
F(41)-C(70)-C(65)	118.3(4)
F(41)-C(70)-C(69)	118.4(5)
C(69)-C(70)-C(65)	123.2(5)
O(11)-C(71)-C(72)	110.6(4)
C(73)-C(72)-C(71)	121.9(5)
C(77)-C(72)-C(71)	121.5(5)
C(77)-C(72)-C(73)	116.3(5)
F(55)-C(73)-C(72)	120.4(5)
F(55)-C(73)-C(74)	117.2(5)
C(74)-C(73)-C(72)	122.4(5)
F(54)-C(74)-C(73)	120.7(5)
F(54)-C(74)-C(75)	119.9(5)
C(73)-C(74)-C(75)	119.4(5)
F(53)-C(75)-C(74)	120.6(5)
F(53)-C(75)-C(76)	119.3(5)
C(74)-C(75)-C(76)	120.1(5)
F(52)-C(76)-C(75)	120.0(5)
F(52)-C(76)-C(77)	121.4(5)
C(77)-C(76)-C(75)	118.6(5)
F(51)-C(77)-C(72)	118.5(5)
F(51)-C(77)-C(76)	118.3(5)
C(76)-C(77)-C(72)	123.2(5)
O(6)-B(1)-B(2)	122.2(4)
O(6)-B(1)-B(3)	125.7(4)
O(6)-B(1)-B(4)	123.0(4)
O(6)-B(1)-B(5)	118.2(4)
O(6)-B(1)-B(6)	117.4(4)
B(3)-B(1)-B(2)	59.6(3)
B(3)-B(1)-B(4)	61.2(3)

B(3)-B(1)-B(5)	109.3(4)
B(3)-B(1)-B(6)	107.3(4)
B(4)-B(1)-B(2)	108.8(4)
B(5)-B(1)-B(2)	108.0(3)
B(5)-B(1)-B(4)	60.8(3)
B(6)-B(1)-B(2)	58.5(3)
B(6)-B(1)-B(4)	109.6(3)
B(6)-B(1)-B(5)	61.2(3)
O(9)-B(2)-B(1)	120.8(4)
O(9)-B(2)-B(3)	124.3(4)
O(9)-B(2)-B(6)	117.5(4)
O(9)-B(2)-B(7)	120.5(4)
O(9)-B(2)-B(10)	124.6(4)
B(1)-B(2)-B(10)	107.5(4)
B(3)-B(2)-B(1)	59.3(3)
B(3)-B(2)-B(7)	108.7(4)
B(3)-B(2)-B(10)	60.3(3)
B(6)-B(2)-B(1)	60.1(3)
B(6)-B(2)-B(3)	108.3(4)
B(6)-B(2)-B(7)	60.1(3)
B(6)-B(2)-B(10)	108.8(4)
B(7)-B(2)-B(1)	107.7(4)
B(7)-B(2)-B(10)	60.7(3)
O(8)-B(3)-B(1)	118.8(4)
O(8)-B(3)-B(2)	119.9(4)
O(8)-B(3)-B(4)	120.9(4)
O(8)-B(3)-B(10)	123.2(4)
O(8)-B(3)-B(12)	124.4(4)
B(1)-B(3)-B(2)	61.1(3)
B(1)-B(3)-B(4)	60.1(3)
B(1)-B(3)-B(10)	109.4(3)
B(1)-B(3)-B(12)	107.5(3)
B(2)-B(3)-B(4)	109.1(4)
B(2)-B(3)-B(10)	60.9(3)
B(2)-B(3)-B(12)	108.3(3)
B(4)-B(3)-B(12)	59.2(3)

B(10)-B(3)-B(4)	108.0(3)
B(10)-B(3)-B(12)	59.6(3)
O(5)-B(4)-B(1)	114.4(4)
O(5)-B(4)-B(3)	120.5(4)
O(5)-B(4)-B(5)	118.7(4)
O(5)-B(4)-B(11)	129.5(4)
O(5)-B(4)-B(12)	128.6(4)
B(1)-B(4)-B(3)	58.7(3)
B(1)-B(4)-B(5)	59.3(3)
B(1)-B(4)-B(12)	107.9(4)
B(5)-B(4)-B(3)	106.2(3)
B(11)-B(4)-B(1)	105.9(3)
B(11)-B(4)-B(3)	105.8(3)
B(11)-B(4)-B(5)	59.6(3)
B(11)-B(4)-B(12)	58.3(3)
B(12)-B(4)-B(3)	61.2(3)
B(12)-B(4)-B(5)	107.2(3)
O(4)-B(5)-B(1)	128.0(4)
O(4)-B(5)-B(4)	122.4(4)
O(4)-B(5)-B(6)	124.9(4)
O(4)-B(5)-B(9)	116.8(4)
O(4)-B(5)-B(11)	118.0(4)
B(1)-B(5)-B(4)	59.8(3)
B(1)-B(5)-B(6)	59.2(3)
B(1)-B(5)-B(9)	108.8(4)
B(1)-B(5)-B(11)	106.4(3)
B(4)-B(5)-B(6)	107.3(3)
B(9)-B(5)-B(4)	108.0(4)
B(9)-B(5)-B(6)	61.5(3)
B(11)-B(5)-B(4)	59.7(3)
B(11)-B(5)-B(6)	106.4(4)
B(11)-B(5)-B(9)	58.5(3)
O(7)-B(6)-B(1)	126.2(4)
O(7)-B(6)-B(2)	124.3(4)
O(7)-B(6)-B(5)	121.0(4)
O(7)-B(6)-B(7)	118.4(4)

O(7)-B(6)-B(9)	117.2(4)
B(1)-B(6)-B(5)	59.6(3)
B(1)-B(6)-B(7)	109.7(4)
B(1)-B(6)-B(9)	106.9(3)
B(2)-B(6)-B(1)	61.4(3)
B(2)-B(6)-B(5)	109.0(4)
B(2)-B(6)-B(7)	61.3(3)
B(2)-B(6)-B(9)	108.5(4)
B(5)-B(6)-B(9)	58.8(3)
B(7)-B(6)-B(5)	107.7(4)
B(7)-B(6)-B(9)	59.7(3)
O(10)-B(7)-B(2)	126.1(4)
O(10)-B(7)-B(6)	126.6(4)
O(10)-B(7)-B(8)	115.9(4)
O(10)-B(7)-B(9)	120.2(4)
O(10)-B(7)-B(10)	119.6(4)
B(2)-B(7)-B(8)	107.7(3)
B(2)-B(7)-B(9)	108.2(4)
B(2)-B(7)-B(10)	60.1(3)
B(6)-B(7)-B(2)	58.6(3)
B(6)-B(7)-B(8)	109.2(4)
B(6)-B(7)-B(9)	62.0(3)
B(6)-B(7)-B(10)	107.1(3)
B(8)-B(7)-B(10)	59.2(3)
B(9)-B(7)-B(8)	59.9(3)
B(9)-B(7)-B(10)	107.3(3)
O(12)-B(8)-B(7)	123.5(4)
O(12)-B(8)-B(9)	125.6(4)
O(12)-B(8)-B(10)	118.8(4)
O(12)-B(8)-B(11)	123.9(4)
O(12)-B(8)-B(12)	118.4(4)
B(9)-B(8)-B(7)	59.9(3)
B(10)-B(8)-B(7)	60.8(3)
B(10)-B(8)-B(9)	108.4(4)
B(10)-B(8)-B(12)	60.6(3)
B(11)-B(8)-B(7)	106.1(4)

B(11)-B(8)-B(9)	58.7(3)
B(11)-B(8)-B(10)	106.7(3)
B(11)-B(8)-B(12)	58.8(3)
B(12)-B(8)-B(7)	108.6(3)
B(12)-B(8)-B(9)	107.2(3)
O(3)-B(9)-B(5)	121.3(4)
O(3)-B(9)-B(6)	124.4(4)
O(3)-B(9)-B(7)	123.1(4)
O(3)-B(9)-B(8)	120.9(4)
O(3)-B(9)-B(11)	121.2(4)
B(5)-B(9)-B(6)	59.7(3)
B(5)-B(9)-B(7)	107.3(3)
B(5)-B(9)-B(8)	108.7(3)
B(7)-B(9)-B(6)	58.3(3)
B(7)-B(9)-B(8)	60.2(3)
B(8)-B(9)-B(6)	106.5(3)
B(11)-B(9)-B(5)	60.6(3)
B(11)-B(9)-B(6)	106.6(3)
B(11)-B(9)-B(7)	107.0(4)
B(11)-B(9)-B(8)	59.5(3)
O(11)-B(10)-B(2)	117.7(4)
O(11)-B(10)-B(3)	119.2(4)
O(11)-B(10)-B(7)	122.2(4)
O(11)-B(10)-B(8)	126.0(4)
O(11)-B(10)-B(12)	124.5(4)
B(2)-B(10)-B(7)	59.2(3)
B(3)-B(10)-B(2)	58.7(3)
B(3)-B(10)-B(7)	106.3(4)
B(3)-B(10)-B(12)	61.2(3)
B(8)-B(10)-B(2)	107.6(4)
B(8)-B(10)-B(3)	108.4(4)
B(8)-B(10)-B(7)	60.0(3)
B(8)-B(10)-B(12)	59.8(3)
B(12)-B(10)-B(2)	107.8(4)
B(12)-B(10)-B(7)	107.3(4)
N(1)-B(11)-B(4)	121.6(4)

N(1)-B(11)-B(5)	120.2(4)
N(1)-B(11)-B(8)	119.2(4)
N(1)-B(11)-B(9)	118.0(4)
N(1)-B(11)-B(12)	120.9(4)
B(5)-B(11)-B(4)	60.7(3)
B(8)-B(11)-B(4)	111.0(4)
B(8)-B(11)-B(5)	110.6(4)
B(9)-B(11)-B(4)	110.8(4)
B(9)-B(11)-B(5)	60.9(3)
B(9)-B(11)-B(8)	61.7(3)
B(12)-B(11)-B(4)	61.3(3)
B(12)-B(11)-B(5)	110.6(4)
B(12)-B(11)-B(8)	61.5(3)
B(12)-B(11)-B(9)	111.7(4)
O(13)-B(12)-B(3)	116.7(4)
O(13)-B(12)-B(4)	118.6(4)
O(13)-B(12)-B(8)	126.9(4)
O(13)-B(12)-B(10)	120.3(4)
O(13)-B(12)-B(11)	127.6(4)
B(4)-B(12)-B(3)	59.6(3)
B(4)-B(12)-B(10)	107.9(3)
B(8)-B(12)-B(3)	106.7(3)
B(8)-B(12)-B(4)	108.9(3)
B(8)-B(12)-B(10)	59.7(3)
B(10)-B(12)-B(3)	59.1(3)
B(11)-B(12)-B(3)	106.2(4)
B(11)-B(12)-B(4)	60.5(3)
B(11)-B(12)-B(8)	59.7(3)
B(11)-B(12)-B(10)	106.6(3)
B(9')-O(3')-C(50')	120.5(4)
B(5')-O(4')-C(1')	121.8(4)
B(4')-O(5')-C(8')	123.6(4)
B(1')-O(6')-C(15')	119.7(4)
B(6')-O(7')-C(36')	119.6(3)
B(3')-O(8')-C(35')	120.1(4)
B(2')-O(9')-C(28')	119.6(4)

B(7')-O(10')-C(43')	122.2(4)
B(10')-O(11')-C(71')	122.0(4)
B(8')-O(12')-C(57')	119.1(4)
B(12')-O(13')-C(64')	119.9(4)
O(1')-N(1')-B(11')	120.0(4)
O(2')-N(1')-O(1')	120.0(4)
O(2')-N(1')-B(11')	120.0(4)
O(4')-C(1')-C(2')	107.1(4)
C(3')-C(2')-C(1')	120.6(5)
C(7')-C(2')-C(1')	122.0(5)
C(7')-C(2')-C(3')	117.4(5)
F(1')-C(3')-C(2')	117.8(5)
F(1')-C(3')-C(4')	119.3(6)
C(4')-C(3')-C(2')	122.9(6)
C(3')-C(4')-F(2')	119.5(7)
C(5')-C(4')-F(2')	121.4(7)
C(5')-C(4')-C(3')	119.0(7)
F(3')-C(5')-C(6')	118.2(8)
C(4')-C(5')-F(3')	119.5(8)
C(4')-C(5')-C(6')	122.3(7)
F(4')-C(6')-C(5')	121.3(7)
F(4')-C(6')-C(7')	121.7(7)
C(5')-C(6')-C(7')	116.8(7)
F(5')-C(7')-C(2')	121.8(6)
F(5')-C(7')-C(6')	116.7(6)
C(2')-C(7')-C(6')	121.5(6)
O(5')-C(8')-C(9')	106.6(4)
C(10')-C(9')-C(8')	120.6(4)
C(14')-C(9')-C(8')	122.9(4)
C(14')-C(9')-C(10')	116.4(4)
F(10')-C(10')-C(9')	119.9(4)
F(10')-C(10')-C(11')	117.4(4)
C(11')-C(10')-C(9')	122.6(5)
F(9')-C(11')-C(10')	120.6(5)
F(9')-C(11')-C(12')	120.0(4)
C(12')-C(11')-C(10')	119.4(5)

F(8')-C(12')-C(11')	120.0(5)
F(8')-C(12')-C(13')	119.7(5)
C(13')-C(12')-C(11')	120.3(5)
F(7')-C(13')-C(12')	121.0(5)
F(7')-C(13')-C(14')	120.4(5)
C(12')-C(13')-C(14')	118.6(5)
F(6')-C(14')-C(9')	120.2(4)
F(6')-C(14')-C(13')	117.1(4)
C(9')-C(14')-C(13')	122.7(5)
O(6')-C(15')-C(16')	106.6(4)
C(17')-C(16')-C(15')	123.0(4)
C(17')-C(16')-C(21')	116.5(5)
C(21')-C(16')-C(15')	120.5(4)
F(11')-C(17')-C(16')	120.3(5)
F(11')-C(17')-C(18')	117.6(5)
C(16')-C(17')-C(18')	122.1(5)
F(12')-C(18')-C(17')	120.6(5)
F(12')-C(18')-C(19')	119.5(5)
C(19')-C(18')-C(17')	119.9(5)
F(13')-C(19')-C(18')	120.3(6)
F(13')-C(19')-C(20')	120.2(6)
C(18')-C(19')-C(20')	119.6(5)
F(14')-C(20')-C(19')	119.2(5)
F(14')-C(20')-C(21')	120.8(5)
C(21')-C(20')-C(19')	120.0(5)
F(15')-C(21')-C(16')	119.2(5)
F(15')-C(21')-C(20')	118.9(5)
C(20')-C(21')-C(16')	121.9(5)
F(25')-C(22')-C(23')	118.8(5)
F(25')-C(22')-C(27')	118.6(4)
C(23')-C(22')-C(27')	122.6(5)
F(24')-C(23')-C(22')	120.5(5)
F(24')-C(23')-C(24')	120.1(5)
C(24')-C(23')-C(22')	119.4(5)
F(23')-C(24')-C(23')	119.9(5)
F(23')-C(24')-C(25')	120.4(5)

C(25')-C(24')-C(23')	119.8(5)
F(22')-C(25')-C(24')	119.9(5)
F(22')-C(25')-C(26')	120.4(5)
C(24')-C(25')-C(26')	119.7(5)
F(21')-C(26')-C(25')	117.6(5)
F(21')-C(26')-C(27')	120.2(5)
C(27')-C(26')-C(25')	122.2(5)
C(22')-C(27')-C(35')	121.4(5)
C(26')-C(27')-C(22')	116.3(5)
C(26')-C(27')-C(35')	122.3(5)
O(9')-C(28')-C(29')	107.6(4)
C(30')-C(29')-C(28')	122.5(6)
C(30')-C(29')-C(34')	116.5(5)
C(34')-C(29')-C(28')	121.0(6)
F(16')-C(30')-C(29')	119.4(5)
F(16')-C(30')-C(31')	118.1(6)
C(31')-C(30')-C(29')	122.5(6)
F(17')-C(31')-C(30')	120.8(6)
F(17')-C(31')-C(32')	119.9(5)
C(30')-C(31')-C(32')	119.3(6)
F(18')-C(32')-C(31')	119.8(6)
F(18')-C(32')-C(33')	119.7(6)
C(33')-C(32')-C(31')	120.5(6)
F(19')-C(33')-C(32')	121.1(5)
F(19')-C(33')-C(34')	119.8(6)
C(32')-C(33')-C(34')	119.1(6)
F(20')-C(34')-C(29')	119.7(5)
F(20')-C(34')-C(33')	118.2(6)
C(33')-C(34')-C(29')	122.1(6)
O(8')-C(35')-C(27')	108.0(4)
O(7')-C(36')-C(37')	107.7(4)
C(38')-C(37')-C(36')	122.7(4)
C(38')-C(37')-C(42')	116.4(4)
C(42')-C(37')-C(36')	121.0(4)
F(26')-C(38')-C(37')	119.6(4)
F(26')-C(38')-C(39')	118.1(5)

C(39')-C(38')-C(37')	122.3(5)
F(27')-C(39')-C(38')	121.4(5)
F(27')-C(39')-C(40')	119.0(5)
C(38')-C(39')-C(40')	119.6(5)
F(28')-C(40')-C(39')	120.1(5)
F(28')-C(40')-C(41')	119.9(5)
C(41')-C(40')-C(39')	119.9(4)
F(29')-C(41')-C(40')	119.6(4)
F(29')-C(41')-C(42')	121.2(5)
C(40')-C(41')-C(42')	119.2(5)
F(30')-C(42')-C(37')	119.6(4)
F(30')-C(42')-C(41')	117.8(4)
C(41')-C(42')-C(37')	122.6(5)
O(10')-C(43')-C(44')	106.6(4)
C(45')-C(44')-C(43')	123.4(5)
C(45')-C(44')-C(49')	116.0(5)
C(49')-C(44')-C(43')	120.5(5)
F(31')-C(45')-C(44')	118.9(5)
F(31')-C(45')-C(46')	117.4(5)
C(44')-C(45')-C(46')	123.6(5)
F(32')-C(46')-C(45')	120.9(5)
F(32')-C(46')-C(47')	120.5(5)
C(47')-C(46')-C(45')	118.5(5)
F(33')-C(47')-C(46')	119.6(5)
F(33')-C(47')-C(48')	120.2(5)
C(48')-C(47')-C(46')	120.1(5)
F(34')-C(48')-C(47')	118.9(5)
F(34')-C(48')-C(49')	120.5(5)
C(47')-C(48')-C(49')	120.6(5)
F(35')-C(49')-C(44')	120.2(5)
F(35')-C(49')-C(48')	118.7(5)
C(48')-C(49')-C(44')	121.1(5)
O(3')-C(50')-C(51')	108.4(4)
C(52')-C(51')-C(50')	120.3(5)
C(56')-C(51')-C(50')	123.9(5)
C(56')-C(51')-C(52')	115.8(5)

F(36')-C(52')-C(51')	119.4(4)
F(36')-C(52')-C(53')	118.5(4)
C(53')-C(52')-C(51')	122.0(5)
F(37')-C(53')-C(52')	119.6(5)
F(37')-C(53')-C(54')	119.9(5)
C(54')-C(53')-C(52')	120.4(5)
F(38')-C(54')-C(53')	119.4(5)
F(38')-C(54')-C(55')	121.1(5)
C(55')-C(54')-C(53')	119.6(5)
F(39')-C(55')-C(54')	119.9(5)
F(39')-C(55')-C(56')	120.8(5)
C(54')-C(55')-C(56')	119.2(5)
F(40')-C(56')-C(51')	119.7(5)
F(40')-C(56')-C(55')	117.4(5)
C(51')-C(56')-C(55')	122.9(5)
O(12')-C(57')-C(58')	106.7(4)
C(59')-C(58')-C(57')	123.9(5)
C(59')-C(58')-C(63')	115.7(5)
C(63')-C(58')-C(57')	120.3(4)
F(46')-C(59')-C(58')	119.8(5)
F(46')-C(59')-C(60')	117.9(5)
C(58')-C(59')-C(60')	122.4(5)
F(47')-C(60')-C(59')	120.1(5)
F(47')-C(60')-C(61')	119.8(5)
C(61')-C(60')-C(59')	120.0(5)
F(48')-C(61')-C(60')	120.5(5)
F(48')-C(61')-C(62')	119.3(5)
C(60')-C(61')-C(62')	120.2(5)
F(49')-C(62')-C(61')	121.2(5)
F(49')-C(62')-C(63')	120.4(5)
C(61')-C(62')-C(63')	118.4(5)
F(50')-C(63')-C(58')	119.4(4)
F(50')-C(63')-C(62')	117.4(4)
C(58')-C(63')-C(62')	123.2(5)
O(13')-C(64')-C(65')	107.4(4)
C(66')-C(65')-C(64')	121.6(5)

C(66')-C(65')-C(70')	116.0(4)
C(70')-C(65')-C(64')	122.4(5)
F(45')-C(66')-C(65')	119.4(4)
F(45')-C(66')-C(67')	117.8(5)
C(65')-C(66')-C(67')	122.8(5)
F(44')-C(67')-C(66')	120.3(5)
F(44')-C(67')-C(68')	120.3(4)
C(68')-C(67')-C(66')	119.4(5)
F(43')-C(68')-C(67')	119.9(5)
F(43')-C(68')-C(69')	120.1(5)
C(67')-C(68')-C(69')	120.0(5)
F(42')-C(69')-C(68')	119.9(5)
F(42')-C(69')-C(70')	120.6(5)
C(68')-C(69')-C(70')	119.4(5)
F(41')-C(70')-C(65')	119.8(5)
F(41')-C(70')-C(69')	117.8(5)
C(69')-C(70')-C(65')	122.4(5)
O(11')-C(71')-C(72')	110.1(4)
C(73')-C(72')-C(71')	121.6(5)
C(77')-C(72')-C(71')	121.2(5)
C(77')-C(72')-C(73')	117.1(5)
F(55')-C(73')-C(72')	121.9(5)
F(55')-C(73')-C(74')	116.6(5)
C(72')-C(73')-C(74')	121.5(5)
F(54')-C(74')-C(73')	121.5(6)
F(54')-C(74')-C(75')	120.2(6)
C(75')-C(74')-C(73')	118.3(5)
F(53')-C(75')-C(74')	119.6(6)
F(53')-C(75')-C(76')	120.0(6)
C(76')-C(75')-C(74')	120.3(6)
F(52')-C(76')-C(75')	119.4(6)
F(52')-C(76')-C(77')	120.8(6)
C(77')-C(76')-C(75')	119.8(6)
F(51')-C(77')-C(72')	118.2(5)
F(51')-C(77')-C(76')	118.9(5)
C(76')-C(77')-C(72')	122.9(6)

O(6')-B(1')-B(2')	122.6(4)
O(6')-B(1')-B(3')	125.7(4)
O(6')-B(1')-B(4')	122.7(4)
O(6')-B(1')-B(5')	118.4(4)
O(6')-B(1')-B(6')	118.0(4)
B(2')-B(1')-B(4')	108.5(4)
B(3')-B(1')-B(2')	59.2(3)
B(3')-B(1')-B(4')	61.2(3)
B(3')-B(1')-B(5')	108.9(4)
B(3')-B(1')-B(6')	107.1(4)
B(5')-B(1')-B(2')	107.9(3)
B(5')-B(1')-B(4')	60.5(3)
B(6')-B(1')-B(2')	58.9(3)
B(6')-B(1')-B(4')	109.2(4)
B(6')-B(1')-B(5')	60.9(3)
O(9')-B(2')-B(1')	123.5(4)
O(9')-B(2')-B(3')	125.6(4)
O(9')-B(2')-B(6')	117.9(4)
O(9')-B(2')-B(7')	117.6(4)
O(9')-B(2')-B(10')	122.7(4)
B(1')-B(2')-B(7')	107.9(4)
B(1')-B(2')-B(10')	107.5(4)
B(3')-B(2')-B(1')	59.9(3)
B(3')-B(2')-B(7')	109.0(4)
B(3')-B(2')-B(10')	59.8(3)
B(6')-B(2')-B(1')	60.1(3)
B(6')-B(2')-B(3')	108.7(4)
B(6')-B(2')-B(7')	59.9(3)
B(6')-B(2')-B(10')	108.6(4)
B(7')-B(2')-B(10')	60.9(3)
O(8')-B(3')-B(1')	119.4(4)
O(8')-B(3')-B(2')	121.2(4)
O(8')-B(3')-B(4')	120.3(4)
O(8')-B(3')-B(10')	123.4(4)
O(8')-B(3')-B(12')	123.3(4)
B(1')-B(3')-B(4')	59.9(3)

B(1')-B(3')-B(10')	109.4(3)
B(1')-B(3')-B(12')	106.9(3)
B(2')-B(3')-B(1')	60.9(3)
B(2')-B(3')-B(4')	108.8(3)
B(2')-B(3')-B(10')	61.3(3)
B(2')-B(3')-B(12')	108.6(3)
B(4')-B(3')-B(12')	58.6(3)
B(10')-B(3')-B(4')	107.7(3)
B(10')-B(3')-B(12')	60.0(3)
O(5')-B(4')-B(1')	114.2(4)
O(5')-B(4')-B(3')	119.8(4)
O(5')-B(4')-B(5')	119.4(4)
O(5')-B(4')-B(11')	129.8(4)
O(5')-B(4')-B(12')	128.0(4)
B(1')-B(4')-B(3')	58.9(3)
B(1')-B(4')-B(5')	59.6(3)
B(5')-B(4')-B(3')	106.4(3)
B(11')-B(4')-B(1')	106.3(3)
B(11')-B(4')-B(3')	105.8(3)
B(11')-B(4')-B(5')	59.5(3)
B(11')-B(4')-B(12')	58.1(3)
B(12')-B(4')-B(1')	108.3(4)
B(12')-B(4')-B(3')	61.3(3)
B(12')-B(4')-B(5')	107.2(3)
O(4')-B(5')-B(1')	128.1(4)
O(4')-B(5')-B(4')	123.2(4)
O(4')-B(5')-B(6')	123.9(4)
O(4')-B(5')-B(9')	115.9(4)
O(4')-B(5')-B(11')	118.1(4)
B(1')-B(5')-B(4')	59.9(3)
B(1')-B(5')-B(6')	59.3(3)
B(1')-B(5')-B(9')	109.0(4)
B(4')-B(5')-B(6')	107.5(4)
B(9')-B(5')-B(4')	108.1(4)
B(9')-B(5')-B(6')	61.7(3)
B(11')-B(5')-B(1')	106.6(4)

B(11')-B(5')-B(4')	59.7(3)
B(11')-B(5')-B(6')	106.7(4)
B(11')-B(5')-B(9')	58.6(3)
O(7')-B(6')-B(1')	126.1(4)
O(7')-B(6')-B(2')	125.4(4)
O(7')-B(6')-B(5')	120.2(4)
O(7')-B(6')-B(7')	118.7(4)
O(7')-B(6')-B(9')	116.5(4)
B(1')-B(6')-B(5')	59.8(3)
B(1')-B(6')-B(9')	107.1(3)
B(2')-B(6')-B(1')	61.0(3)
B(2')-B(6')-B(5')	108.7(3)
B(2')-B(6')-B(7')	61.2(3)
B(2')-B(6')-B(9')	108.5(4)
B(5')-B(6')-B(9')	58.8(3)
B(7')-B(6')-B(1')	109.7(4)
B(7')-B(6')-B(5')	107.9(4)
B(7')-B(6')-B(9')	60.0(3)
O(10')-B(7')-B(2')	126.4(4)
O(10')-B(7')-B(6')	127.6(4)
O(10')-B(7')-B(8')	115.5(4)
O(10')-B(7')-B(9')	120.6(4)
O(10')-B(7')-B(10')	119.3(4)
B(2')-B(7')-B(8')	107.3(3)
B(2')-B(7')-B(9')	108.2(4)
B(2')-B(7')-B(10')	59.7(3)
B(6')-B(7')-B(2')	58.9(3)
B(6')-B(7')-B(8')	108.6(4)
B(6')-B(7')-B(9')	62.0(3)
B(6')-B(7')-B(10')	106.8(3)
B(8')-B(7')-B(10')	59.0(3)
B(9')-B(7')-B(8')	59.4(3)
B(9')-B(7')-B(10')	106.6(3)
O(12')-B(8')-B(7')	123.0(4)
O(12')-B(8')-B(9')	125.1(4)
O(12')-B(8')-B(10')	118.9(4)

O(12')-B(8')-B(11')	124.3(4)
O(12')-B(8')-B(12')	118.8(4)
B(9')-B(8')-B(7')	60.2(3)
B(9')-B(8')-B(12')	107.2(4)
B(10')-B(8')-B(7')	60.8(3)
B(10')-B(8')-B(9')	108.7(4)
B(10')-B(8')-B(12')	60.6(3)
B(11')-B(8')-B(7')	106.3(4)
B(11')-B(8')-B(9')	58.9(3)
B(11')-B(8')-B(10')	106.4(3)
B(11')-B(8')-B(12')	58.4(3)
B(12')-B(8')-B(7')	108.7(4)
O(3')-B(9')-B(5')	121.2(4)
O(3')-B(9')-B(6')	124.8(4)
O(3')-B(9')-B(7')	123.7(4)
O(3')-B(9')-B(8')	121.0(4)
O(3')-B(9')-B(11')	120.8(4)
B(5')-B(9')-B(6')	59.5(3)
B(5')-B(9')-B(7')	106.9(4)
B(5')-B(9')-B(8')	108.4(3)
B(7')-B(9')-B(6')	58.1(3)
B(8')-B(9')-B(6')	106.4(4)
B(8')-B(9')-B(7')	60.4(3)
B(11')-B(9')-B(5')	60.4(3)
B(11')-B(9')-B(6')	106.3(3)
B(11')-B(9')-B(7')	107.1(4)
B(11')-B(9')-B(8')	59.6(3)
O(11')-B(10')-B(2')	117.4(4)
O(11')-B(10')-B(3')	118.7(4)
O(11')-B(10')-B(7')	121.8(4)
O(11')-B(10')-B(8')	125.9(4)
O(11')-B(10')-B(12')	124.6(4)
B(2')-B(10')-B(7')	59.3(3)
B(2')-B(10')-B(12')	108.1(4)
B(3')-B(10')-B(2')	58.9(3)
B(3')-B(10')-B(7')	107.0(4)

B(3')-B(10')-B(8')	109.1(4)
B(3')-B(10')-B(12')	61.7(3)
B(8')-B(10')-B(2')	107.9(4)
B(8')-B(10')-B(7')	60.1(3)
B(8')-B(10')-B(12')	59.8(3)
B(12')-B(10')-B(7')	107.6(4)
N(1')-B(11')-B(4')	122.0(4)
N(1')-B(11')-B(5')	118.5(4)
N(1')-B(11')-B(8')	120.0(4)
N(1')-B(11')-B(9')	116.4(4)
N(1')-B(11')-B(12')	122.7(4)
B(5')-B(11')-B(4')	60.8(3)
B(8')-B(11')-B(4')	110.9(4)
B(8')-B(11')-B(5')	110.4(4)
B(9')-B(11')-B(4')	111.0(4)
B(9')-B(11')-B(5')	61.0(3)
B(9')-B(11')-B(8')	61.5(3)
B(12')-B(11')-B(4')	61.2(3)
B(12')-B(11')-B(5')	110.6(4)
B(12')-B(11')-B(8')	61.7(3)
B(12')-B(11')-B(9')	112.0(4)
O(13')-B(12')-B(3')	117.4(4)
O(13')-B(12')-B(4')	119.3(4)
O(13')-B(12')-B(8')	125.9(4)
O(13')-B(12')-B(10')	120.4(4)
O(13')-B(12')-B(11')	127.0(4)
B(4')-B(12')-B(3')	60.1(3)
B(4')-B(12')-B(8')	109.1(4)
B(4')-B(12')-B(10')	107.6(4)
B(8')-B(12')-B(3')	106.4(3)
B(8')-B(12')-B(10')	59.7(3)
B(10')-B(12')-B(3')	58.3(3)
B(11')-B(12')-B(3')	106.8(4)
B(11')-B(12')-B(4')	60.7(3)
B(11')-B(12')-B(8')	59.8(3)
B(11')-B(12')-B(10')	106.7(4)

C(78)-N(2)-C(82)	110.9(4)
C(78)-N(2)-C(86)	107.3(4)
C(78)-N(2)-C(90)	112.4(4)
C(82)-N(2)-C(86)	103.3(4)
C(90)-N(2)-C(82)	112.0(4)
C(90)-N(2)-C(86)	110.5(4)
N(2)-C(78)-C(79)	118.5(5)
C(78)-C(79)-C(80)	112.3(5)
C(81)-C(80)-C(79)	116.9(6)
C(83)-C(82)-N(2)	118.1(4)
C(82)-C(83)-C(84)	109.0(5)
C(85)-C(84)-C(83)	112.8(5)
C(87)-C(86)-N(2)	116.2(5)
C(86)-C(87)-C(88)	110.5(6)
C(87)-C(88)-C(89)	111.0(6)
N(2)-C(90)-C(91)	118.3(5)
C(90)-C(91)-C(92)	111.2(5)
C(93)-C(92)-C(91)	112.7(6)
C(94)-N(3)-C(98)	110.8(5)
C(94)-N(3)-C(106)	89.3(6)
C(94)-N(3)-C(110)	121.0(7)
C(98)-N(3)-C(106)	111.0(5)
C(98)-N(3)-C(110)	102.6(6)
C(102)-N(3)-C(94)	111.9(5)
C(102)-N(3)-C(98)	110.8(5)
C(102)-N(3)-C(106)	121.1(6)
C(102)-N(3)-C(110)	98.8(6)
C(95)-C(94)-N(3)	118.4(5)
C(94)-C(95)-C(96)	110.1(7)
C(97)-C(96)-C(95)	114.5(9)
C(99)-C(98)-N(3)	118.1(5)
C(98)-C(99)-C(100)	109.5(5)
C(99)-C(100)-C(101)	113.4(5)
N(3)-C(102)-C(103)	116.1(6)
C(104)-C(103)-C(102)	111.6(7)
C(103)-C(104)-C(105)	111.9(8)

C(107)-C(106)-N(3)	107.9(9)
C(109)-C(107)-C(106)	111.6(11)
C(107)-C(109)-C(108)	111.1(12)
C(111)-C(110)-N(3)	113.9(9)
C(110)-C(111)-C(112)	109.8(9)
C(113)-C(112)-C(111)	109.2(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[2b]^{1-}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	30(2)	68(3)	81(3)	53(2)	24(2)	19(2)
F(2)	85(3)	38(2)	83(3)	16(2)	-8(2)	-18(2)
F(3)	148(5)	43(2)	72(3)	0(2)	54(3)	29(3)
F(4)	68(3)	77(3)	114(4)	47(3)	67(3)	38(2)
F(5)	32(2)	40(2)	100(3)	34(2)	-7(2)	-5(2)
F(6)	33(2)	36(2)	20(2)	12(1)	-2(1)	3(1)
F(7)	53(2)	23(2)	38(2)	-1(1)	10(2)	5(2)
F(8)	51(2)	24(2)	68(3)	26(2)	5(2)	13(2)
F(9)	48(2)	43(2)	42(2)	35(2)	-5(2)	6(2)
F(10)	33(2)	24(2)	19(2)	9(1)	1(1)	0(1)
F(11)	30(2)	40(2)	64(2)	23(2)	6(2)	-1(2)
F(12)	57(3)	59(2)	121(4)	68(3)	33(2)	28(2)
F(13)	32(2)	132(4)	128(4)	109(4)	8(2)	30(2)
F(14)	28(2)	110(3)	73(3)	57(3)	-21(2)	-16(2)
F(15)	36(2)	46(2)	42(2)	15(2)	0(2)	-5(2)
F(16)	53(2)	67(3)	52(2)	28(2)	-3(2)	-4(2)
F(17)	100(4)	124(4)	64(3)	48(3)	-17(3)	25(3)
F(18)	55(3)	140(5)	55(3)	2(3)	-27(2)	23(3)
F(19)	39(2)	84(3)	74(3)	-3(2)	-16(2)	-23(2)
F(20)	59(3)	56(2)	64(3)	21(2)	-2(2)	-15(2)
F(21)	55(2)	32(2)	38(2)	21(2)	15(2)	10(2)
F(22)	67(3)	35(2)	31(2)	-2(2)	4(2)	7(2)
F(23)	73(3)	65(2)	14(2)	11(2)	8(2)	19(2)
F(24)	89(3)	47(2)	33(2)	26(2)	21(2)	23(2)
F(25)	54(2)	25(2)	28(2)	5(1)	13(2)	7(2)
F(26)	28(2)	33(2)	55(2)	-1(2)	6(2)	3(1)
F(27)	31(2)	29(2)	103(3)	14(2)	-6(2)	-10(2)
F(28)	17(2)	65(2)	98(3)	61(2)	7(2)	-8(2)
F(29)	17(2)	78(2)	35(2)	38(2)	10(1)	10(2)

F(30)	19(2)	40(2)	21(2)	10(1)	1(1)	2(1)
F(31)	84(3)	63(3)	36(2)	6(2)	9(2)	13(2)
F(32)	65(3)	39(2)	86(3)	-19(2)	14(2)	5(2)
F(33)	89(4)	31(2)	158(5)	49(3)	58(3)	30(2)
F(34)	138(5)	66(3)	84(3)	62(3)	40(3)	39(3)
F(35)	94(3)	37(2)	42(2)	20(2)	32(2)	24(2)
F(36)	27(2)	41(2)	35(2)	16(2)	7(1)	13(1)
F(37)	31(2)	51(2)	36(2)	34(2)	5(1)	13(2)
F(38)	38(2)	66(2)	19(2)	18(2)	8(1)	12(2)
F(39)	55(2)	40(2)	43(2)	3(2)	14(2)	15(2)
F(40)	46(2)	50(2)	56(2)	33(2)	17(2)	23(2)
F(41)	36(2)	31(2)	35(2)	-6(1)	-4(1)	9(1)
F(42)	35(2)	20(2)	75(3)	12(2)	-18(2)	-9(1)
F(43)	17(2)	55(2)	72(3)	46(2)	-1(2)	-11(2)
F(44)	21(2)	55(2)	29(2)	21(2)	9(1)	8(1)
F(45)	18(2)	26(2)	22(2)	4(1)	2(1)	1(1)
F(46)	46(2)	28(2)	45(2)	21(2)	-14(2)	-7(2)
F(47)	70(3)	25(2)	49(2)	20(2)	8(2)	16(2)
F(48)	34(2)	63(2)	51(2)	40(2)	12(2)	34(2)
F(49)	17(2)	57(2)	34(2)	26(2)	-2(1)	2(1)
F(50)	21(2)	24(2)	32(2)	15(1)	2(1)	1(1)
F(51)	44(2)	43(2)	49(2)	17(2)	21(2)	11(2)
F(52)	52(2)	39(2)	70(3)	24(2)	24(2)	4(2)
F(53)	58(2)	27(2)	54(2)	12(2)	12(2)	11(2)
F(54)	55(2)	37(2)	42(2)	10(2)	22(2)	16(2)
F(55)	50(2)	36(2)	41(2)	19(2)	17(2)	6(2)
O(1)	65(3)	32(2)	27(2)	17(2)	-15(2)	-27(2)
O(2)	43(2)	28(2)	15(2)	9(2)	-9(2)	8(2)
O(3)	12(2)	28(2)	17(2)	15(1)	6(1)	9(1)
O(4)	20(2)	22(2)	14(2)	11(1)	4(1)	12(1)
O(5)	13(2)	16(2)	20(2)	11(1)	1(1)	0(1)
O(6)	11(2)	25(2)	16(2)	16(1)	2(1)	4(1)
O(7)	10(2)	31(2)	17(2)	18(2)	1(1)	3(1)
O(8)	14(2)	26(2)	12(2)	13(1)	4(1)	7(1)
O(9)	13(2)	27(2)	14(2)	4(1)	2(1)	-3(1)
O(10)	17(2)	17(2)	26(2)	14(1)	1(1)	-2(1)

O(11)	15(2)	17(2)	17(2)	5(1)	4(1)	6(1)
O(12)	12(2)	24(2)	16(2)	16(1)	5(1)	8(1)
O(13)	7(2)	25(2)	12(2)	11(1)	1(1)	4(1)
N(1)	13(2)	21(2)	14(2)	6(2)	2(2)	3(2)
C(1)	51(4)	35(3)	27(3)	8(2)	-7(3)	28(3)
C(2)	26(3)	25(2)	23(3)	12(2)	2(2)	15(2)
C(3)	25(3)	34(3)	44(3)	22(2)	10(2)	8(2)
C(4)	55(4)	24(3)	49(3)	14(2)	6(3)	0(2)
C(5)	66(4)	31(3)	48(4)	12(3)	24(3)	16(3)
C(6)	50(4)	41(3)	62(4)	20(3)	33(3)	19(3)
C(7)	26(3)	27(3)	51(3)	20(2)	8(2)	9(2)
C(8)	13(2)	17(2)	25(3)	14(2)	3(2)	-1(2)
C(9)	10(2)	19(2)	23(2)	13(2)	2(2)	3(2)
C(10)	15(3)	24(2)	20(2)	13(2)	3(2)	2(2)
C(11)	23(3)	27(2)	31(3)	22(2)	1(2)	4(2)
C(12)	24(3)	22(2)	44(3)	19(2)	4(2)	7(2)
C(13)	24(3)	21(2)	33(3)	9(2)	5(2)	2(2)
C(14)	15(3)	23(2)	20(2)	10(2)	2(2)	1(2)
C(15)	22(3)	40(3)	20(3)	22(2)	5(2)	9(2)
C(16)	20(2)	38(3)	20(2)	23(2)	2(2)	4(2)
C(17)	21(3)	41(3)	46(3)	29(2)	7(2)	6(2)
C(18)	29(3)	61(3)	70(4)	56(3)	17(3)	16(2)
C(19)	24(3)	79(4)	72(4)	64(3)	7(3)	17(3)
C(20)	16(3)	79(4)	51(4)	49(3)	-1(2)	3(2)
C(21)	22(3)	48(3)	27(3)	25(2)	0(2)	0(2)
C(22)	30(3)	24(2)	19(2)	9(2)	10(2)	7(2)
C(23)	39(3)	33(3)	24(2)	19(2)	11(2)	10(2)
C(24)	37(3)	40(3)	13(2)	6(2)	8(2)	11(2)
C(25)	32(3)	30(3)	23(2)	4(2)	6(2)	6(2)
C(26)	20(3)	28(2)	27(2)	12(2)	7(2)	1(2)
C(27)	15(2)	27(2)	16(2)	9(2)	6(2)	3(2)
C(28)	31(3)	39(3)	19(3)	0(2)	-2(2)	1(2)
C(29)	28(3)	45(3)	19(3)	1(2)	1(2)	2(2)
C(30)	37(3)	50(3)	28(3)	9(3)	1(2)	4(3)
C(31)	49(4)	74(4)	34(3)	10(3)	-7(3)	18(3)
C(32)	37(3)	79(4)	36(3)	-2(3)	-11(3)	10(3)

C(33)	29(3)	70(4)	39(3)	-7(3)	-4(3)	-1(3)
C(34)	30(3)	48(3)	31(3)	4(3)	-2(2)	-9(2)
C(35)	14(2)	40(3)	16(2)	12(2)	4(2)	4(2)
C(36)	10(2)	24(3)	18(2)	12(2)	2(2)	2(2)
C(37)	9(2)	25(2)	27(2)	18(2)	0(2)	4(2)
C(38)	19(3)	23(3)	40(3)	8(2)	-1(2)	2(2)
C(39)	21(3)	25(3)	61(3)	22(2)	-6(2)	-7(2)
C(40)	9(2)	39(3)	60(3)	39(2)	-1(2)	-2(2)
C(41)	14(2)	47(3)	34(3)	33(2)	2(2)	3(2)
C(42)	14(2)	30(2)	17(2)	16(2)	-1(2)	2(2)
C(43)	20(3)	22(2)	33(3)	14(2)	1(2)	-4(2)
C(44)	18(3)	19(2)	37(3)	11(2)	8(2)	-2(2)
C(45)	32(3)	26(3)	46(3)	4(2)	9(2)	-2(2)
C(46)	31(3)	22(3)	65(4)	2(2)	13(3)	-2(2)
C(47)	39(4)	24(3)	86(4)	20(3)	23(3)	11(3)
C(48)	61(5)	34(3)	67(4)	33(3)	25(3)	15(3)
C(49)	40(3)	27(3)	40(3)	16(2)	20(2)	15(2)
C(50)	15(2)	52(3)	20(2)	24(2)	6(2)	11(2)
C(51)	12(2)	44(3)	22(2)	20(2)	9(2)	10(2)
C(52)	9(2)	40(3)	20(2)	18(2)	1(2)	4(2)
C(53)	12(2)	41(3)	25(2)	21(2)	3(2)	7(2)
C(54)	17(3)	45(3)	21(2)	17(2)	2(2)	7(2)
C(55)	22(3)	39(3)	30(3)	9(2)	8(2)	9(2)
C(56)	21(3)	37(3)	31(3)	20(2)	7(2)	10(2)
C(57)	16(2)	28(3)	20(2)	18(2)	5(2)	9(2)
C(58)	15(2)	20(2)	14(2)	11(2)	5(2)	4(2)
C(59)	30(3)	22(2)	20(3)	13(2)	-1(2)	2(2)
C(60)	43(3)	31(3)	27(3)	20(2)	10(2)	15(2)
C(61)	25(3)	42(3)	23(3)	23(2)	10(2)	20(2)
C(62)	18(2)	40(3)	19(2)	19(2)	9(2)	11(2)
C(63)	19(2)	25(2)	18(2)	15(2)	6(2)	8(2)
C(64)	12(2)	23(3)	14(2)	9(2)	-2(2)	6(2)
C(65)	12(2)	20(2)	18(2)	11(2)	-2(2)	2(2)
C(66)	13(2)	17(2)	19(2)	11(2)	-2(2)	2(2)
C(67)	13(2)	33(3)	24(2)	18(2)	3(2)	5(2)
C(68)	13(2)	31(3)	38(3)	26(2)	-3(2)	0(2)

C(69)	18(2)	19(2)	43(3)	15(2)	-12(2)	-2(2)
C(70)	19(2)	18(2)	28(3)	6(2)	-4(2)	6(2)
C(71)	19(3)	29(3)	25(3)	7(2)	2(2)	10(2)
C(72)	26(3)	28(3)	19(2)	6(2)	-3(2)	10(2)
C(73)	31(3)	27(3)	39(3)	16(2)	9(2)	6(2)
C(74)	40(3)	32(3)	30(3)	9(2)	11(2)	12(2)
C(75)	41(3)	20(3)	41(3)	8(2)	7(3)	8(2)
C(76)	27(3)	34(3)	41(3)	16(2)	7(2)	6(2)
C(77)	19(3)	31(3)	27(3)	0(2)	8(2)	4(2)
B(1)	8(2)	21(2)	14(2)	11(2)	3(2)	3(2)
B(2)	13(2)	21(2)	17(2)	12(2)	4(2)	4(2)
B(3)	10(2)	20(2)	11(2)	10(2)	1(2)	2(2)
B(4)	12(2)	18(2)	11(2)	8(2)	3(2)	4(2)
B(5)	12(2)	17(2)	12(2)	8(2)	4(2)	4(2)
B(6)	12(2)	20(2)	13(2)	10(2)	2(2)	3(2)
B(7)	11(2)	18(2)	17(2)	10(2)	3(2)	4(2)
B(8)	11(2)	18(2)	14(2)	10(2)	2(2)	3(2)
B(9)	10(2)	19(2)	14(2)	10(2)	2(2)	5(2)
B(10)	10(2)	18(2)	14(2)	10(2)	-1(2)	1(2)
B(11)	14(2)	20(2)	12(2)	10(2)	2(2)	4(2)
B(12)	10(2)	17(2)	12(2)	9(2)	2(2)	4(2)
F(1')	34(2)	53(2)	64(2)	32(2)	17(2)	11(2)
F(2')	112(4)	44(3)	123(5)	-5(3)	16(3)	-36(3)
F(3')	295(11)	67(4)	239(9)	-86(5)	182(9)	-37(5)
F(4')	168(6)	94(4)	191(7)	8(4)	157(6)	30(4)
F(5')	43(2)	50(2)	108(4)	36(2)	25(2)	2(2)
F(6')	39(2)	31(2)	20(2)	12(1)	-7(1)	-3(1)
F(7')	48(2)	19(2)	35(2)	1(1)	6(2)	2(1)
F(8')	49(2)	22(2)	58(2)	22(2)	-1(2)	9(2)
F(9')	50(2)	35(2)	28(2)	24(2)	-7(1)	3(2)
F(10')	33(2)	21(2)	20(2)	6(1)	0(1)	-1(1)
F(11')	35(2)	32(2)	50(2)	17(2)	-3(2)	-9(1)
F(12')	61(3)	37(2)	86(3)	41(2)	26(2)	18(2)
F(13')	32(2)	93(3)	137(4)	91(3)	9(2)	22(2)
F(14')	33(2)	81(3)	110(4)	64(3)	-39(2)	-21(2)
F(15')	39(2)	29(2)	47(2)	17(2)	-14(2)	-6(1)

F(16')	66(3)	32(2)	49(2)	6(2)	-3(2)	8(2)
F(17')	43(2)	45(2)	59(2)	6(2)	-12(2)	4(2)
F(18')	46(2)	32(2)	71(3)	-1(2)	-7(2)	-5(2)
F(19')	50(2)	35(2)	76(3)	11(2)	-1(2)	6(2)
F(20')	42(2)	47(2)	59(3)	12(2)	-10(2)	-3(2)
F(21')	82(3)	28(2)	48(2)	19(2)	27(2)	12(2)
F(22')	92(3)	29(2)	40(2)	-5(2)	23(2)	5(2)
F(23')	71(3)	66(3)	15(2)	6(2)	12(2)	8(2)
F(24')	82(3)	52(2)	28(2)	27(2)	17(2)	18(2)
F(25')	57(2)	25(2)	27(2)	8(1)	11(2)	7(2)
F(26')	32(2)	27(2)	45(2)	-3(2)	11(2)	0(1)
F(27')	34(2)	25(2)	67(2)	9(2)	1(2)	-14(1)
F(28')	21(2)	55(2)	61(2)	40(2)	9(2)	-4(2)
F(29')	22(2)	52(2)	26(2)	22(2)	12(1)	15(1)
F(30')	25(2)	24(2)	19(2)	8(1)	1(1)	4(1)
F(31')	53(2)	35(2)	27(2)	11(1)	-8(2)	-5(2)
F(32')	56(2)	30(2)	35(2)	-3(2)	2(2)	0(2)
F(33')	67(3)	24(2)	60(2)	18(2)	-1(2)	8(2)
F(34')	69(3)	43(2)	36(2)	25(2)	-7(2)	4(2)
F(35')	60(2)	25(2)	24(2)	5(1)	8(2)	0(2)
F(36')	21(2)	29(2)	27(2)	14(1)	1(1)	7(1)
F(37')	28(2)	56(2)	31(2)	32(2)	3(1)	10(2)
F(38')	63(3)	73(3)	16(2)	12(2)	12(2)	20(2)
F(39')	105(4)	43(2)	41(2)	2(2)	25(2)	24(2)
F(40')	76(3)	37(2)	46(2)	22(2)	19(2)	26(2)
F(41')	35(2)	31(2)	49(2)	4(2)	5(2)	9(2)
F(42')	36(2)	22(2)	81(3)	18(2)	-3(2)	-8(1)
F(43')	18(2)	51(2)	74(3)	43(2)	6(2)	-3(2)
F(44')	24(2)	50(2)	39(2)	25(2)	13(1)	11(2)
F(45')	25(2)	25(2)	31(2)	12(1)	1(1)	3(1)
F(46')	44(2)	27(2)	49(2)	19(2)	-5(2)	-3(2)
F(47')	63(2)	29(2)	59(2)	27(2)	6(2)	13(2)
F(48')	35(2)	59(2)	50(2)	39(2)	12(2)	31(2)
F(49')	15(2)	52(2)	38(2)	25(2)	1(1)	5(1)
F(50')	22(2)	28(2)	34(2)	17(1)	4(1)	4(1)
F(51')	49(2)	52(2)	83(3)	36(2)	44(2)	20(2)

F(52')	57(3)	39(2)	141(4)	44(3)	37(3)	8(2)
F(53')	84(3)	30(2)	78(3)	0(2)	-1(2)	21(2)
F(54')	80(3)	83(3)	49(2)	26(2)	37(2)	49(2)
F(55')	57(3)	65(3)	85(3)	53(2)	42(2)	20(2)
O(1')	73(3)	19(2)	26(2)	12(2)	-16(2)	-11(2)
O(2')	42(2)	31(2)	21(2)	14(2)	-13(2)	2(2)
O(3')	13(2)	25(2)	13(2)	11(1)	5(1)	7(1)
O(4')	18(2)	16(2)	18(2)	7(1)	2(1)	9(1)
O(5')	17(2)	16(2)	19(2)	11(1)	-1(1)	-2(1)
O(6')	14(2)	21(2)	15(2)	12(1)	1(1)	3(1)
O(7')	13(2)	24(2)	16(2)	14(1)	2(1)	1(1)
O(8')	16(2)	23(2)	11(2)	10(1)	5(1)	2(1)
O(9')	22(2)	17(2)	17(2)	4(1)	4(1)	-2(1)
O(10')	17(2)	18(2)	22(2)	12(1)	3(1)	-1(1)
O(11')	21(2)	16(2)	24(2)	10(1)	8(1)	7(1)
O(12')	18(2)	23(2)	17(2)	15(1)	5(1)	6(1)
O(13')	12(2)	28(2)	16(2)	15(1)	3(1)	4(1)
N(1')	15(2)	19(2)	18(2)	10(2)	2(2)	1(2)
C(1')	31(3)	26(3)	31(3)	1(2)	-7(2)	18(2)
C(2')	28(3)	22(2)	28(3)	9(2)	2(2)	11(2)
C(3')	33(3)	30(3)	40(3)	13(2)	6(2)	4(2)
C(4')	79(5)	35(3)	65(5)	-3(3)	19(4)	-12(3)
C(5')	128(6)	39(4)	98(7)	-22(4)	56(5)	-7(4)
C(6')	93(6)	51(4)	100(6)	-2(4)	73(5)	13(3)
C(7')	39(3)	33(3)	61(4)	16(3)	25(3)	7(2)
C(8')	15(2)	20(2)	29(3)	15(2)	1(2)	-2(2)
C(9')	9(2)	19(2)	23(2)	11(2)	-1(2)	-1(2)
C(10')	14(3)	20(2)	23(2)	9(2)	1(2)	-2(2)
C(11')	16(3)	26(2)	28(2)	18(2)	-2(2)	-1(2)
C(12')	27(3)	18(2)	37(3)	15(2)	0(2)	1(2)
C(13')	22(3)	17(2)	30(2)	6(2)	2(2)	-1(2)
C(14')	18(3)	22(2)	22(2)	11(2)	-2(2)	-3(2)
C(15')	19(3)	32(3)	17(2)	16(2)	3(2)	7(2)
C(16')	18(2)	26(2)	17(2)	16(2)	2(2)	1(2)
C(17')	22(3)	28(2)	29(3)	15(2)	7(2)	2(2)
C(18')	35(3)	32(3)	51(4)	30(3)	16(2)	13(2)

C(19')	27(3)	52(3)	60(4)	44(3)	4(2)	11(2)
C(20')	23(3)	53(3)	56(4)	39(3)	-7(2)	-1(2)
C(21')	27(3)	28(3)	28(3)	20(2)	-3(2)	-2(2)
C(22')	26(3)	23(2)	21(2)	8(2)	8(2)	0(2)
C(23')	44(4)	35(3)	21(2)	14(2)	9(2)	4(2)
C(24')	39(3)	41(3)	19(2)	6(2)	13(2)	3(2)
C(25')	47(4)	30(3)	30(3)	2(2)	14(2)	1(2)
C(26')	36(3)	24(2)	32(3)	11(2)	14(2)	2(2)
C(27')	20(3)	25(2)	19(2)	7(2)	10(2)	1(2)
C(28')	44(3)	29(3)	15(2)	1(2)	4(2)	-6(2)
C(29')	40(3)	35(3)	21(3)	7(2)	7(2)	-6(2)
C(30')	45(3)	30(3)	24(3)	3(2)	5(2)	3(2)
C(31')	34(3)	32(3)	45(4)	6(2)	-1(2)	-2(2)
C(32')	33(3)	28(3)	44(4)	2(2)	-2(2)	-3(2)
C(33')	40(3)	31(3)	45(4)	9(2)	5(3)	1(2)
C(34')	36(3)	35(3)	34(3)	8(2)	-1(2)	-2(2)
C(35')	19(3)	33(3)	18(2)	9(2)	10(2)	5(2)
C(36')	14(2)	21(3)	18(2)	10(2)	-1(2)	1(2)
C(37')	13(2)	22(2)	20(2)	14(2)	2(2)	6(2)
C(38')	20(2)	23(2)	31(3)	10(2)	5(2)	4(2)
C(39')	23(3)	22(2)	44(3)	17(2)	-1(2)	-3(2)
C(40')	14(2)	33(3)	39(3)	24(2)	5(2)	1(2)
C(41')	13(2)	35(3)	23(2)	22(2)	4(2)	8(2)
C(42')	15(2)	20(2)	18(2)	14(2)	3(2)	6(2)
C(43')	16(3)	20(2)	38(3)	11(2)	8(2)	-1(2)
C(44')	13(2)	22(2)	31(2)	12(2)	10(2)	-1(2)
C(45')	26(3)	28(2)	25(2)	11(2)	0(2)	2(2)
C(46')	31(3)	20(2)	31(3)	4(2)	2(2)	1(2)
C(47')	37(3)	19(2)	38(3)	10(2)	2(2)	2(2)
C(48')	44(3)	23(2)	30(3)	14(2)	2(2)	2(2)
C(49')	36(3)	19(2)	24(2)	8(2)	5(2)	-3(2)
C(50')	18(3)	37(3)	17(2)	16(2)	10(2)	10(2)
C(51')	18(3)	30(2)	19(2)	12(2)	9(2)	12(2)
C(52')	12(2)	31(2)	21(2)	13(2)	5(2)	9(2)
C(53')	18(3)	41(3)	20(2)	19(2)	2(2)	7(2)
C(54')	33(3)	48(3)	20(2)	11(2)	11(2)	11(2)

C(55')	48(4)	34(3)	27(3)	6(2)	11(2)	12(3)
C(56')	40(3)	31(3)	29(3)	14(2)	15(2)	16(2)
C(57')	20(3)	29(3)	22(3)	20(2)	6(2)	6(2)
C(58')	25(2)	24(2)	19(2)	16(2)	11(2)	9(2)
C(59')	31(3)	21(2)	25(3)	13(2)	3(2)	2(2)
C(60')	44(3)	29(3)	34(3)	25(2)	14(2)	15(2)
C(61')	28(3)	35(3)	26(3)	21(2)	10(2)	16(2)
C(62')	23(3)	37(3)	22(3)	18(2)	9(2)	9(2)
C(63')	19(2)	26(2)	17(2)	13(2)	10(2)	11(2)
C(64')	16(2)	34(3)	25(3)	19(2)	1(2)	6(2)
C(65')	14(2)	25(2)	28(2)	18(2)	2(2)	3(2)
C(66')	21(2)	18(2)	26(2)	15(2)	2(2)	5(2)
C(67')	16(2)	32(3)	35(3)	26(2)	6(2)	9(2)
C(68')	17(3)	31(3)	47(3)	29(2)	0(2)	-1(2)
C(69')	20(3)	27(3)	50(3)	21(2)	-6(2)	1(2)
C(70')	23(3)	24(2)	35(3)	13(2)	-1(2)	7(2)
C(71')	26(3)	30(3)	46(3)	15(2)	4(2)	9(2)
C(72')	26(3)	27(2)	26(3)	13(2)	3(2)	9(2)
C(73')	34(3)	42(3)	36(3)	26(2)	13(2)	14(2)
C(74')	47(4)	49(3)	30(3)	13(2)	12(3)	28(3)
C(75')	46(4)	27(3)	48(3)	5(2)	0(3)	13(2)
C(76')	38(3)	33(3)	66(4)	23(3)	7(3)	7(2)
C(77')	26(3)	32(3)	47(3)	19(2)	12(2)	8(2)
B(1')	15(2)	16(2)	12(2)	6(2)	3(2)	2(2)
B(2')	14(2)	14(2)	14(2)	7(2)	4(2)	2(2)
B(3')	14(2)	17(2)	11(2)	7(2)	4(2)	2(2)
B(4')	14(2)	15(2)	14(2)	9(2)	2(2)	3(2)
B(5')	16(2)	18(2)	15(2)	10(2)	3(2)	4(2)
B(6')	12(2)	16(2)	13(2)	9(2)	2(2)	1(2)
B(7')	16(2)	18(2)	16(2)	9(2)	5(2)	4(2)
B(8')	15(2)	16(2)	17(2)	12(2)	5(2)	4(2)
B(9')	12(2)	20(2)	16(2)	10(2)	4(2)	5(2)
B(10')	13(2)	19(2)	17(2)	10(2)	4(2)	1(2)
B(11')	15(2)	17(2)	14(2)	9(2)	0(2)	3(2)
B(12')	14(2)	16(2)	18(2)	12(2)	3(2)	4(2)
N(2)	36(3)	24(2)	20(2)	3(2)	-2(2)	-5(2)

C(78)	43(3)	37(3)	36(3)	15(3)	0(3)	1(2)
C(79)	37(3)	44(3)	39(4)	19(3)	5(3)	4(3)
C(80)	65(5)	51(4)	90(6)	40(4)	21(4)	20(4)
C(81)	74(5)	73(6)	127(8)	62(6)	46(5)	38(5)
C(82)	37(3)	28(3)	20(3)	2(2)	-1(2)	3(2)
C(83)	35(3)	42(3)	27(3)	14(3)	2(2)	3(3)
C(84)	58(4)	37(3)	29(3)	14(3)	9(3)	16(3)
C(85)	68(5)	66(5)	49(4)	28(4)	21(4)	6(4)
C(86)	42(3)	32(3)	34(3)	6(3)	-9(2)	-10(2)
C(87)	37(3)	42(4)	52(4)	18(3)	0(3)	-4(3)
C(88)	41(4)	53(4)	83(5)	30(4)	7(3)	-5(3)
C(89)	46(5)	99(7)	92(6)	43(5)	14(4)	2(4)
C(90)	33(3)	31(3)	23(3)	8(2)	0(2)	-5(2)
C(91)	39(3)	35(3)	38(3)	10(2)	3(3)	-2(2)
C(92)	41(4)	42(3)	36(3)	9(3)	9(3)	-4(3)
C(93)	49(4)	42(4)	56(5)	-1(3)	-3(3)	-3(3)
N(3)	29(2)	25(2)	44(3)	-1(2)	1(2)	0(2)
C(94)	67(4)	29(3)	38(3)	1(3)	-13(3)	14(3)
C(95)	82(5)	37(4)	31(3)	16(3)	5(3)	16(3)
C(96)	197(9)	54(5)	35(4)	24(4)	31(5)	54(5)
C(97)	212(11)	68(6)	70(6)	41(5)	64(7)	50(6)
C(98)	29(3)	29(3)	49(4)	6(3)	-1(3)	-3(2)
C(99)	30(3)	29(3)	28(3)	9(2)	3(2)	-3(2)
C(100)	42(3)	30(3)	37(3)	12(3)	2(3)	-1(2)
C(101)	51(4)	35(3)	43(4)	12(3)	8(3)	8(3)
C(102)	44(3)	38(3)	28(3)	4(2)	9(2)	-15(2)
C(103)	66(5)	35(3)	50(4)	-2(3)	25(3)	-11(3)
C(104)	105(6)	46(4)	37(4)	2(3)	9(4)	-32(4)
C(105)	134(8)	41(4)	55(5)	-9(3)	26(5)	-36(4)
C(106)	32(4)	21(6)	31(5)	4(5)	-12(4)	0(4)
C(107)	33(5)	36(5)	45(5)	15(4)	-5(4)	-3(4)
C(108)	46(9)	45(8)	79(10)	17(7)	-15(8)	-5(7)
C(109)	33(5)	36(5)	45(5)	15(4)	-5(4)	-3(4)
C(110)	24(4)	29(6)	34(6)	6(5)	-3(4)	2(4)
C(111)	23(4)	31(4)	33(4)	6(3)	-2(3)	-1(3)
C(112)	23(5)	34(7)	35(7)	-10(5)	-4(5)	-4(5)

C(113)	23(4)	31(4)	33(4)	6(3)	-2(3)	-1(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[2b]^{1-}$.

	x	y	z	U(eq)
H(1A)	8504	5731	9217	44
H(1B)	9482	6068	9160	44
H(8A)	5458	5755	9199	20
H(8B)	5438	5953	9780	20
H(15A)	7937	6264	10323	28
H(15B)	8400	6843	10683	28
H(28A)	7796	8042	10865	39
H(28B)	8174	8576	10770	39
H(35A)	5510	6898	10488	27
H(35B)	5744	7518	10575	27
H(36A)	10439	7008	9688	20
H(36B)	10168	7562	10042	20
H(43A)	9614	8405	9404	29
H(43B)	9172	8547	9923	29
H(50A)	9334	6867	8418	30
H(50B)	9364	7491	8538	30
H(57A)	6528	7429	8231	22
H(57B)	6990	8004	8603	22
H(64A)	4639	6689	8909	19
H(64B)	4456	7268	9251	19
H(71A)	5118	8042	10069	29
H(71B)	5564	8117	9600	29
H(1'A)	8935	911	4262	37
H(1'B)	9666	1182	3981	37
H(8'A)	5485	687	4154	24
H(8'B)	5387	914	4731	24
H(15C)	7883	1328	5317	24
H(15D)	8390	1905	5663	24

H(28C)	8371	2914	5890	39
H(28D)	7560	3184	5711	39
H(35C)	5383	1911	5407	28
H(35D)	5617	2523	5467	28
H(36C)	10316	2054	4652	21
H(36D)	10077	2637	4947	21
H(43C)	9379	3328	4175	30
H(43D)	9075	3508	4725	30
H(50C)	9119	1701	3313	26
H(50D)	9252	2315	3374	26
H(57C)	6344	2298	3107	24
H(57D)	6798	2881	3465	24
H(64C)	4548	1580	3823	27
H(64D)	4362	2168	4140	27
H(71C)	4945	2999	4881	39
H(71D)	5504	3126	4460	39
H(78A)	4290	181	2063	46
H(78B)	4547	428	2635	46
H(79A)	2961	297	2781	47
H(79B)	2666	-16	2214	47
H(80A)	3503	1062	2591	76
H(80B)	3084	743	2043	76
H(81A)	1548	723	2285	121
H(81B)	2075	1321	2463	121
H(81C)	1950	1018	2840	121
H(82A)	4596	-660	2918	36
H(82B)	4299	-82	3118	36
H(83A)	2999	-1030	2686	42
H(83B)	2685	-451	2866	42
H(84A)	3666	-839	3512	48
H(84B)	3216	-299	3674	48
H(85A)	2168	-1334	3335	88
H(85B)	1666	-819	3413	88
H(85C)	2181	-900	3867	88
H(86A)	5762	-63	2634	47
H(86B)	5604	-693	2391	47

H(87A)	5705	1	1861	53
H(87B)	5546	-631	1617	53
H(88A)	7089	-632	2015	70
H(88B)	7252	1	2194	70
H(89A)	7194	-714	1197	116
H(89B)	8062	-265	1483	116
H(89C)	7096	-105	1314	116
H(90A)	3910	-742	1656	36
H(90B)	3115	-836	2000	36
H(91A)	4082	-1436	2173	46
H(91B)	4699	-1393	1737	46
H(92A)	2698	-1801	1641	50
H(92B)	3232	-1699	1204	50
H(93A)	3092	-2601	1140	82
H(93B)	3762	-2424	1633	82
H(93C)	4184	-2348	1160	82
H(94A)	4472	4423	7841	57
H(94B)	4243	5010	8101	57
H(95A)	2865	4102	7678	58
H(95B)	2598	4690	7896	58
H(96A)	3625	4237	8463	107
H(96B)	3231	4792	8669	107
H(97A)	1657	4254	8386	163
H(97B)	2169	4284	8888	163
H(97C)	2205	3781	8406	163
H(98A)	4438	5586	7691	46
H(98B)	4139	5404	7125	46
H(99A)	2817	5441	7843	36
H(99B)	2515	5256	7273	36
H(10A)	3188	6104	7281	44
H(10B)	3463	6287	7853	44
H(10C)	1552	6030	7415	65
H(10D)	2068	6615	7723	65
H(10E)	1814	6197	7986	65
H(10F)	3524	4497	6668	48
H(10G)	2823	4389	7048	48

H(10H)	4295	3789	6629	67
H(10I)	3770	3715	7080	67
H(10J)	2759	3564	6177	84
H(10K)	2303	3435	6621	84
H(10L)	2585	2636	6042	131
H(10M)	3322	2760	6504	131
H(10N)	3678	2870	6033	131
H(10O)	5560	5020	7705	36
H(10P)	5339	4391	7428	36
H(10Q)	5376	4509	6661	47
H(10R)	5566	5138	6931	47
H(10S)	7146	5596	7321	90
H(10T)	7989	5271	7368	90
H(10U)	7100	5286	7694	90
H(10V)	7004	4760	6658	47
H(10W)	6892	4463	7041	47
H(11A)	5273	4367	7041	37
H(11B)	5023	4775	6791	37
H(11C)	5956	5120	7737	37
H(11D)	5842	5476	7410	37
H(11E)	7006	4636	7205	45
H(11F)	6813	4919	6823	45
H(11G)	8298	5319	7303	47
H(11H)	7730	5477	7784	47
H(11I)	7572	5744	7388	47

Table 6. Crystal data and structure refinement for $[3]^{1-}$

Identification code	Pentafluorobenzyloxy-dodecaborane radical w TBA
Empirical formula	$C_{100}H_{60}B_{12}F_{60}NO_{12}$
Formula weight	2737.21
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	13.3889(3)
b/Å	13.8983(3)
c/Å	29.7778(7)
α/°	97.6210(10)
β/°	100.2900(10)
γ/°	93.5830(10)
Volume/Å^3	5382.7(2)
Z	2
ρ_{calc}g/cm^3	1.689
μ/mm^{-1}	1.606
F(000)	2726.0
Crystal size/mm^3	0.20 × 0.16 × 0.05
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	3.048 to 136.464
Index ranges	$-16 \leq h \leq 16$, $-16 \leq k \leq 16$, $-35 \leq l \leq 35$
Reflections collected	92226
Independent reflections	18759 [R_{int} = 0.0465, R_{sigma} = 0.0419]
Data/restraints/parameters	18759/8/1768
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.1276
Final R indexes [all data]	R_1 = 0.0712, wR_2 = 0.1357
Largest diff. peak/hole / e Å^{-3}	0.57/-0.63

Table 7. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $[3]^{1-}$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5400.6(11)	713.0(11)	9080.4(5)	23.0(4)
O2	3064.4(11)	260.6(11)	9271.1(5)	22.7(4)
O3	4455.4(12)	2118.2(10)	9876.1(6)	23.8(4)
O4	6833.6(11)	1587.9(11)	10093.6(5)	21.9(3)
O5	6875.6(11)	-709.0(11)	9602.3(5)	23.9(4)
O6	4533.3(12)	-1595.7(11)	9130.2(5)	25.1(4)
O7	6788.3(12)	1519.4(11)	4926.4(6)	24.7(4)
O8	5297.7(12)	1961.8(11)	5680.6(5)	25.7(4)
O9	4339.4(12)	1877.9(11)	4587.6(6)	27.3(4)
O10	3034.5(12)	-222.0(11)	4223.8(6)	26.0(4)
O11	5328.9(12)	124.0(11)	3993.4(6)	26.7(4)
O12	6941.9(12)	-820.7(11)	4710.1(6)	25.9(4)
B1	5249(2)	397.1(19)	9501.1(9)	20.4(6)
B2	3957(2)	166.8(19)	9592.4(9)	21.1(6)
B3	4749(2)	1171.3(18)	9935.9(9)	19.9(5)
B4	6031(2)	857.0(18)	10061.5(9)	19.6(5)
B5	6050.6(19)	-404.9(18)	9797.4(9)	19.4(5)
B6	4748(2)	-831.5(19)	9502.1(9)	20.7(6)
B7	6004(2)	805.2(19)	4956.0(9)	21.9(6)
B8	5202(2)	1074.1(19)	5384.9(10)	23.3(6)
B9	4678(2)	1061.6(19)	4791.2(9)	22.5(6)
B10	3955(2)	-112.3(19)	4555.8(10)	23.2(6)
B11	5199(2)	106.2(19)	4449.4(9)	23.3(6)
B12	6080(2)	-483.4(19)	4860.7(9)	23.7(6)
F1	5085.1(14)	2511.6(13)	8602.1(6)	58.9(5)
F2	4920.3(16)	2661.5(18)	7694.1(7)	83.6(7)
F3	6034.2(14)	1587.4(16)	7175.2(6)	66.1(6)

F4	7327.0(14)	383.2(12)	7564.6(6)	53.2(5)
F5	7505.8(13)	231.0(12)	8468.9(6)	49.0(4)
F6	1847.7(11)	-411.7(10)	8270.1(5)	38.0(4)
F7	-94.9(12)	-167.1(12)	7900.0(6)	48.6(4)
F8	-909.8(11)	1523.8(13)	8147.2(6)	50.3(4)
F9	203.0(12)	2934.1(12)	8784.9(6)	49.2(4)
F10	2098.9(11)	2656.2(10)	9194.6(5)	39.8(4)
F11	4077.6(12)	3751.2(10)	9299.2(5)	39.2(4)
F12	2770.3(13)	5132.4(12)	9373.8(6)	52.8(5)
F13	2475.7(12)	5923.5(11)	10220.7(7)	52.9(5)
F14	3510.1(14)	5327.2(12)	10990.0(6)	54.7(5)
F15	4810.5(13)	3941.4(11)	10917.5(6)	48.9(4)
F16	8142.4(11)	3292.8(10)	11132.2(5)	36.2(4)
F17	9514.4(12)	4786.7(10)	11137.9(5)	38.6(4)
F18	10601.2(11)	4788.0(10)	10450.2(6)	39.1(4)
F19	10240.8(12)	3301.1(11)	9735.3(5)	42.4(4)
F20	8808.9(12)	1839.3(10)	9704.0(5)	38.1(4)
F21	9016.2(11)	28.9(10)	9767.1(6)	40.2(4)
F22	10353.4(12)	-90.5(12)	9189.4(6)	50.5(5)
F23	10333.7(12)	-1767.0(14)	8598.8(6)	52.3(5)
F24	8995.4(12)	-3311.9(12)	8601.2(5)	46.5(4)
F25	7643.0(11)	-3179.3(10)	9171.2(5)	38.4(4)
F26	6510.4(13)	-1687.7(15)	8546.5(7)	67.1(6)
F27	7076.6(14)	-3349.4(19)	8129.6(7)	90.7(8)
F28	5684.5(19)	-4878.6(15)	7784.6(6)	84.3(7)
F29	3680.6(18)	-4682.9(14)	7793.0(8)	85.8(7)
F30	3108.3(13)	-3029.0(14)	8205.3(6)	62.3(5)
F31	8303.3(14)	2651.2(14)	5819.0(6)	61.2(5)
F32	9708.8(16)	4177.4(13)	5938.3(8)	89.5(8)
F33	10749.8(15)	4449.9(14)	5259.9(11)	108.4(10)
F34	10349.9(18)	3218(2)	4453.8(10)	109.9(10)
F35	8911.8(16)	1708.5(16)	4326.3(7)	71.5(6)
F36	4158.6(13)	2274.2(12)	6565.8(6)	53.0(5)

F37	3678.8(14)	3987.9(16)	6963.4(7)	76.1(7)
F38	4862.9(17)	5652.2(13)	6964.7(6)	71.3(6)
F39	6625.2(19)	5542.6(12)	6639.0(7)	78.8(7)
F40	7130.3(14)	3837.1(12)	6258.7(7)	62.4(5)
F41	5199.1(14)	4077.7(11)	5526.8(6)	51.3(5)
F42	3916(2)	5386.7(13)	5724.1(9)	90.6(8)
F43	2319.9(17)	5666.4(16)	5077.5(12)	118.3(12)
F44	1988.7(15)	4564.5(18)	4224.3(11)	116.6(11)
F45	3287.1(16)	3212.4(13)	4031.0(7)	71.6(6)
F46	1682.8(14)	1756.1(12)	3948.4(6)	53.1(5)
F47	-224.7(15)	1719.9(17)	3467.5(7)	78.8(7)
F48	-1046.2(13)	135.5(19)	2855.4(7)	85.7(7)
F49	53.7(14)	-1426.1(15)	2717.7(6)	68.1(6)
F50	1978.4(13)	-1381.0(11)	3189.4(5)	44.3(4)
F51	5028(2)	1543(2)	3323.2(12)	50.0(8)
F52	4786(2)	1197(2)	2390.6(10)	71.0(11)
F53	5868(2)	-138(3)	1986.1(9)	66.5(10)
F54	7167(2)	-1127(2)	2506.0(11)	61.6(10)
F55	7436(2)	-786(2)	3435.8(12)	44.2(8)
F51A	5039(5)	1291(5)	2994(3)	60(2)
F52A	5408(5)	464(5)	2173(2)	64(2)
F53A	6724(6)	-918(4)	2132(2)	68(2)
F54A	7725(4)	-1465(4)	2927(2)	64(2)
F55A	7427(5)	-592(5)	3751(3)	55.5(17)
F56	7056.9(11)	-3437.4(10)	4102.5(5)	38.1(4)
F57	8264.9(13)	-3702.4(11)	3469.7(6)	48.1(4)
F58	9841.7(13)	-2385.1(13)	3481.0(6)	50.5(4)
F59	10262.7(11)	-802.8(11)	4154.8(6)	46.3(4)
F60	9102.0(11)	-560.2(10)	4802.4(6)	39.4(4)
C1	6329.6(19)	1251.8(19)	9061.8(9)	30.7(6)
C2	6295.0(19)	1363.9(18)	8563.5(9)	29.4(6)
C3	5650(2)	1982(2)	8353.8(10)	39.8(7)
C4	5558(2)	2057(2)	7893.0(11)	49.8(8)

C5	6119(2)	1520(2)	7627.4(10)	43.5(7)
C6	6778(2)	910(2)	7825.2(9)	36.4(6)
C7	6858(2)	840.5(18)	8286.7(9)	31.6(6)
C8	3114.2(17)	956.2(17)	8956.1(8)	25.2(5)
C9	2036.0(17)	1112.9(17)	8743.0(8)	24.7(5)
C10	1454.8(19)	416.9(18)	8408.9(8)	27.3(5)
C11	459(2)	540.5(19)	8214.0(9)	32.9(6)
C12	49.1(19)	1385(2)	8341.8(10)	36.0(7)
C13	601(2)	2097(2)	8668.8(9)	33.9(6)
C14	1584.9(19)	1947.2(18)	8870.0(9)	29.6(6)
C15	5140.2(18)	2964.5(16)	10054.0(9)	28.2(6)
C16	4473.0(18)	3790.7(16)	10105.7(9)	26.6(5)
C17	3934.5(19)	4116.9(17)	9721.2(9)	30.2(6)
C18	3262(2)	4816.9(19)	9755.2(10)	36.4(7)
C19	3122(2)	5225.8(18)	10184.7(11)	36.9(7)
C20	3645(2)	4929.3(19)	10571.4(10)	37.1(7)
C21	4314(2)	4218.9(18)	10528.0(10)	33.2(6)
C22	7727.7(18)	1613.2(18)	10434.5(9)	29.2(6)
C23	8435.5(17)	2492.6(16)	10421.2(8)	23.7(5)
C24	8633.3(18)	3276.2(17)	10774.1(9)	25.9(5)
C25	9334.6(19)	4049.4(17)	10782.9(9)	27.1(5)
C26	9882.1(18)	4055.0(17)	10434.0(9)	27.9(6)
C27	9701.3(19)	3304.2(18)	10074.8(9)	28.3(6)
C28	8984.5(18)	2549.7(17)	10068.1(8)	26.0(5)
C29	7500.2(17)	-1417.3(17)	9787.4(9)	25.5(5)
C30	8286.7(17)	-1560.3(17)	9485.6(9)	25.6(5)
C31	8995.9(18)	-800.9(18)	9478.9(9)	28.9(6)
C32	9679.7(19)	-854(2)	9185.0(10)	35.7(7)
C33	9666(2)	-1695(2)	8885.9(9)	36.1(7)
C34	8991(2)	-2478(2)	8886.8(9)	33.8(6)
C35	8305.5(18)	-2400.1(18)	9186.2(9)	28.7(6)
C36	4489(2)	-1413.4(18)	8665.8(8)	31.7(6)
C37	4792.5(19)	-2305.6(18)	8402.5(8)	27.8(6)

C38	5794(2)	-2427(2)	8368.0(10)	40.4(7)
C39	6095(2)	-3275(3)	8156.6(10)	52.2(9)
C40	5392(3)	-4035(2)	7979.4(11)	53.3(9)
C41	4388(3)	-3941(2)	7988.2(11)	49.9(8)
C42	4107(2)	-3094(2)	8199.0(10)	38.9(7)
C43	7815.4(19)	1258.5(19)	5023.5(10)	36.0(6)
C44	8548.6(18)	2141.3(17)	5070.2(9)	28.5(6)
C45	8780(2)	2800(2)	5466.5(10)	38.2(7)
C46	9498(2)	3570(2)	5534.2(13)	52.9(9)
C47	10016(3)	3706(2)	5195.0(16)	62.8(11)
C48	9825(2)	3093(3)	4789.5(15)	63.0(11)
C49	9083(2)	2310(2)	4725.3(11)	43.4(7)
C50	5869(2)	2043.3(17)	6141.0(8)	30.1(6)
C51	5657.4(19)	3000.0(18)	6398.2(8)	28.2(6)
C52	4785(2)	3071.7(19)	6584.8(9)	35.0(6)
C53	4526(2)	3950(2)	6784.6(10)	46.2(8)
C54	5133(3)	4788(2)	6791.9(10)	47.1(8)
C55	6014(3)	4733.1(19)	6622.3(10)	46.0(8)
C56	6260(2)	3842.8(19)	6426.7(10)	38.4(7)
C57	4943.8(19)	2786.8(17)	4672.3(9)	30.4(6)
C58	4266.7(19)	3576.7(17)	4771.8(10)	31.2(6)
C59	4398(2)	4157.3(19)	5198.4(11)	39.5(7)
C60	3751(3)	4843(2)	5301.4(15)	60.1(10)
C61	2956(3)	4984(3)	4985(2)	74.8(14)
C62	2769(2)	4444(3)	4554.1(18)	68.3(13)
C63	3442(2)	3745(2)	4452.4(12)	48.7(8)
C64	2994.2(19)	245.2(18)	3820.2(9)	28.7(6)
C65	1902.6(19)	194(2)	3579.3(9)	32.4(6)
C66	1303(2)	957(2)	3647.0(10)	40.9(7)
C67	314(2)	936(3)	3407.6(12)	52.9(9)
C68	-88(2)	141(3)	3099.1(12)	55.4(9)
C69	457(2)	-636(2)	3027.5(10)	47.0(8)
C70	1450(2)	-605(2)	3266.9(9)	36.2(6)

C71	6233(2)	602(2)	3908.9(10)	51.1(8)
C72	6231.4(18)	382.9(18)	3403.2(7)	27.5(6)
C73	5554(2)	885(2)	3131.4(13)	36.8(17)
C74	5440(3)	710(4)	2653.7(12)	43.6(13)
C75	6004(5)	33(5)	2447.8(8)	43(3)
C76	6681(5)	-469(5)	2719.7(16)	42(3)
C77	6795(3)	-294(3)	3197.4(15)	31.3(17)
C73A	5720(8)	655(8)	2997(4)	24(2)
C74A	5896(10)	219(10)	2571(4)	30(3)
C75A	6544(11)	-514(10)	2553(5)	24(3)
C76A	7084(8)	-749(8)	2959(4)	42(3)
C77A	6857(13)	-281(13)	3367(6)	59(5)
C78	7293.4(19)	-1741.6(18)	4791.5(9)	29.3(6)
C79	8017.5(19)	-1966.2(17)	4464.7(9)	26.8(5)
C80	7840.9(19)	-2763.4(18)	4122.4(9)	29.4(6)
C81	8446(2)	-2909.8(19)	3795.2(9)	34.5(6)
C82	9248(2)	-2240(2)	3799.9(9)	35.1(6)
C83	9460(2)	-1449(2)	4139.8(10)	35.0(6)
C84	8860.1(19)	-1326.8(18)	4468.6(9)	29.9(6)
N1	55.4(19)	5510.7(15)	7374.5(8)	40.9(6)
C85	-829(3)	4719(2)	7277.2(13)	60.1(10)
C86	-1086(7)	4549(5)	7784(3)	37(2)
C87	-2037(8)	3863(6)	7705(3)	57(2)
C86A	-1603(8)	4629(5)	7576(4)	43(2)
C87A	-1436(9)	3732(6)	7819(3)	47(2)
C88	-2202(3)	3744(2)	8185.3(13)	73.0(12)
C89	-306(2)	6499.1(19)	7528.8(10)	44.9(8)
C90	-1279(2)	6757(2)	7237.5(12)	51.8(8)
C91	-1544(2)	7765(2)	7412.2(12)	54.1(9)
C92	-2589(3)	7969(2)	7171.5(13)	62.6(10)
C93	446(2)	5522(2)	6926.1(10)	37.6(7)
C94	1372(2)	6233(2)	6948.6(10)	41.8(7)
C95	1656(3)	6202(2)	6475.0(13)	58.5(10)

C96	2548(3)	6933(3)	6472.4(17)	83.5(14)
C97	882(3)	5308(2)	7760.2(10)	53.0(9)
C98	1380(3)	4365(2)	7676.6(11)	48.1(8)
C99	1981(3)	4134(2)	8129.1(11)	56.9(9)
C100	2571(3)	3240(2)	8058.2(13)	63.1(10)

Table 8. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[3]^{1-}$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	20.9(8)	25.8(9)	23.5(9)	6.3(7)	5.3(7)	1.5(7)
O2	21.4(8)	21.9(8)	25.6(9)	9.3(6)	1.4(7)	4.8(7)
O3	25.5(9)	13.4(8)	32.5(10)	2.5(6)	4.3(7)	6.7(7)
O4	20.0(8)	20.2(8)	24.7(9)	5.1(6)	1.1(7)	1.1(7)
O5	24.1(9)	23.3(9)	27.1(10)	5.9(7)	7.7(7)	11.6(7)
O6	33.1(9)	20.6(9)	21.2(9)	-0.9(6)	6.0(7)	4.3(7)
O7	25.9(9)	22.2(9)	26.2(9)	4.2(7)	5.1(7)	2.6(7)
O8	34.6(9)	21.0(9)	20.0(9)	-0.9(6)	3.1(7)	4.1(8)
O9	32.6(9)	17.8(9)	30.9(10)	4.6(7)	3.4(8)	3.2(7)
O10	27.6(9)	27.2(9)	22.3(9)	5.6(7)	1.3(7)	0.4(7)
O11	29.2(9)	29.2(9)	22.7(9)	3.2(7)	8.4(7)	1.3(8)
O12	29.0(9)	20.0(9)	31.0(10)	3.7(7)	9.9(7)	6.8(7)
B1	24.2(14)	19.5(14)	19.2(14)	3.2(10)	7.6(11)	4.9(11)
B2	22.2(13)	17.3(14)	23.9(15)	2.3(10)	4.3(11)	3.7(11)
B3	21.0(13)	15.4(14)	23.6(15)	1.0(10)	4.5(11)	6.9(11)
B4	21.0(13)	16.1(13)	22.2(14)	2.3(10)	4.9(11)	4.2(11)
B5	21.2(13)	17.1(14)	20.3(14)	-0.5(10)	5.8(11)	5.3(11)
B6	20.6(13)	19.1(14)	22.9(15)	1.8(10)	5.2(11)	4.7(11)
B7	25.9(14)	17.7(14)	21.3(15)	0.9(10)	3.1(11)	2.8(12)
B8	26.3(14)	21.5(15)	22.6(15)	3.2(11)	5.8(12)	3.5(12)
B9	26.7(14)	18.6(14)	21.5(15)	1.9(10)	3.4(11)	2.2(12)
B10	25.1(14)	19.9(14)	24.1(15)	3.1(11)	4.2(11)	1.3(12)

B11	29.7(15)	19.6(14)	20.9(15)	-0.5(10)	7.1(12)	4.8(12)
B12	27.8(14)	20.0(14)	22.7(15)	1.0(11)	4.9(12)	2.0(12)
F1	69.9(12)	71.7(13)	54.2(12)	29.4(9)	35.8(10)	40.3(11)
F2	78.4(14)	133(2)	66.8(14)	65.8(14)	30.7(12)	60.8(14)
F3	65.7(13)	112.0(16)	27.9(10)	27.1(10)	13.9(9)	14.8(12)
F4	69.2(12)	54.4(11)	41.1(11)	0.9(8)	28.6(9)	6.8(9)
F5	57.9(11)	50.8(10)	49.2(11)	20.5(8)	23.0(9)	23.0(9)
F6	42.8(9)	29.3(8)	39.5(9)	1.8(6)	2.3(7)	7.4(7)
F7	43.3(10)	51.6(10)	41.8(10)	4.2(8)	-9.3(8)	-8.7(8)
F8	26.0(8)	74.9(12)	49.9(11)	18.6(9)	-3.3(8)	13.2(8)
F9	47.3(10)	53.2(11)	50.9(11)	9.0(8)	9.1(8)	30.5(9)
F10	42.8(9)	33.2(9)	38.6(10)	-3.0(7)	-0.8(7)	7.9(7)
F11	45.4(9)	34.4(9)	37.6(9)	4.2(7)	5.9(7)	9.4(7)
F12	50.9(10)	48.3(10)	61.1(12)	19.8(9)	-0.5(9)	25.0(9)
F13	45.8(10)	32.1(9)	88.5(14)	12.1(9)	24.3(10)	21.7(8)
F14	74.2(13)	40.6(10)	54.8(12)	-2.3(8)	29.7(10)	16.5(9)
F15	67.4(12)	41.6(10)	39.7(10)	8.2(7)	7.6(9)	21.4(9)
F16	39.8(9)	36.7(9)	36.9(9)	5.1(7)	18.2(7)	9.5(7)
F17	51.4(10)	23.8(8)	36.7(9)	-6.2(6)	6.3(7)	2.7(7)
F18	36.7(8)	27.2(8)	51.7(10)	7.2(7)	6.8(7)	-8.2(7)
F19	49.4(10)	40.0(9)	44.8(10)	7.3(7)	25.9(8)	6.0(8)
F20	54.3(10)	23.1(8)	34.3(9)	-4.6(6)	9.4(7)	-0.1(7)
F21	31.4(8)	24.8(8)	64.6(12)	0.8(7)	11.9(8)	7.3(7)
F22	33.8(9)	53.1(11)	74.6(13)	31.1(9)	20.2(9)	5.5(8)
F23	39.8(9)	88.6(13)	41.9(10)	24.0(9)	24.8(8)	29.3(9)
F24	43.7(9)	58.7(11)	34.8(10)	-10.2(8)	6.0(7)	27.1(8)
F25	35.5(8)	27.0(8)	51.5(10)	-1.6(7)	9.2(7)	5.9(7)
F26	42.3(10)	88.5(14)	56.8(13)	-18.5(10)	1.5(9)	-15.4(10)
F27	44.2(11)	161(2)	57.3(14)	-23.8(13)	0.0(10)	49.9(14)
F28	139(2)	70.2(13)	42.6(12)	-12.2(10)	9.3(12)	67.2(14)
F29	116.5(19)	48.3(12)	83.5(17)	-34.1(10)	38.8(14)	-29.5(12)
F30	44.3(10)	73.5(13)	62.6(13)	-27.2(10)	25.7(9)	-12.5(9)
F31	58.0(12)	84.0(14)	40.3(11)	-4.3(9)	10.7(9)	20.8(10)

F32	75.3(14)	44.1(11)	116(2)	-30.4(11)	-44.5(13)	19.7(11)
F33	51.6(13)	56.3(13)	205(3)	60.3(15)	-28.5(15)	-25.5(11)
F34	70.4(15)	157(2)	128(2)	85.9(19)	45.6(16)	-6.2(15)
F35	75.2(14)	99.8(16)	40.9(12)	3.5(10)	20.4(10)	5.9(12)
F36	46.8(10)	54.4(11)	53.3(12)	-9.6(8)	16.9(9)	-14.0(9)
F37	47.4(11)	106.7(17)	67.4(14)	-29.6(12)	19.3(10)	20.8(11)
F38	116.6(17)	46.3(11)	47.2(12)	-9.6(8)	3.5(11)	47.3(12)
F39	131(2)	27.2(10)	76.9(15)	-4.1(9)	32.5(14)	-17.7(11)
F40	64.9(12)	49.1(11)	75.1(14)	-11.2(9)	39.3(11)	-12.9(9)
F41	78.0(13)	29.3(9)	42.7(11)	4.1(7)	3.3(9)	0.4(9)
F42	155(2)	27.1(10)	115(2)	3.4(10)	96.3(18)	10.6(12)
F43	87.0(17)	56.3(14)	259(4)	73.8(18)	107(2)	49.0(13)
F44	37.2(11)	110.2(19)	216(3)	120(2)	-11.6(15)	7.9(12)
F45	79.5(14)	59.0(12)	65.1(14)	34.7(10)	-27.4(11)	-16.7(11)
F46	60.3(12)	46.3(11)	56.0(12)	7.4(8)	15.6(9)	18.3(9)
F47	61.5(13)	116.2(18)	77.1(15)	42.9(13)	24.8(11)	56.0(13)
F48	27.9(10)	165(2)	66.8(15)	48.5(15)	-7.2(9)	6.9(12)
F49	60.0(12)	96.6(15)	36.6(11)	11.4(10)	-7.2(9)	-34.9(11)
F50	53.9(10)	40.8(9)	35.2(10)	2.9(7)	4.9(8)	-3.7(8)
F51	54.0(17)	47.1(17)	60(2)	22.1(15)	21.8(16)	25.1(14)
F52	64.5(19)	108(3)	53(2)	55.5(18)	6.6(15)	23.7(18)
F53	71(2)	104(3)	23.1(16)	4.9(15)	13.5(14)	-9.5(19)
F54	70(2)	58.3(19)	57(2)	-20.6(16)	34.6(18)	0.5(17)
F55	41.1(16)	43.6(17)	52(2)	13.3(14)	11.5(15)	15.1(13)
F51A	57(4)	54(4)	76(6)	25(4)	16(4)	29(3)
F52A	84(5)	75(5)	29(4)	30(3)	-15(3)	1(4)
F53A	112(6)	67(4)	32(4)	-6(3)	43(4)	-8(4)
F54A	53(4)	60(4)	94(5)	20(3)	38(4)	28(3)
F55A	55(4)	66(4)	45(4)	24(3)	-4(3)	11(3)
F56	40.8(9)	28.0(8)	44.3(10)	0.2(6)	8.9(7)	1.7(7)
F57	53.7(10)	44.5(10)	42.7(10)	-12.2(7)	10.5(8)	13.2(8)
F58	49.3(10)	66.1(12)	46.4(11)	13.3(8)	26.7(8)	22.7(9)
F59	31.9(9)	46.9(10)	66.1(12)	19.0(8)	16.8(8)	5.7(8)

F60	33.8(8)	31.3(8)	50.0(10)	-3.2(7)	6.2(7)	2.8(7)
C1	29.1(13)	36.0(15)	27.4(15)	7.8(11)	6.5(11)	-2.7(12)
C2	26.2(13)	35.9(15)	26.1(14)	6.5(11)	5.6(11)	-3.8(12)
C3	40.0(16)	51.3(19)	36.0(17)	16.8(13)	17.9(13)	13.0(14)
C4	49.1(18)	69(2)	42.1(19)	30.1(16)	14.4(15)	22.4(17)
C5	46.5(17)	63(2)	22.7(15)	13.8(13)	7.8(13)	-0.2(16)
C6	40.7(16)	40.3(16)	29.6(16)	1.6(12)	14.0(13)	0.6(13)
C7	32.0(14)	32.2(15)	31.1(15)	7.6(11)	5.0(12)	1.5(12)
C8	22.9(12)	26.5(13)	28.3(14)	11.9(10)	4.1(10)	4.8(11)
C9	23.2(12)	28.3(14)	24.5(13)	11.2(10)	3.5(10)	5.6(11)
C10	31.5(13)	27.3(14)	24.9(14)	7.7(10)	5.8(11)	7.4(12)
C11	33.9(14)	36.0(15)	25.7(15)	6.2(11)	-1.5(11)	-4.0(13)
C12	22.3(13)	53.7(19)	35.0(16)	17.7(13)	2.9(12)	10.5(13)
C13	34.8(15)	36.5(16)	34.9(16)	9.1(12)	10.7(12)	18.0(13)
C14	30.9(14)	31.4(15)	28.0(15)	8.2(11)	5.4(11)	7.8(12)
C15	28.1(13)	14.3(13)	41.6(16)	2.3(10)	5.6(11)	4.8(11)
C16	27.4(13)	15.1(12)	37.3(16)	4.0(10)	5.8(11)	2.4(10)
C17	30.3(14)	15.7(13)	44.4(17)	1.4(11)	7.8(12)	4.7(11)
C18	33.1(15)	27.5(15)	49.1(19)	11.3(12)	2.9(13)	8.0(12)
C19	31.0(14)	17.4(14)	66(2)	8.4(12)	13.0(14)	14.1(12)
C20	44.6(16)	23.3(14)	46.8(18)	-0.6(12)	21.5(14)	4.3(13)
C21	38.7(15)	21.7(14)	40.9(17)	8.3(11)	7.1(13)	8.6(12)
C22	24.7(13)	24.9(13)	36.3(16)	9.0(11)	-2.8(11)	4.0(11)
C23	22.3(12)	18.3(12)	30.7(14)	5.5(10)	1.9(10)	7.0(10)
C24	24.6(12)	25.7(14)	30.0(14)	6.0(10)	8.4(11)	9.8(11)
C25	31.6(13)	17.7(13)	29.8(14)	-0.9(10)	2.3(11)	5.6(11)
C26	25.1(13)	19.2(13)	39.8(16)	7.6(10)	5.4(11)	0.5(11)
C27	30.0(13)	26.9(14)	31.1(15)	6.7(10)	11.0(11)	5.3(11)
C28	30.0(13)	19.6(13)	27.5(14)	1.4(10)	2.7(11)	6.6(11)
C29	25.0(12)	23.5(13)	31.5(14)	6.7(10)	9.3(11)	12.2(11)
C30	22.4(12)	26.4(14)	31.1(15)	8.1(10)	6.9(11)	11.9(11)
C31	24.2(13)	25.5(14)	39.7(16)	6.4(11)	9.0(11)	11.0(11)
C32	26.6(14)	38.8(17)	48.2(18)	21.0(13)	10.4(13)	12.7(13)

C33	28.7(14)	55.1(19)	33.8(16)	19.3(13)	15.0(12)	21.4(14)
C34	34.3(15)	41.0(17)	27.8(15)	2.4(11)	5.9(12)	22.3(13)
C35	27.0(13)	25.8(14)	34.0(15)	4.9(11)	4.9(11)	9.4(11)
C36	47.7(16)	24.4(14)	22.2(14)	1.3(10)	4.0(12)	9.5(12)
C37	35.5(14)	28.5(14)	18.8(13)	-0.5(10)	5.8(11)	5.4(12)
C38	35.0(15)	51.9(18)	28.0(16)	-5.2(13)	-2.0(12)	0.9(14)
C39	39.3(17)	83(3)	32.1(17)	-6.9(16)	2.3(14)	31.8(18)
C40	80(3)	47(2)	33.9(18)	-7.1(14)	10.6(17)	36(2)
C41	71(2)	34.0(17)	40.9(19)	-10.9(13)	17.4(17)	-6.2(16)
C42	44.0(17)	36.9(16)	36.0(17)	-7.4(12)	18.7(13)	0.5(14)
C43	29.2(14)	27.0(15)	53.7(19)	13.1(12)	7.2(13)	4.1(12)
C44	25.9(13)	24.2(13)	35.7(15)	8.4(11)	3.2(11)	2.8(11)
C45	33.7(15)	38.1(17)	41.5(18)	5.0(13)	1.5(13)	12.3(13)
C46	42.1(18)	27.7(16)	75(3)	-2.7(15)	-21.6(17)	8.7(15)
C47	39.4(19)	39(2)	104(3)	32(2)	-15(2)	-8.6(16)
C48	37.7(18)	81(3)	83(3)	51(2)	17.3(19)	0.3(19)
C49	38.2(16)	51.7(19)	41.8(19)	14.8(14)	5.8(14)	3.6(15)
C50	37.0(15)	26.4(14)	22.8(14)	-3.1(10)	-0.2(11)	3.2(12)
C51	34.7(14)	25.5(13)	21.9(14)	-1.1(10)	1.7(11)	3.8(12)
C52	38.7(15)	33.1(15)	29.9(15)	-3.2(11)	3.6(12)	1.8(13)
C53	42.6(17)	59(2)	33.4(17)	-9.2(14)	4.8(13)	20.5(16)
C54	70(2)	35.2(17)	31.9(17)	-5.6(12)	-2.1(15)	25.6(17)
C55	74(2)	22.0(15)	39.5(18)	1.3(12)	6.2(16)	-0.1(15)
C56	48.8(17)	31.1(15)	34.1(17)	-3.0(11)	11.2(13)	0.8(14)
C57	32.9(14)	21.5(13)	38.3(16)	5.4(11)	9.5(12)	3.1(11)
C58	31.9(14)	18.6(13)	46.1(17)	11.7(11)	9.2(12)	4.7(11)
C59	47.8(17)	19.7(14)	59(2)	12.0(13)	25.3(16)	7.3(13)
C60	79(3)	27.1(18)	93(3)	18.7(17)	56(2)	10.3(18)
C61	56(2)	37(2)	154(5)	39(3)	55(3)	20(2)
C62	28.2(17)	52(2)	135(4)	66(2)	3(2)	8.4(17)
C63	38.4(17)	41.1(18)	66(2)	25.3(16)	-3.2(16)	-3.6(15)
C64	30.8(14)	30.3(14)	25.4(14)	8.7(10)	2.8(11)	3.6(11)
C65	31.7(14)	41.8(16)	26.3(15)	13.2(11)	6.8(12)	3.8(13)

C66	41.4(17)	50.3(19)	36.1(17)	16.8(14)	10.4(14)	12.7(15)
C67	43.6(18)	77(3)	48(2)	27.7(18)	14.7(16)	26.1(19)
C68	28.6(16)	95(3)	47(2)	30.1(19)	2.2(15)	9.1(18)
C69	43.3(17)	66(2)	27.4(16)	13.8(14)	-1.3(13)	-16.2(16)
C70	38.0(15)	44.8(17)	27.7(15)	8.9(12)	9.2(12)	2.2(14)
C71	59(2)	58(2)	33.9(18)	-6.4(14)	22.1(15)	-27.1(16)
C72	28.9(13)	27.8(14)	26.1(14)	5.2(10)	6.7(11)	-1.4(12)
C73	40(3)	41(4)	34(3)	7(3)	15(3)	6(3)
C74	37(3)	61(4)	38(3)	27(3)	6(3)	6(3)
C75	50(4)	59(5)	18(4)	-3(3)	13(3)	-11(4)
C76	39(4)	62(4)	20(5)	-12(4)	7(4)	-11(3)
C77	37(3)	26(3)	34(5)	-3(3)	21(3)	0(2)
C73A	30(5)	19(5)	29(7)	13(4)	13(5)	10(4)
C74A	34(7)	48(8)	9(5)	12(5)	-3(5)	5(6)
C75A	34(6)	22(6)	14(8)	-4(4)	3(5)	1(5)
C76A	44(6)	57(7)	22(6)	12(5)	-1(5)	-1(5)
C77A	58(9)	80(11)	39(10)	-6(7)	27(7)	-24(8)
C78	35.2(14)	24.8(14)	31.1(15)	7.6(10)	10.0(12)	9.2(12)
C79	29.1(13)	24.8(13)	28.4(14)	7.1(10)	5.7(11)	9.3(11)
C80	31.2(14)	23.8(14)	34.0(15)	5.0(11)	5.9(11)	7.5(12)
C81	41.7(16)	33.2(15)	28.7(15)	0.4(11)	5.8(12)	15.2(13)
C82	34.2(15)	43.4(17)	34.3(16)	12.0(12)	14.5(12)	17.1(13)
C83	29.1(14)	33.5(16)	46.0(18)	15.0(12)	8.0(13)	8.8(12)
C84	30.2(14)	24.1(14)	34.7(15)	1.8(11)	3.8(11)	10.3(12)
N1	57.2(16)	26.4(12)	40.7(15)	-6.1(10)	23.5(12)	-0.1(11)
C85	66(2)	28.8(17)	91(3)	-13.1(16)	50(2)	-5.0(16)
C86	30(4)	38(4)	43(4)	3(3)	11(3)	6(3)
C87	49(5)	50(5)	70(5)	-3(4)	22(4)	-12(4)
C86A	34(5)	39(4)	60(6)	7(4)	20(4)	13(3)
C87A	59(6)	34(4)	54(5)	8(3)	23(5)	10(5)
C88	105(3)	46(2)	77(3)	6.0(18)	50(3)	-10(2)
C89	67(2)	27.1(15)	43.2(19)	-7.3(12)	27.2(16)	1.1(15)
C90	55(2)	35.7(17)	65(2)	-7.6(15)	23.6(17)	3.7(16)

C91	59(2)	33.3(17)	68(2)	-10.9(15)	21.8(18)	0.7(16)
C92	69(2)	35.5(19)	85(3)	0.3(17)	25(2)	8.6(17)
C93	45.4(16)	36.7(16)	31.7(16)	-3.2(12)	14.6(13)	6.2(13)
C94	41.8(17)	38.4(17)	47.6(19)	7.2(13)	13.6(14)	5.5(14)
C95	74(2)	43.8(19)	72(3)	16.0(16)	43(2)	12.6(18)
C96	89(3)	58(2)	130(4)	35(2)	72(3)	17(2)
C97	90(3)	37.7(18)	33.5(18)	3.7(13)	17.3(17)	12.5(18)
C98	68(2)	34.7(17)	44.9(19)	-0.6(13)	23.9(17)	7.7(16)
C99	87(3)	44.7(19)	46(2)	10.3(15)	27.0(19)	16.6(19)
C100	85(3)	51(2)	66(3)	16.4(17)	35(2)	23(2)

Table 9. Bond Lengths for $[3]^{1-}$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	B1	1.424(3)	F51A	C73A	1.309(11)
O1	C1	1.425(3)	F52A	C74A	1.341(11)
O2	B2	1.416(3)	F53A	C75A	1.373(13)
O2	C8	1.440(3)	F54A	C76A	1.359(12)
O3	B3	1.421(3)	F55A	C77A	1.394(18)
O3	C15	1.425(3)	F56	C80	1.350(3)
O4	B4	1.413(3)	F57	C81	1.346(3)
O4	C22	1.420(3)	F58	C82	1.347(3)
O5	B5	1.399(3)	F59	C83	1.347(3)
O5	C29	1.433(3)	F60	C84	1.337(3)
O6	B6	1.405(3)	C1	C2	1.505(3)
O6	C36	1.430(3)	C2	C7	1.381(3)
O7	B7	1.422(3)	C2	C3	1.384(4)
O7	C43	1.433(3)	C3	C4	1.374(4)
O8	B8	1.402(3)	C4	C5	1.368(4)
O8	C50	1.432(3)	C5	C6	1.373(4)
O9	B9	1.417(3)	C6	C7	1.376(4)
O9	C57	1.424(3)	C8	C9	1.511(3)
O10	B10	1.422(3)	C9	C10	1.380(3)

O10	C64	1.434(3)	C9	C14	1.380(3)
O11	B11	1.403(3)	C10	C11	1.386(3)
O11	C71	1.422(3)	C11	C12	1.364(4)
O12	B12	1.396(3)	C12	C13	1.367(4)
O12	C78	1.427(3)	C13	C14	1.387(3)
B1	B6	1.796(4)	C15	C16	1.507(3)
B1	B5	1.802(4)	C16	C21	1.376(4)
B1	B2	1.813(4)	C16	C17	1.385(4)
B1	B4	1.817(4)	C17	C18	1.372(3)
B1	B3	1.820(4)	C18	C19	1.379(4)
B2	B3	1.780(4)	C19	C20	1.364(4)
B2	B5[1]	1.806(4)	C20	C21	1.383(4)
B2	B6	1.817(3)	C22	C23	1.508(3)
B2	B4[1]	1.864(4)	C23	C24	1.386(3)
B3	B4	1.785(4)	C23	C28	1.394(3)
B3	B5[1]	1.816(4)	C24	C25	1.376(3)
B3	B6[1]	1.823(4)	C25	C26	1.375(3)
B4	B6[1]	1.808(4)	C26	C27	1.368(3)
B4	B5	1.828(4)	C27	C28	1.372(3)
B4	B2[1]	1.864(4)	C29	C30	1.508(3)
B5	B2[1]	1.806(4)	C30	C35	1.376(3)
B5	B3[1]	1.816(4)	C30	C31	1.380(3)
B5	B6	1.831(4)	C31	C32	1.374(3)
B6	B4[1]	1.808(4)	C32	C33	1.369(4)
B6	B3[1]	1.823(4)	C33	C34	1.371(4)
B7	B12	1.788(4)	C34	C35	1.389(3)
B7	B11	1.811(4)	C36	C37	1.495(3)
B7	B9	1.825(4)	C37	C38	1.382(4)
B7	B8	1.827(4)	C37	C42	1.382(4)
B7	B10[2]	1.842(4)	C38	C39	1.379(4)
B8	B9	1.779(4)	C39	C40	1.353(5)
B8	B10[2]	1.809(4)	C40	C41	1.363(5)
B8	B12[2]	1.836(4)	C41	C42	1.365(4)

B8	B11[2]	1.850(4)	C43	C44	1.498(3)
B9	B12[2]	1.802(4)	C44	C45	1.369(4)
B9	B11	1.815(4)	C44	C49	1.388(4)
B9	B10	1.830(4)	C45	C46	1.362(4)
B10	B11	1.765(4)	C46	C47	1.350(5)
B10	B8[2]	1.809(4)	C47	C48	1.356(5)
B10	B12[2]	1.833(4)	C48	C49	1.396(5)
B10	B7[2]	1.842(4)	C50	C51	1.513(3)
B11	B8[2]	1.850(4)	C51	C56	1.364(4)
B11	B12	1.853(4)	C51	C52	1.383(3)
B12	B9[2]	1.802(4)	C52	C53	1.379(4)
B12	B10[2]	1.833(4)	C53	C54	1.373(5)
B12	B8[2]	1.836(4)	C54	C55	1.366(4)
F1	C3	1.336(3)	C55	C56	1.381(4)
F2	C4	1.352(3)	C57	C58	1.500(3)
F3	C5	1.347(3)	C58	C63	1.376(4)
F4	C6	1.341(3)	C58	C59	1.388(4)
F5	C7	1.346(3)	C59	C60	1.368(4)
F6	C10	1.342(3)	C60	C61	1.332(6)
F7	C11	1.345(3)	C61	C62	1.372(6)
F8	C12	1.348(3)	C62	C63	1.406(5)
F9	C13	1.339(3)	C64	C65	1.502(3)
F10	C14	1.343(3)	C65	C70	1.381(4)
F11	C17	1.343(3)	C65	C66	1.384(4)
F12	C18	1.348(3)	C66	C67	1.383(4)
F13	C19	1.345(3)	C67	C68	1.354(5)
F14	C20	1.342(3)	C68	C69	1.355(4)
F15	C21	1.346(3)	C69	C70	1.386(4)
F16	C24	1.348(3)	C71	C72	1.496(3)
F17	C25	1.348(3)	C72	C77A	1.292(17)
F18	C26	1.347(3)	C72	C73A	1.390(10)
F19	C27	1.343(3)	C72	C73	1.3900
F20	C28	1.342(3)	C72	C77	1.3900

F21	C31	1.339(3)	C73	C74	1.3900
F22	C32	1.346(3)	C74	C75	1.3900
F23	C33	1.342(3)	C75	C76	1.3900
F24	C34	1.345(3)	C76	C77	1.3900
F25	C35	1.347(3)	C73A	C74A	1.400(13)
F26	C38	1.344(3)	C74A	C75A	1.380(13)
F27	C39	1.341(3)	C75A	C76A	1.384(12)
F28	C40	1.350(3)	C76A	C77A	1.392(13)
F29	C41	1.349(4)	C78	C79	1.509(3)
F30	C42	1.349(3)	C79	C80	1.380(3)
F31	C45	1.354(3)	C79	C84	1.389(3)
F32	C46	1.349(4)	C80	C81	1.377(3)
F33	C47	1.351(4)	C81	C82	1.374(4)
F34	C48	1.343(4)	C82	C83	1.370(4)
F35	C49	1.334(3)	C83	C84	1.374(4)
F36	C52	1.337(3)	N1	C97	1.515(4)
F37	C53	1.337(3)	N1	C93	1.520(3)
F38	C54	1.340(3)	N1	C85	1.526(4)
F39	C55	1.339(3)	N1	C89	1.526(3)
F40	C56	1.348(3)	C85	C86A	1.491(7)
F41	C59	1.337(3)	C85	C86	1.648(7)
F42	C60	1.354(4)	C86	C87	1.506(12)
F43	C61	1.347(4)	C87	C88	1.515(8)
F44	C62	1.335(4)	C86A	C87A	1.531(14)
F45	C63	1.344(4)	C87A	C88	1.625(9)
F46	C66	1.342(3)	C89	C90	1.522(4)
F47	C67	1.354(3)	C90	C91	1.514(4)
F48	C68	1.355(3)	C91	C92	1.516(5)
F49	C69	1.353(4)	C93	C94	1.522(4)
F50	C70	1.344(3)	C94	C95	1.521(4)
F51	C73	1.320(4)	C95	C96	1.520(5)
F52	C74	1.344(4)	C97	C98	1.519(4)
F53	C75	1.341(3)	C98	C99	1.524(4)

F54	C76	1.316(4)		C99	C100	1.525(4)	
F55	C77	1.301(4)					

[1]1-X,-Y,2-Z; [2]1-X,-Y,1-Z

Table 10. Bond Angles for [3]$^{1-}$

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
B1	O1	C1	120.02(19)	O3	C15	C16	105.33(19)
B2	O2	C8	118.25(18)	C21	C16	C17	116.5(2)
B3	O3	C15	121.17(18)	C21	C16	C15	122.6(2)
B4	O4	C22	119.50(18)	C17	C16	C15	120.8(2)
B5	O5	C29	121.33(18)	F11	C17	C18	118.2(2)
B6	O6	C36	121.16(18)	F11	C17	C16	119.6(2)
B7	O7	C43	116.92(18)	C18	C17	C16	122.2(3)
B8	O8	C50	119.73(18)	F12	C18	C17	120.5(3)
B9	O9	C57	121.76(19)	F12	C18	C19	119.9(2)
B10	O10	C64	119.10(19)	C17	C18	C19	119.5(3)
B11	O11	C71	119.5(2)	F13	C19	C20	120.2(3)
B12	O12	C78	122.41(19)	F13	C19	C18	119.8(3)
O1	B1	B6	120.13(19)	C20	C19	C18	120.0(2)
O1	B1	B5	123.59(18)	F14	C20	C19	120.1(2)
B6	B1	B5	61.19(14)	F14	C20	C21	120.5(3)
O1	B1	B2	118.9(2)	C19	C20	C21	119.4(3)
B6	B1	B2	60.47(14)	F15	C21	C16	119.9(2)
B5	B1	B2	108.95(18)	F15	C21	C20	117.7(2)
O1	B1	B4	124.1(2)	C16	C21	C20	122.4(3)
B6	B1	B4	109.22(18)	O4	C22	C23	109.53(19)
B5	B1	B4	60.70(14)	C24	C23	C28	115.2(2)
B2	B1	B4	106.95(17)	C24	C23	C22	122.2(2)
O1	B1	B3	122.02(19)	C28	C23	C22	122.5(2)
B6	B1	B3	107.13(17)	F16	C24	C25	117.3(2)
B5	B1	B3	107.23(17)	F16	C24	C23	119.9(2)
B2	B1	B3	58.68(14)	C25	C24	C23	122.8(2)

B4	B1	B3	58.79(14)	F17	C25	C26	119.6(2)
O2	B2	B3	123.99(19)	F17	C25	C24	120.7(2)
O2	B2	B5[1]	119.54(19)	C26	C25	C24	119.7(2)
B3	B2	B5[1]	60.85(15)	F18	C26	C27	120.4(2)
O2	B2	B1	125.0(2)	F18	C26	C25	120.1(2)
B3	B2	B1	60.86(15)	C27	C26	C25	119.5(2)
B5[1]	B2	B1	109.06(18)	F19	C27	C26	119.8(2)
O2	B2	B6	121.6(2)	F19	C27	C28	120.4(2)
B3	B2	B6	107.93(18)	C26	C27	C28	119.8(2)
B5[1]	B2	B6	107.37(18)	F20	C28	C27	118.1(2)
B1	B2	B6	59.30(14)	F20	C28	C23	119.0(2)
O2	B2	B4[1]	118.8(2)	C27	C28	C23	122.9(2)
B3	B2	B4[1]	107.89(18)	O5	C29	C30	105.68(19)
B5[1]	B2	B4[1]	59.75(14)	C35	C30	C31	116.6(2)
B1	B2	B4[1]	106.66(17)	C35	C30	C29	123.5(2)
B6	B2	B4[1]	58.82(14)	C31	C30	C29	119.7(2)
O3	B3	B2	116.92(19)	F21	C31	C32	118.3(2)
O3	B3	B4	125.2(2)	F21	C31	C30	118.9(2)
B2	B3	B4	109.81(17)	C32	C31	C30	122.8(2)
O3	B3	B5[1]	117.77(18)	F22	C32	C33	120.3(2)
B2	B3	B5[1]	60.27(15)	F22	C32	C31	120.6(3)
B4	B3	B5[1]	109.16(18)	C33	C32	C31	119.1(3)
O3	B3	B1	122.7(2)	F23	C33	C32	120.1(3)
B2	B3	B1	60.46(14)	F23	C33	C34	119.6(3)
B4	B3	B1	60.52(14)	C32	C33	C34	120.3(2)
B5[1]	B3	B1	108.30(17)	F24	C34	C33	120.3(2)
O3	B3	B6[1]	123.13(19)	F24	C34	C35	120.4(3)
B2	B3	B6[1]	108.95(18)	C33	C34	C35	119.3(2)
B4	B3	B6[1]	60.13(14)	F25	C35	C30	120.6(2)
B5[1]	B3	B6[1]	60.42(14)	F25	C35	C34	117.5(2)
B1	B3	B6[1]	108.07(17)	C30	C35	C34	121.9(3)
O4	B4	B3	118.69(18)	O6	C36	C37	107.02(19)
O4	B4	B6[1]	122.4(2)	C38	C37	C42	114.8(2)

B3	B4	B6[1]	60.99(14)
O4	B4	B1	119.25(19)
B3	B4	B1	60.70(14)
B6[1]	B4	B1	108.88(18)
O4	B4	B5	123.72(19)
B3	B4	B5	107.60(18)
B6[1]	B4	B5	106.79(18)
B1	B4	B5	59.25(14)
O4	B4	B2[1]	126.2(2)
B3	B4	B2[1]	107.48(18)
B6[1]	B4	B2[1]	59.31(14)
B1	B4	B2[1]	106.28(17)
B5	B4	B2[1]	58.54(14)
O5	B5	B1	117.16(19)
O5	B5	B2[1]	125.4(2)
B1	B5	B2[1]	109.45(17)
O5	B5	B3[1]	124.90(19)
B1	B5	B3[1]	107.69(17)
B2[1]	B5	B3[1]	58.88(14)
O5	B5	B4	121.2(2)
B1	B5	B4	60.06(14)
B2[1]	B5	B4	61.71(14)
B3[1]	B5	B4	107.89(17)
O5	B5	B6	119.80(19)
B1	B5	B6	59.24(14)
B2[1]	B5	B6	107.49(17)
B3[1]	B5	B6	59.99(15)
B4	B5	B6	107.17(17)
O6	B6	B1	127.8(2)
O6	B6	B4[1]	116.5(2)
B1	B6	B4[1]	109.84(17)
O6	B6	B2	125.1(2)
B1	B6	B2	60.23(14)

C38	C37	C36	122.3(2)
C42	C37	C36	122.8(2)
F26	C38	C39	118.2(3)
F26	C38	C37	118.9(3)
C39	C38	C37	122.9(3)
F27	C39	C40	120.2(3)
F27	C39	C38	120.4(3)
C40	C39	C38	119.4(3)
F28	C40	C39	119.8(3)
F28	C40	C41	120.1(3)
C39	C40	C41	120.0(3)
F29	C41	C40	120.1(3)
F29	C41	C42	120.4(3)
C40	C41	C42	119.5(3)
F30	C42	C41	117.9(3)
F30	C42	C37	118.8(2)
C41	C42	C37	123.2(3)
O7	C43	C44	110.1(2)
C45	C44	C49	115.8(3)
C45	C44	C43	122.1(3)
C49	C44	C43	122.0(3)
F31	C45	C46	118.1(3)
F31	C45	C44	118.1(3)
C46	C45	C44	123.7(3)
F32	C46	C47	120.2(3)
F32	C46	C45	120.7(4)
C47	C46	C45	119.1(3)
C46	C47	F33	120.0(4)
C46	C47	C48	121.0(3)
F33	C47	C48	119.0(4)
F34	C48	C47	121.1(4)
F34	C48	C49	119.8(4)
C47	C48	C49	119.1(3)

B4[1]	B6	B2	61.87(14)
O6	B6	B3[1]	116.01(19)
B1	B6	B3[1]	107.62(18)
B4[1]	B6	B3[1]	58.88(14)
B2	B6	B3[1]	107.85(17)
O6	B6	B5	122.35(19)
B1	B6	B5	59.56(14)
B4[1]	B6	B5	107.48(18)
B2	B6	B5	107.48(17)
B3[1]	B6	B5	59.59(14)
O7	B7	B12	125.1(2)
O7	B7	B11	122.4(2)
B12	B7	B11	61.96(15)
O7	B7	B9	118.73(19)
B12	B7	B9	109.04(19)
B11	B7	B9	59.90(14)
O7	B7	B8	118.70(19)
B12	B7	B8	108.26(19)
B11	B7	B8	107.18(19)
B9	B7	B8	58.31(15)
O7	B7	B10[2]	123.4(2)
B12	B7	B10[2]	60.63(15)
B11	B7	B10[2]	109.05(19)
B9	B7	B10[2]	106.02(18)
B8	B7	B10[2]	59.07(15)
O8	B8	B9	118.02(19)
O8	B8	B10[2]	125.7(2)
B9	B8	B10[2]	109.46(18)
O8	B8	B7	123.5(2)
B9	B8	B7	60.79(15)
B10[2]	B8	B7	60.90(15)
O8	B8	B12[2]	118.69(19)
B9	B8	B12[2]	59.77(15)
F35	C49	C44	120.3(3)
F35	C49	C48	118.4(3)
C44	C49	C48	121.3(3)
O8	C50	C51	107.00(19)
C56	C51	C52	116.7(2)
C56	C51	C50	122.5(2)
C52	C51	C50	120.7(2)
F36	C52	C53	118.3(3)
F36	C52	C51	119.7(2)
C53	C52	C51	122.0(3)
F37	C53	C54	120.3(3)
F37	C53	C52	120.1(3)
C54	C53	C52	119.6(3)
F38	C54	C55	120.3(3)
F38	C54	C53	120.2(3)
C55	C54	C53	119.5(3)
F39	C55	C54	120.0(3)
F39	C55	C56	120.3(3)
C54	C55	C56	119.6(3)
F40	C56	C51	120.6(2)
F40	C56	C55	116.9(3)
C51	C56	C55	122.5(3)
O9	C57	C58	107.9(2)
C63	C58	C59	115.3(3)
C63	C58	C57	122.2(3)
C59	C58	C57	122.4(3)
F41	C59	C60	117.0(3)
F41	C59	C58	120.0(2)
C60	C59	C58	122.9(3)
C61	C60	F42	119.4(4)
C61	C60	C59	120.3(4)
F42	C60	C59	120.4(4)
C60	C61	F43	121.2(5)

B10[2]	B8	B12[2]	106.85(18)
B7	B8	B12[2]	107.58(18)
O8	B8	B11[2]	123.2(2)
B9	B8	B11[2]	108.27(19)
B10[2]	B8	B11[2]	57.69(14)
B7	B8	B11[2]	106.63(18)
B12[2]	B8	B11[2]	60.36(15)
O9	B9	B8	125.5(2)
O9	B9	B12[2]	120.0(2)
B8	B9	B12[2]	61.68(15)
O9	B9	B11	119.2(2)
B8	B9	B11	109.07(18)
B12[2]	B9	B11	107.51(18)
O9	B9	B7	125.8(2)
B8	B9	B7	60.89(15)
B12[2]	B9	B7	109.14(18)
B11	B9	B7	59.67(15)
O9	B9	B10	116.4(2)
B8	B9	B10	109.68(19)
B12[2]	B9	B10	60.62(15)
B11	B9	B10	57.94(15)
B7	B9	B10	106.37(17)
O10	B10	B11	126.4(2)
O10	B10	B8[2]	122.7(2)
B11	B10	B8[2]	62.32(15)
O10	B10	B9	123.8(2)
B11	B10	B9	60.62(15)
B8[2]	B10	B9	109.12(18)
O10	B10	B12[2]	117.5(2)
B11	B10	B12[2]	108.31(19)
B8[2]	B10	B12[2]	107.10(19)
B9	B10	B12[2]	58.93(15)
O10	B10	B7[2]	117.2(2)

C60	C61	C62	120.7(4)
F43	C61	C62	118.1(5)
F44	C62	C61	123.0(4)
F44	C62	C63	118.6(5)
C61	C62	C63	118.4(3)
F45	C63	C58	117.8(3)
F45	C63	C62	119.8(3)
C58	C63	C62	122.3(4)
O10	C64	C65	108.5(2)
C70	C65	C66	116.2(3)
C70	C65	C64	121.8(2)
C66	C65	C64	121.9(3)
F46	C66	C67	117.9(3)
F46	C66	C65	119.9(3)
C67	C66	C65	122.2(3)
F47	C67	C68	120.7(3)
F47	C67	C66	120.1(3)
C68	C67	C66	119.2(3)
C67	C68	C69	121.0(3)
C67	C68	F48	119.0(3)
C69	C68	F48	120.0(3)
F49	C69	C68	120.8(3)
F49	C69	C70	119.8(3)
C68	C69	C70	119.4(3)
F50	C70	C65	119.6(2)
F50	C70	C69	118.4(3)
C65	C70	C69	122.0(3)
O11	C71	C72	107.7(2)
C77A	C72	C73A	117.4(8)
C73	C72	C77	120.0
C77A	C72	C71	104.9(8)
C73A	C72	C71	137.6(5)
C73	C72	C71	114.2(3)

B11	B10	B7[2]	109.59(19)
B8[2]	B10	B7[2]	60.04(15)
B9	B10	B7[2]	106.01(18)
B12[2]	B10	B7[2]	58.22(14)
O11	B11	B10	118.7(2)
O11	B11	B7	125.2(2)
B10	B11	B7	109.79(19)
O11	B11	B9	124.7(2)
B10	B11	B9	61.44(15)
B7	B11	B9	60.43(15)
O11	B11	B8[2]	118.25(19)
B10	B11	B8[2]	59.99(15)
B7	B11	B8[2]	106.84(19)
B9	B11	B8[2]	107.96(18)
O11	B11	B12	121.94(19)
B10	B11	B12	107.96(19)
B7	B11	B12	58.41(14)
B9	B11	B12	106.66(18)
B8[2]	B11	B12	59.45(15)
O12	B12	B7	117.7(2)
O12	B12	B9[2]	126.9(2)
B7	B12	B9[2]	109.57(18)
O12	B12	B10[2]	125.5(2)
B7	B12	B10[2]	61.15(15)
B9[2]	B12	B10[2]	60.44(15)
O12	B12	B8[2]	121.5(2)
B7	B12	B8[2]	108.44(18)
B9[2]	B12	B8[2]	58.55(15)
B10[2]	B12	B8[2]	107.07(18)
O12	B12	B11	116.6(2)
B7	B12	B11	59.63(15)
B9[2]	B12	B11	107.17(19)
B10[2]	B12	B11	107.65(17)
C77	C72	C71	125.7(3)
F51	C73	C72	120.6(3)
F51	C73	C74	119.4(3)
C72	C73	C74	120.0
F52	C74	C73	120.0(4)
F52	C74	C75	120.0(4)
C73	C74	C75	120.0
F53	C75	C76	121.0(5)
F53	C75	C74	119.0(5)
C76	C75	C74	120.0
F54	C76	C77	122.6(5)
F54	C76	C75	117.4(5)
C77	C76	C75	120.0
F55	C77	C76	117.6(3)
F55	C77	C72	122.4(3)
C76	C77	C72	120.0
F51A	C73A	C72	122.3(9)
F51A	C73A	C74A	117.5(9)
C72	C73A	C74A	120.1(8)
F52A	C74A	C75A	118.7(14)
F52A	C74A	C73A	121.3(11)
C75A	C74A	C73A	119.8(10)
F53A	C75A	C74A	119.0(13)
F53A	C75A	C76A	121.1(11)
C74A	C75A	C76A	119.5(11)
F54A	C76A	C75A	117.8(11)
F54A	C76A	C77A	125.5(12)
C75A	C76A	C77A	116.4(12)
C72	C77A	C76A	126.5(14)
C72	C77A	F55A	122.1(12)
C76A	C77A	F55A	111.4(14)
O12	C78	C79	105.95(19)
C80	C79	C84	116.1(2)

B8[2]	B12	B11	60.20(15)	C80	C79	C78	122.6(2)
O1	C1	C2	106.5(2)	C84	C79	C78	121.1(2)
C7	C2	C3	116.4(2)	F56	C80	C81	117.7(2)
C7	C2	C1	123.0(2)	F56	C80	C79	120.0(2)
C3	C2	C1	120.5(2)	C81	C80	C79	122.3(3)
F1	C3	C4	118.6(2)	F57	C81	C82	119.2(2)
F1	C3	C2	119.5(2)	F57	C81	C80	121.0(3)
C4	C3	C2	121.8(2)	C82	C81	C80	119.7(2)
F2	C4	C5	118.8(3)	F58	C82	C83	120.6(3)
F2	C4	C3	121.0(3)	F58	C82	C81	119.7(3)
C5	C4	C3	120.2(3)	C83	C82	C81	119.6(2)
F3	C5	C4	120.7(3)	F59	C83	C82	120.1(2)
F3	C5	C6	119.8(3)	F59	C83	C84	120.3(3)
C4	C5	C6	119.5(3)	C82	C83	C84	119.7(3)
F4	C6	C5	119.5(3)	F60	C84	C83	118.2(2)
F4	C6	C7	121.0(2)	F60	C84	C79	119.4(2)
C5	C6	C7	119.5(2)	C83	C84	C79	122.4(2)
F5	C7	C6	118.0(2)	C97	N1	C93	111.6(2)
F5	C7	C2	119.5(2)	C97	N1	C85	110.9(3)
C6	C7	C2	122.4(2)	C93	N1	C85	106.6(2)
O2	C8	C9	107.94(18)	C97	N1	C89	107.2(2)
C10	C9	C14	116.9(2)	C93	N1	C89	110.3(2)
C10	C9	C8	120.9(2)	C85	N1	C89	110.4(2)
C14	C9	C8	122.2(2)	C86A	C85	N1	124.4(4)
F6	C10	C9	119.9(2)	N1	C85	C86	106.2(4)
F6	C10	C11	118.4(2)	C87	C86	C85	108.4(7)
C9	C10	C11	121.8(2)	C86	C87	C88	104.4(7)
F7	C11	C12	120.4(2)	C85	C86A	C87A	109.1(8)
F7	C11	C10	120.1(2)	C86A	C87A	C88	106.9(7)
C12	C11	C10	119.5(2)	C90	C89	N1	115.9(2)
F8	C12	C11	120.1(3)	C91	C90	C89	111.3(3)
F8	C12	C13	119.3(2)	C90	C91	C92	111.7(3)
C11	C12	C13	120.6(2)	N1	C93	C94	115.8(2)

F9	C13	C12	120.4(2)	C95	C94	C93	110.4(3)
F9	C13	C14	120.6(3)	C96	C95	C94	112.7(3)
C12	C13	C14	119.0(2)	N1	C97	C98	116.5(2)
F10	C14	C9	120.5(2)	C97	C98	C99	110.2(2)
F10	C14	C13	117.4(2)	C98	C99	C100	112.2(3)
C9	C14	C13	122.2(3)				

[1]1-X,-Y,2-Z; [2]1-X,-Y,1-Z

Table 11. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å^2×10^3) for [3]1-

Atom	***x***	***y***	***z***	**U(eq)**
H1A	6920	898	9177	37
H1B	6390	1899	9254	37
H8A	3488	706	8713	30
H8B	3477	1579	9123	30
H15A	5603	3081	9838	34
H15B	5555	2891	10356	34
H22A	8073	1012	10376	35
H22B	7544	1646	10743	35
H29A	7086	-2038	9778	31
H29B	7832	-1178	10111	31
H36A	4961	-841	8658	38
H36B	3790	-1282	8529	38
H43A	7933	765	4771	43
H43B	7928	970	5313	43
H50A	6606	2034	6137	36
H50B	5656	1493	6292	36
H57A	5242	2886	4399	37
H57B	5507	2797	4939	37
H64A	3406	-87	3612	34
H64B	3276	934	3909	34
H71A	6840	363	4087	61

H71B	6250	1314	4004	61
H78A	6715	-2251	4730	35
H78B	7648	-1708	5115	35
H85A	-636	4109	7116	72
H85B	-1431	4930	7082	72
H85C	-1215	4766	6966	72
H85D	-522	4089	7252	72
H86A	-510	4269	7964	44
H86B	-1192	5179	7959	44
H87A	-1940	3228	7531	68
H87B	-2624	4142	7532	68
H86C	-2297	4562	7386	51
H86D	-1536	5221	7808	51
H87C	-719	3758	7981	56
H87D	-1588	3129	7592	56
H88A	-1915	4333	8400	110
H88B	-1864	3182	8284	110
H88C	-2934	3640	8183	110
H89A	-412	6517	7850	54
H89B	245	7010	7531	54
H90A	-1191	6731	6913	62
H90B	-1847	6272	7245	62
H91A	-1026	8258	7360	65
H91B	-1528	7822	7748	65
H92A	-2620	7877	6837	94
H92B	-2714	8642	7276	94
H92C	-3109	7521	7246	94
H93A	-114	5680	6689	45
H93B	619	4858	6822	45
H94A	1219	6901	7060	50
H94B	1954	6061	7170	50
H95A	1833	5538	6372	70
H95B	1058	6339	6252	70

H96A	2378	7592	6575	125
H96B	2689	6895	6159	125
H96C	3151	6783	6682	125
H97A	587	5304	8042	64
H97B	1421	5856	7824	64
H98A	1844	4427	7455	58
H98B	850	3825	7541	58
H99A	1504	4021	8339	68
H99B	2464	4703	8278	68
H10A	2096	2676	7909	95
H10B	2929	3108	8358	95
H10C	3067	3361	7862	95

Table 12. Atomic Occupancy for [3]$^{1-}$

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
F51	0.674(4)	F52	0.674(4)	F53	0.674(4)
F54	0.674(4)	F55	0.674(4)	F51A	0.326(4)
F52A	0.326(4)	F53A	0.326(4)	F54A	0.326(4)
F55A	0.326(4)	C73	0.674(4)	C74	0.674(4)
C75	0.674(4)	C76	0.674(4)	C77	0.674(4)
C73A	0.326(4)	C74A	0.326(4)	C75A	0.326(4)
C76A	0.326(4)	C77A	0.326(4)	H85A	0.531(13)
H85B	0.531(13)	H85C	0.469(13)	H85D	0.469(13)
C86	0.531(13)	H86A	0.531(13)	H86B	0.531(13)
C87	0.531(13)	H87A	0.531(13)	H87B	0.531(13)
C86A	0.469(13)	H86C	0.469(13)	H86D	0.469(13)
C87A	0.469(13)	H87C	0.469(13)	H87D	0.469(13)

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(1) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.

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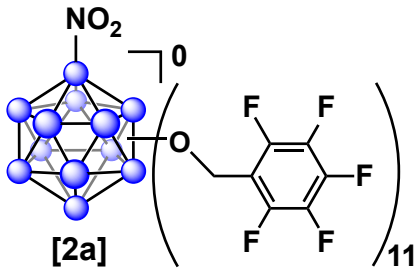
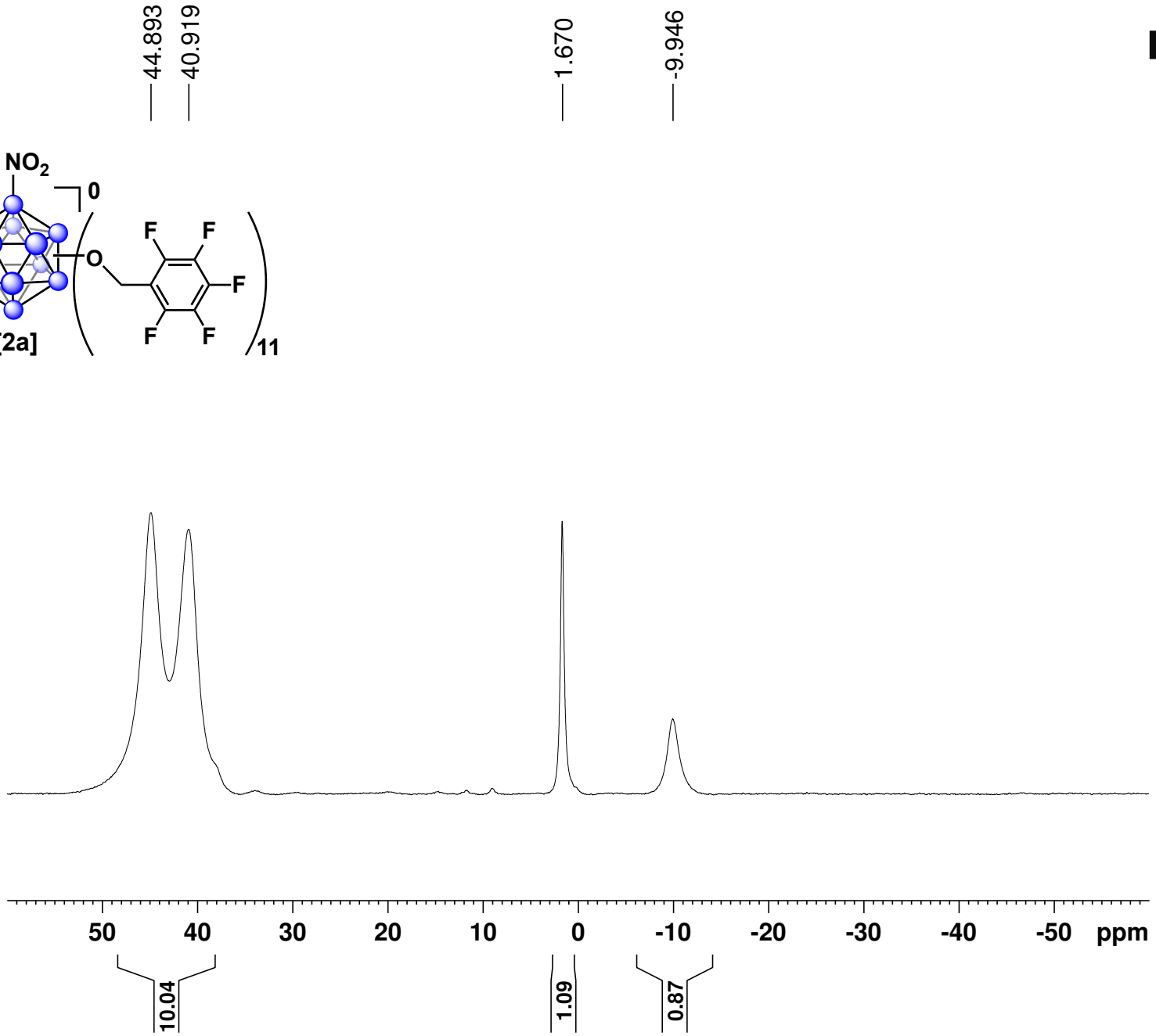
^{11}B NMR Spectra of **[2a]**





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PROCNO 1

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AQ 0.0499408 sec
RG 189.85
DW 9.800 usec
DE 6.50 usec
TE 297.9 K
D1 0.05000000 sec
TD0 1

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NUC1 11B
P1 10.00 usec
PLW1 52.00000000 W

F2 - Processing parameters
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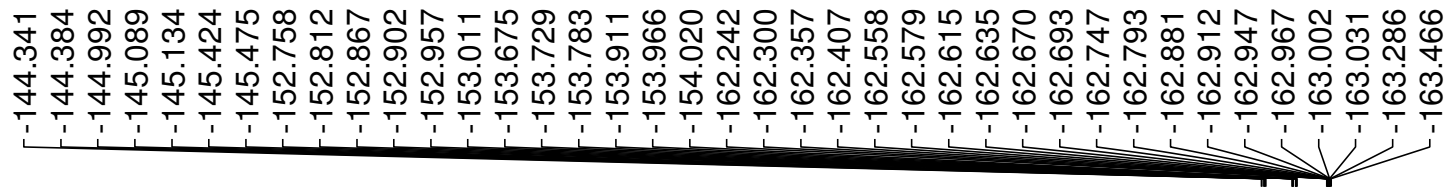
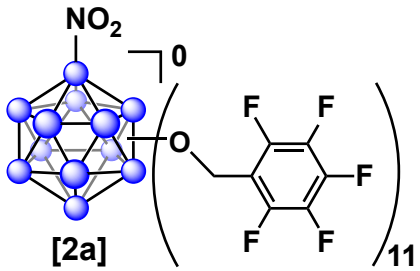
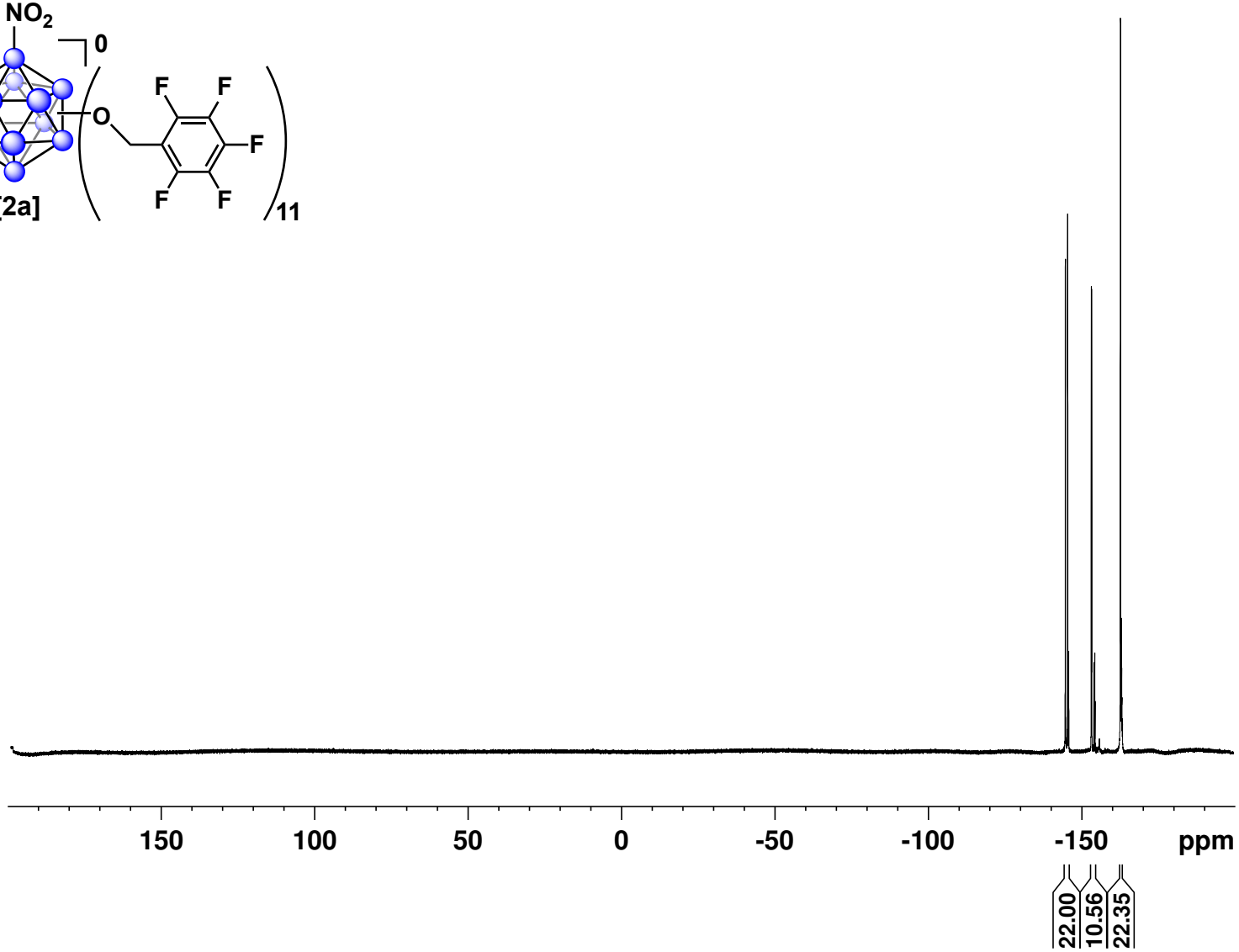
^{19}F NMR Spectra of **[2a]**







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PROCNO 1

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TD 262144
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FIDRES 0.572205 Hz
AQ 0.8738133 sec
RG 189.85
DW 3.333 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

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NUC1 19F
P1 14.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
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WDW EM
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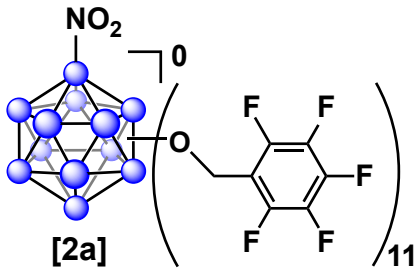
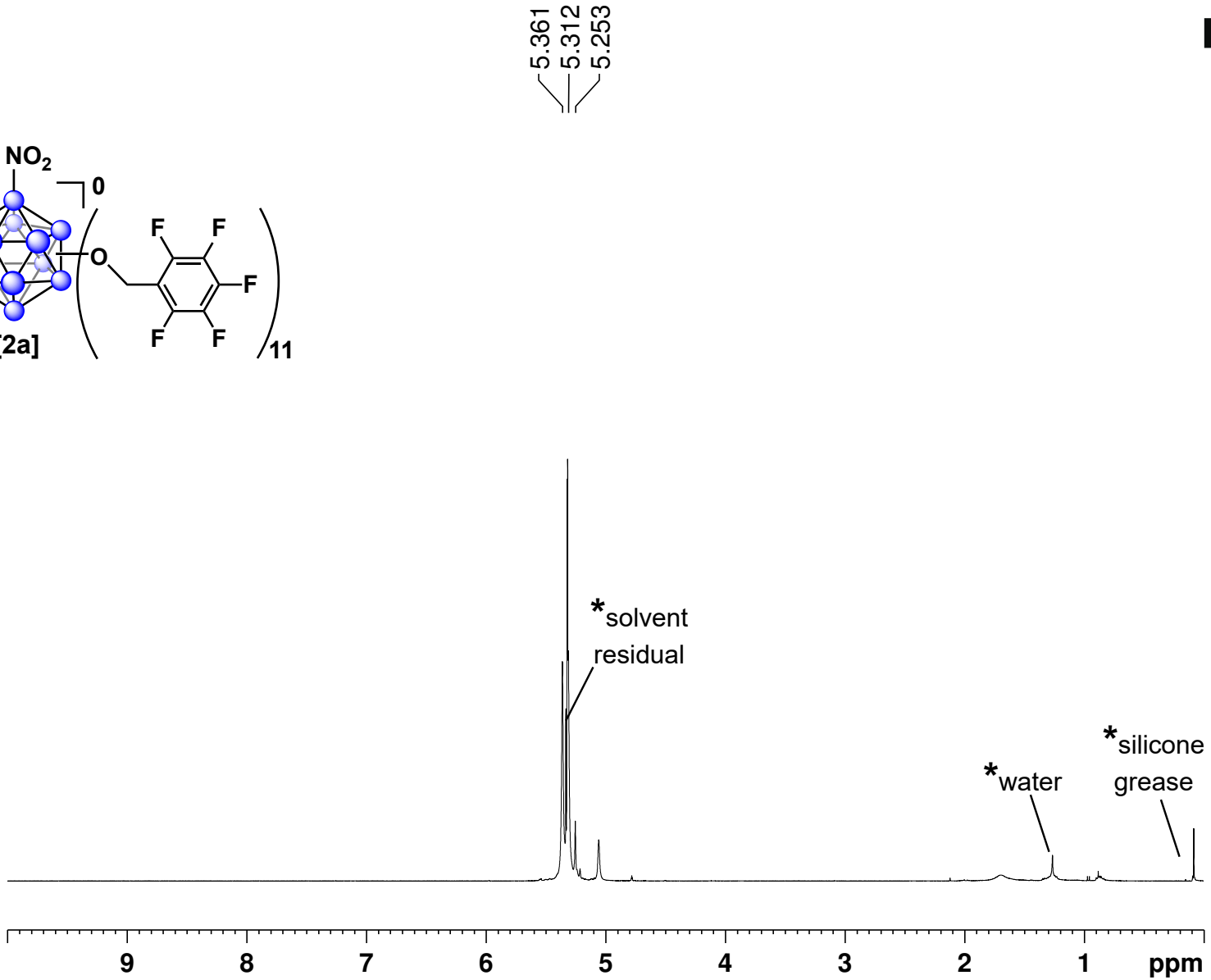
PC 1.00

^{1}H NMR Spectra of **[2a]**



[2a]



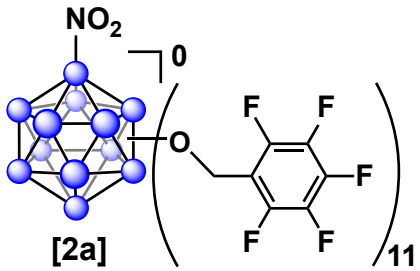
Current Data Parameters
NAME Jan09-2018
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180109
Time 10.06
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CD2Cl2
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 189.85
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

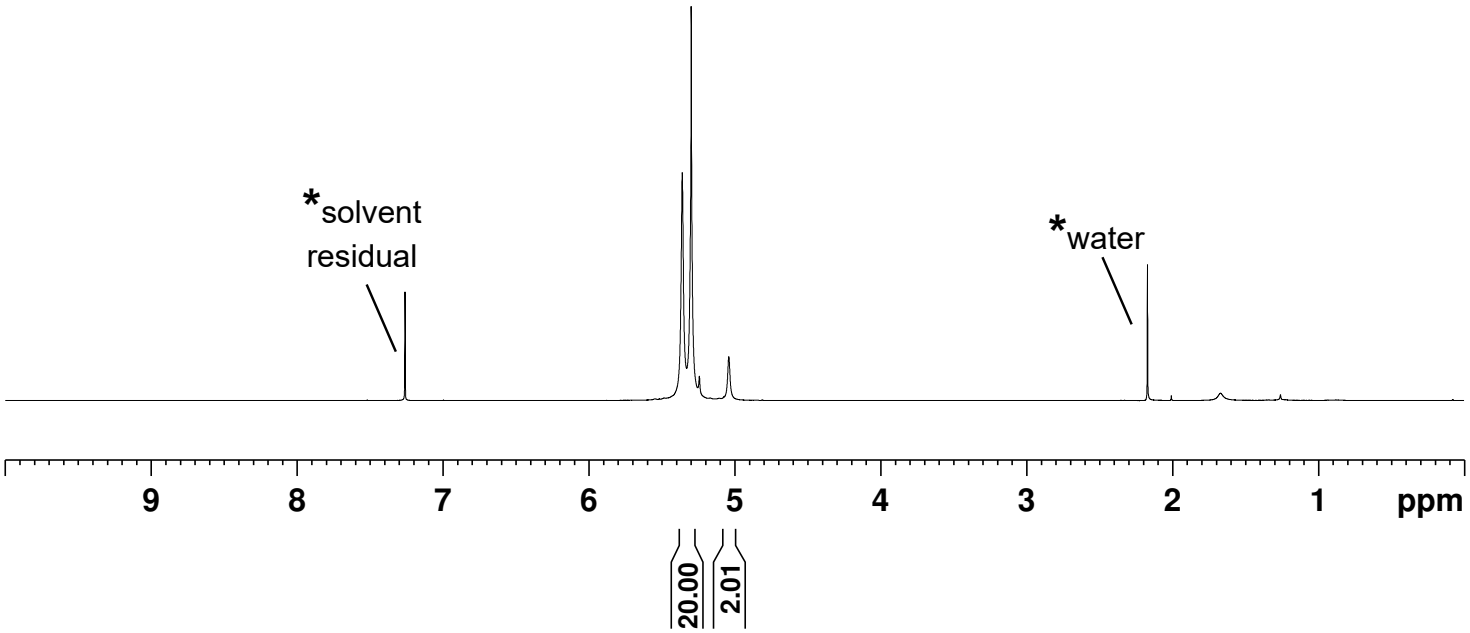
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300154 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR Spectra of **[2a]**



[2a]



Current Data Parameters
NAME Jul02-2017
EXPNO 51
PROCNO 1

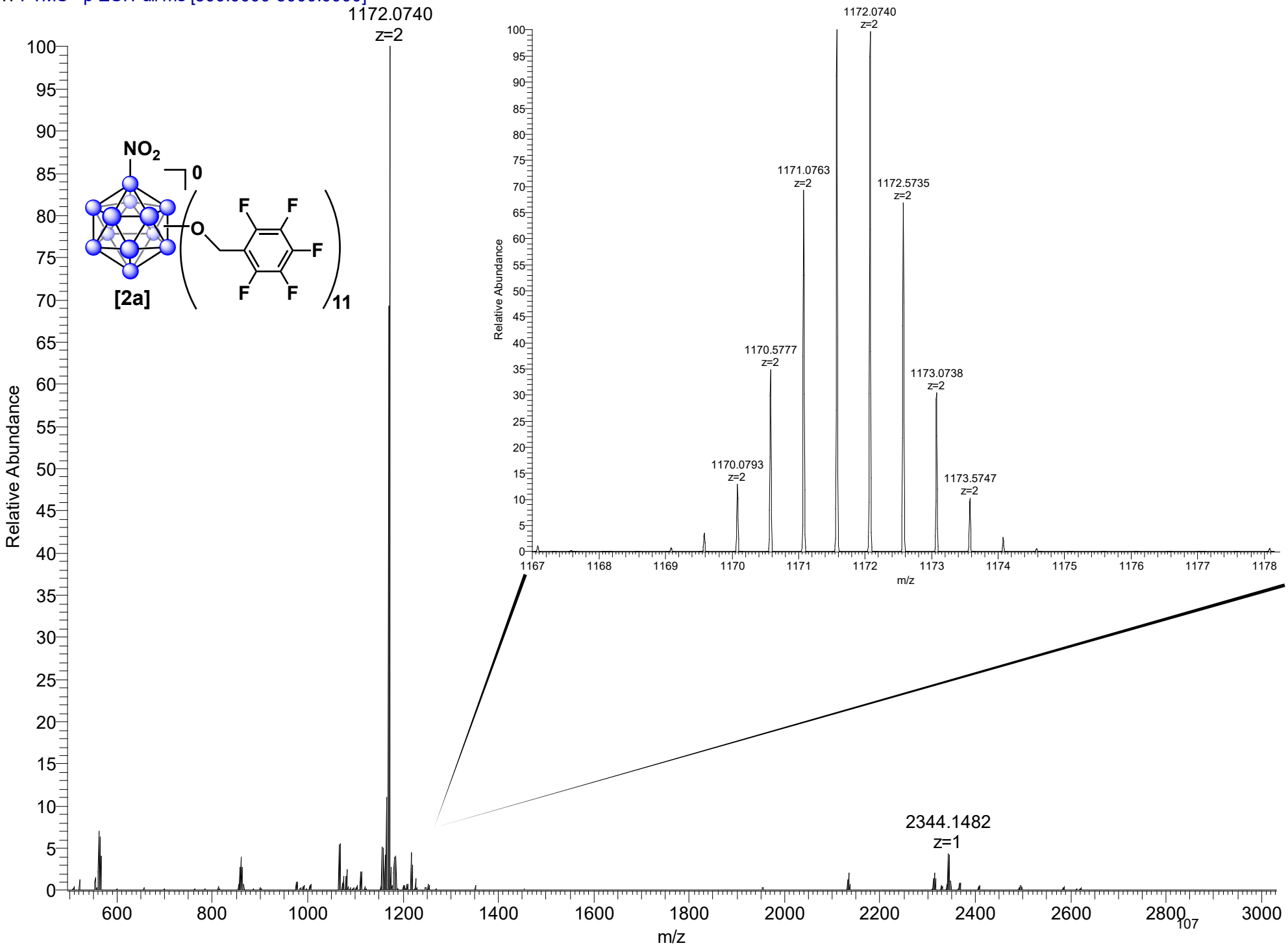
F2 - Acquisition Parameters
Date_ 20170702
Time 19.00
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 155.85
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

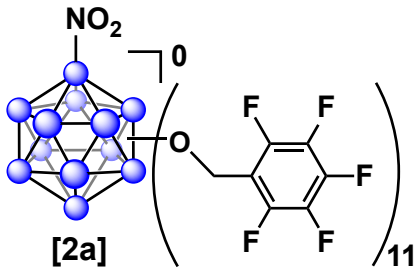
F2 - Processing parameters
SI 65536
SF 400.1300180 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

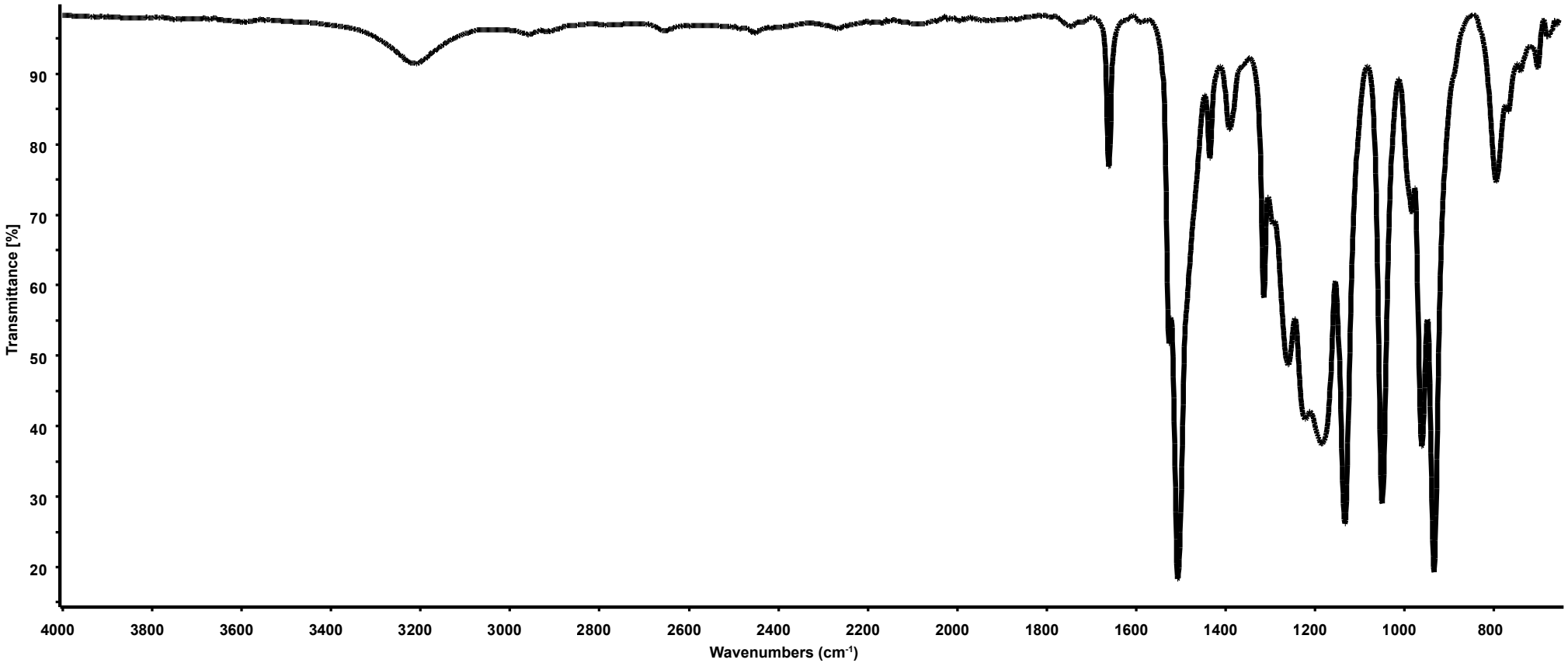
180329 B12NO2PFB11 0 #1-50 RT: 0.01-0.43 AV: 50 NL: 2.22E6
T: FTMS - p ESI Full ms [500.0000-3000.0000]

HRMS of **[2a]**

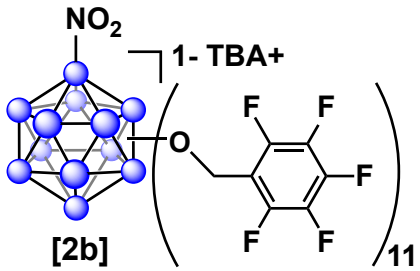


IR Spectra of **[2a]**





^{11}B NMR Spectra of **[2b]**

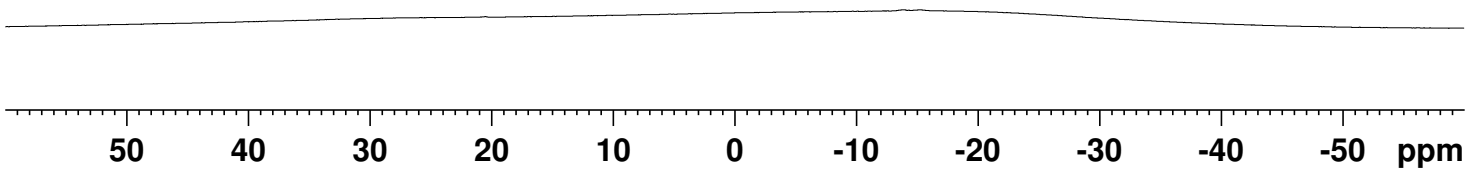


Current Data Parameters
NAME Jan16-2018
EXPNO 172
PROCNO 1

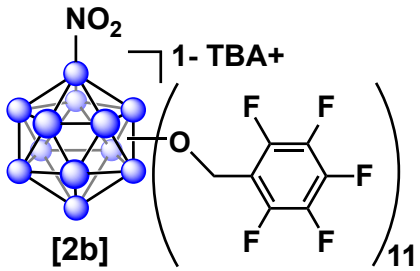
F2 - Acquisition Parameters
Date_ 20180117
Time 0.15
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 5096
SOLVENT CD3CN
NS 1024
DS 0
SWH 51020.406 Hz
FIDRES 10.011854 Hz
AQ 0.0499408 sec
RG 189.85
DW 9.800 usec
DE 6.50 usec
TE 298.2 K
D1 0.05000000 sec
TD0 1

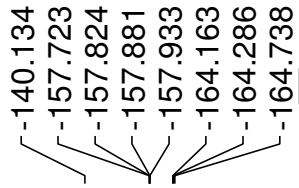
======== CHANNEL f1 ========
SFO1 128.3776052 MHz
NUC1 11B
P1 10.00 usec
PLW1 52.00000000 W

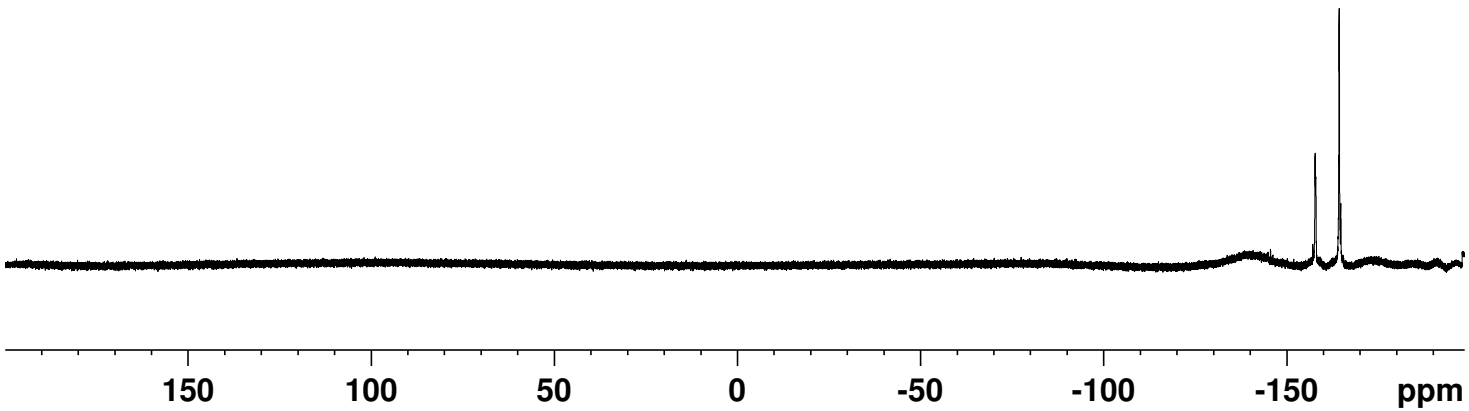
F2 - Processing parameters
SI 32768
SF 128.3775340 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40



^{19}F NMR Spectra of **[2b]**







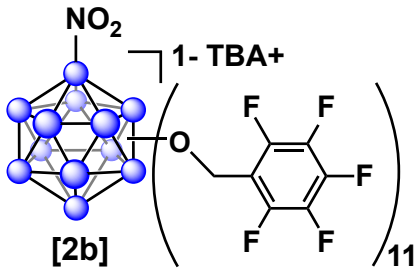
Current Data Parameters
NAME Jan16-2018
EXPNO 171
PROCNO 1

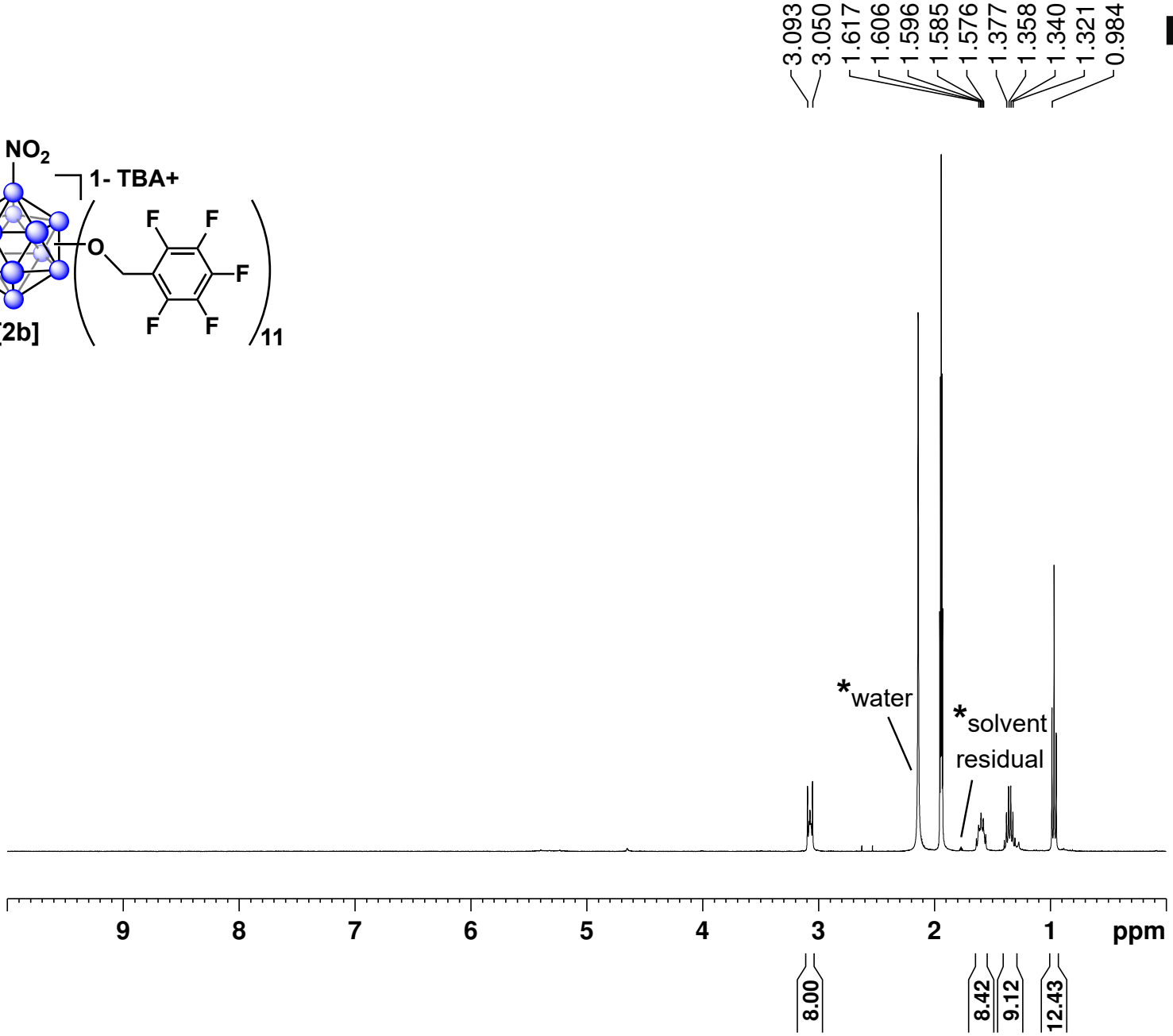
F2 - Acquisition Parameters
Date_ 20180117
Time 0.12
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgflqn30
TD 262144
SOLVENT CD3CN
NS 32
DS 0
SWH 150000.000 Hz
FIDRES 0.572205 Hz
AQ 0.8738133 sec
RG 189.85
DW 3.333 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 376.4983660 MHz
NUC1 19F
P1 14.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 262144
SF 376.4981063 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

^{1}H NMR Spectra of **[2b]**





Current Data Parameters
NAME Jan16-2018
EXPNO 170
PROCNO 1

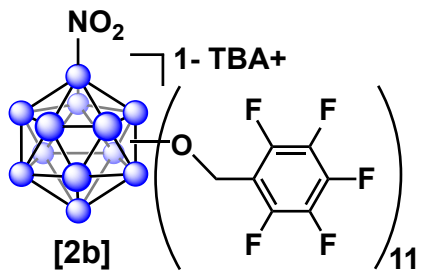
F2 - Acquisition Parameters
Date_ 20180117
Time 0.09
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CD3CN
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 189.85
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

180329 B12NO2PFB11 1- #1-50 RT: 0.01-0.43 AV: 50 NL: 1.75E7
T: FTMS - p ESI Full ms [500.0000-3000.0000]

HRMS of **[2b]**



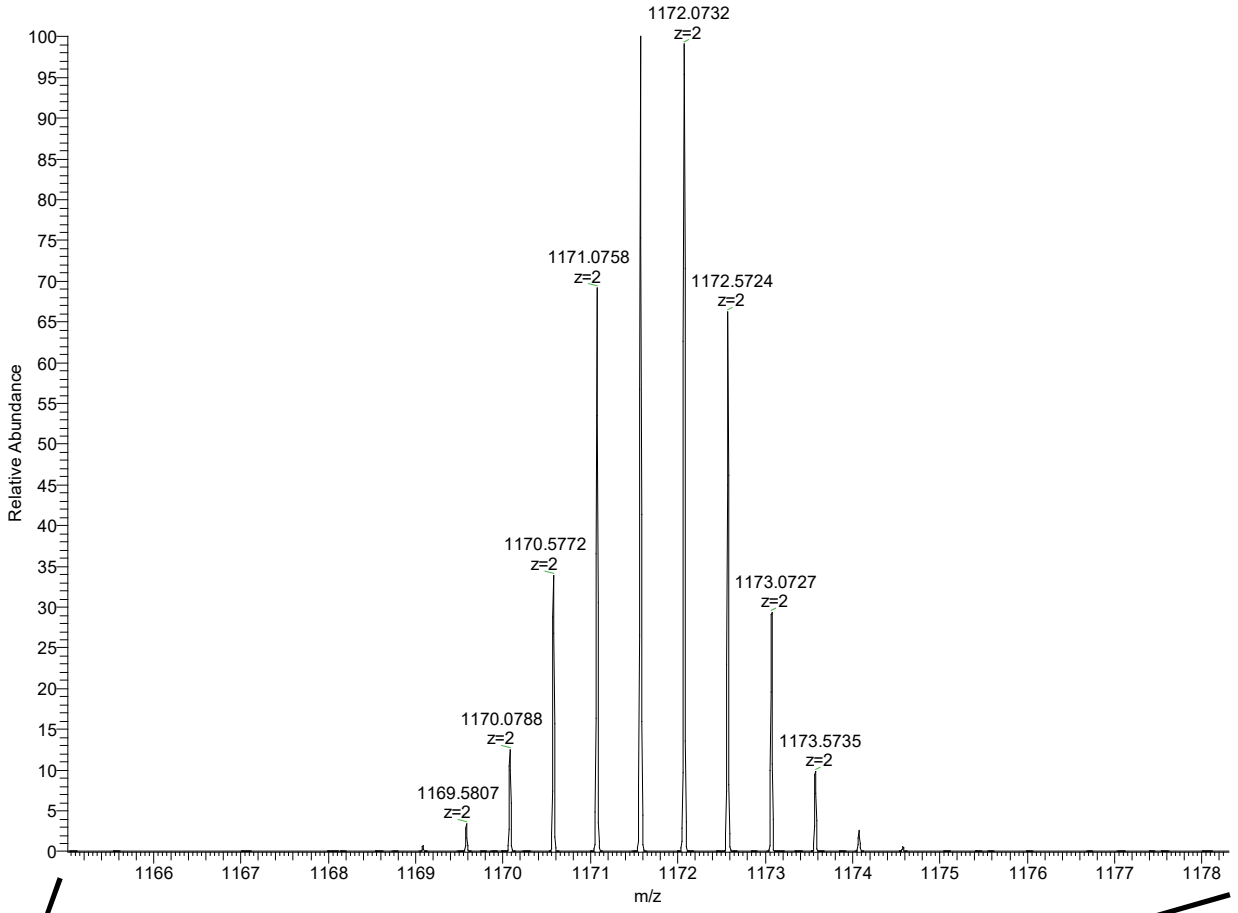
1172.0732
z=2

Relative Abundance

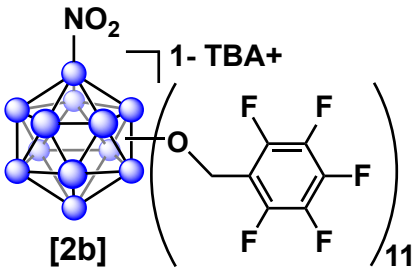
m/z

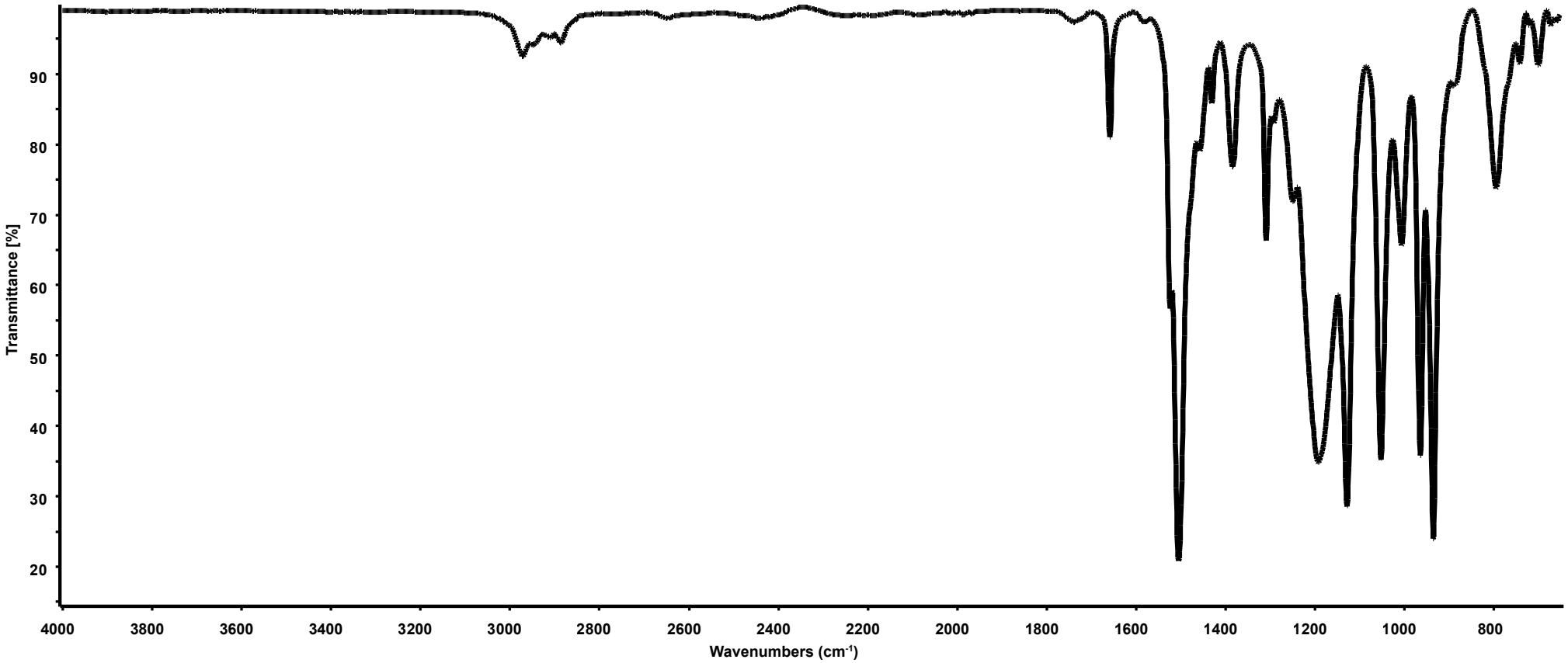
2344.1461
z=1

2586.4206
z=1

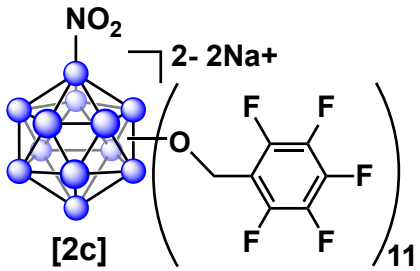


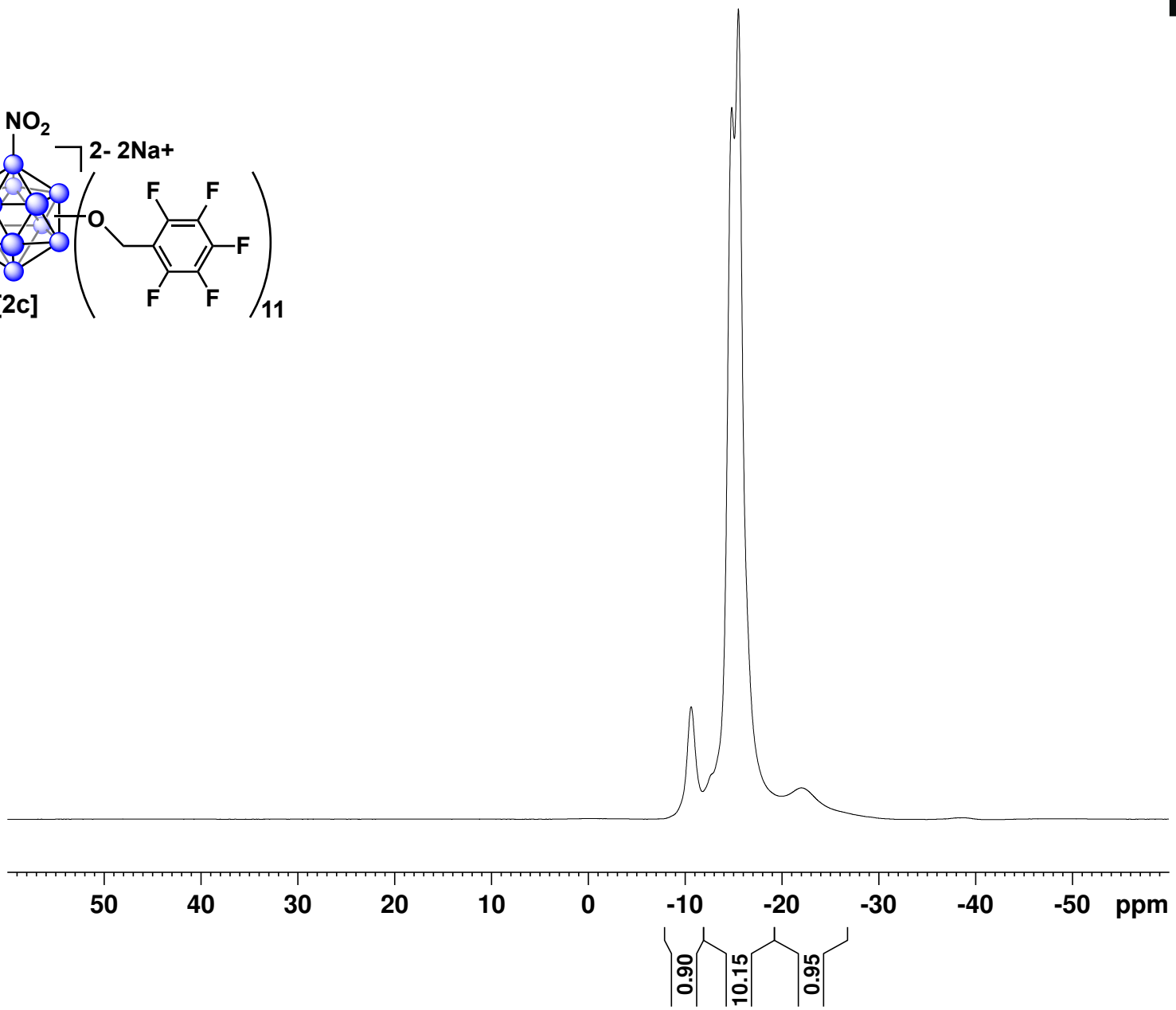
IR Spectra of **[2b]**





^{11}B NMR Spectra of **[2c]**





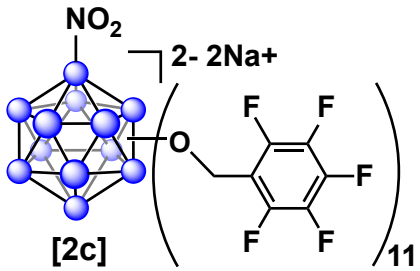
Current Data Parameters
NAME Jan12-2018
EXPNO 71
PROCNO 1

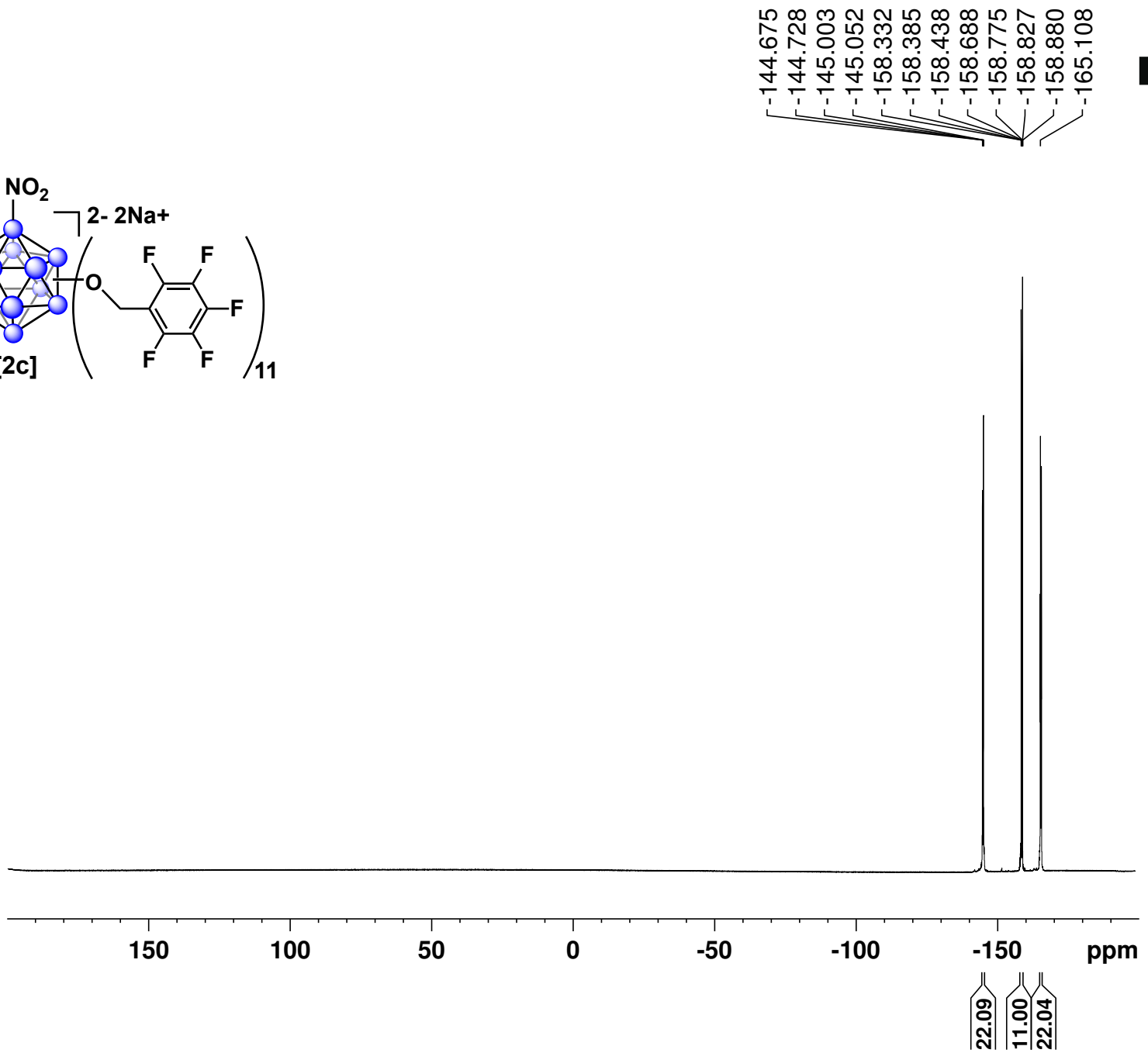
F2 - Acquisition Parameters
Date_ 20180112
Time 14.26
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 5096
SOLVENT CD3CN
NS 1024
DS 0
SWH 51020.406 Hz
FIDRES 10.011854 Hz
AQ 0.0499408 sec
RG 189.85
DW 9.800 usec
DE 6.50 usec
TE 298.2 K
D1 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 128.3776052 MHz
NUC1 11B
P1 10.00 usec
PLW1 52.00000000 W

F2 - Processing parameters
SI 32768
SF 128.3776161 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

^{19}F NMR Spectra of **[2c]**





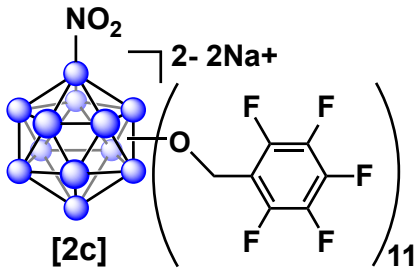
Current Data Parameters
NAME Jan12-2018
EXPNO 72
PROCNO 1

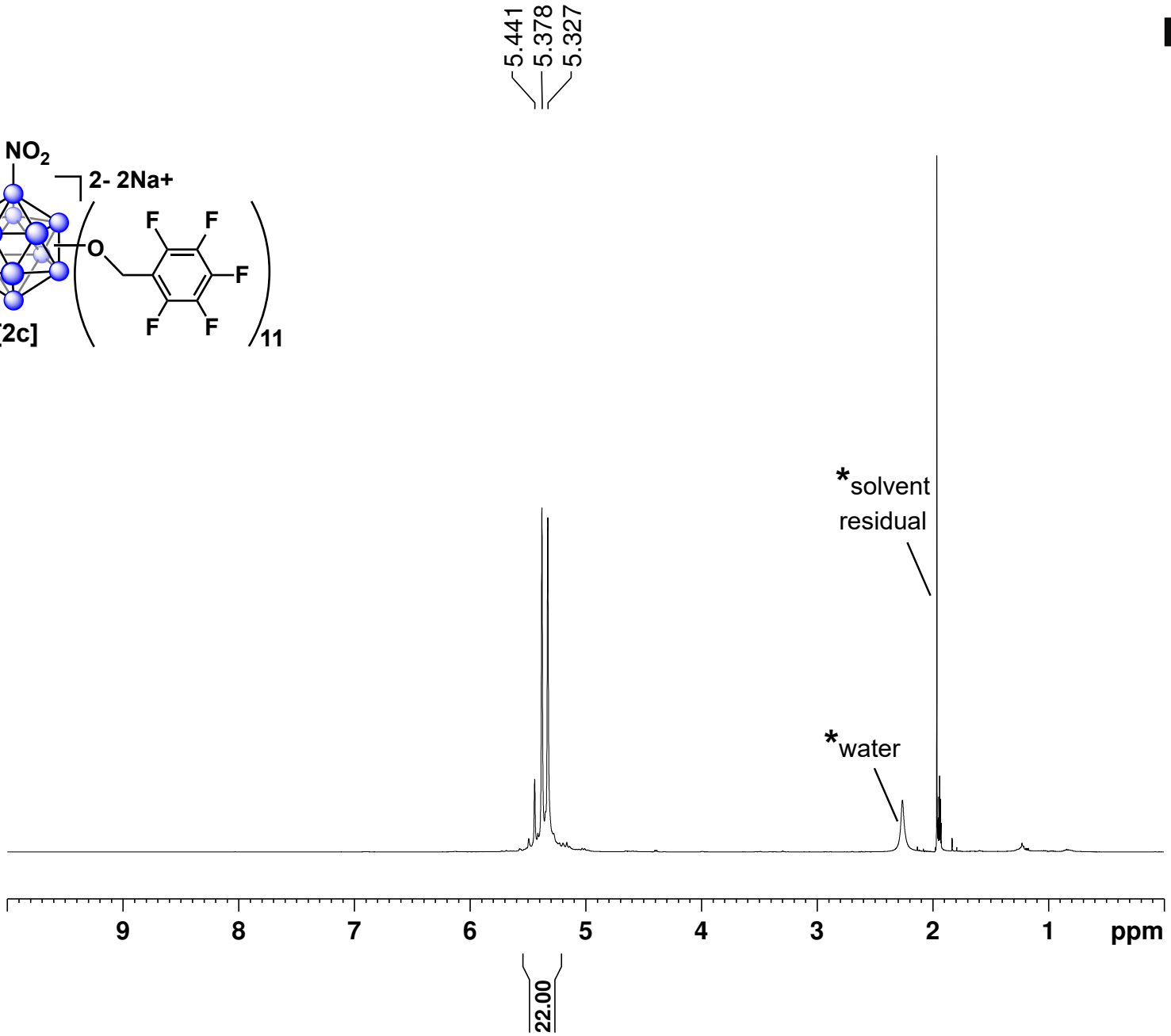
F2 - Acquisition Parameters
Date_ 20180112
Time 14.31
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgflqn30
TD 262144
SOLVENT CD3CN
NS 32
DS 0
SWH 150000.000 Hz
FIDRES 0.572205 Hz
AQ 0.8738133 sec
RG 189.85
DW 3.333 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 376.4983660 MHz
NUC1 19F
P1 14.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 262144
SF 376.4981932 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

^{1}H NMR Spectra of **[2c]**





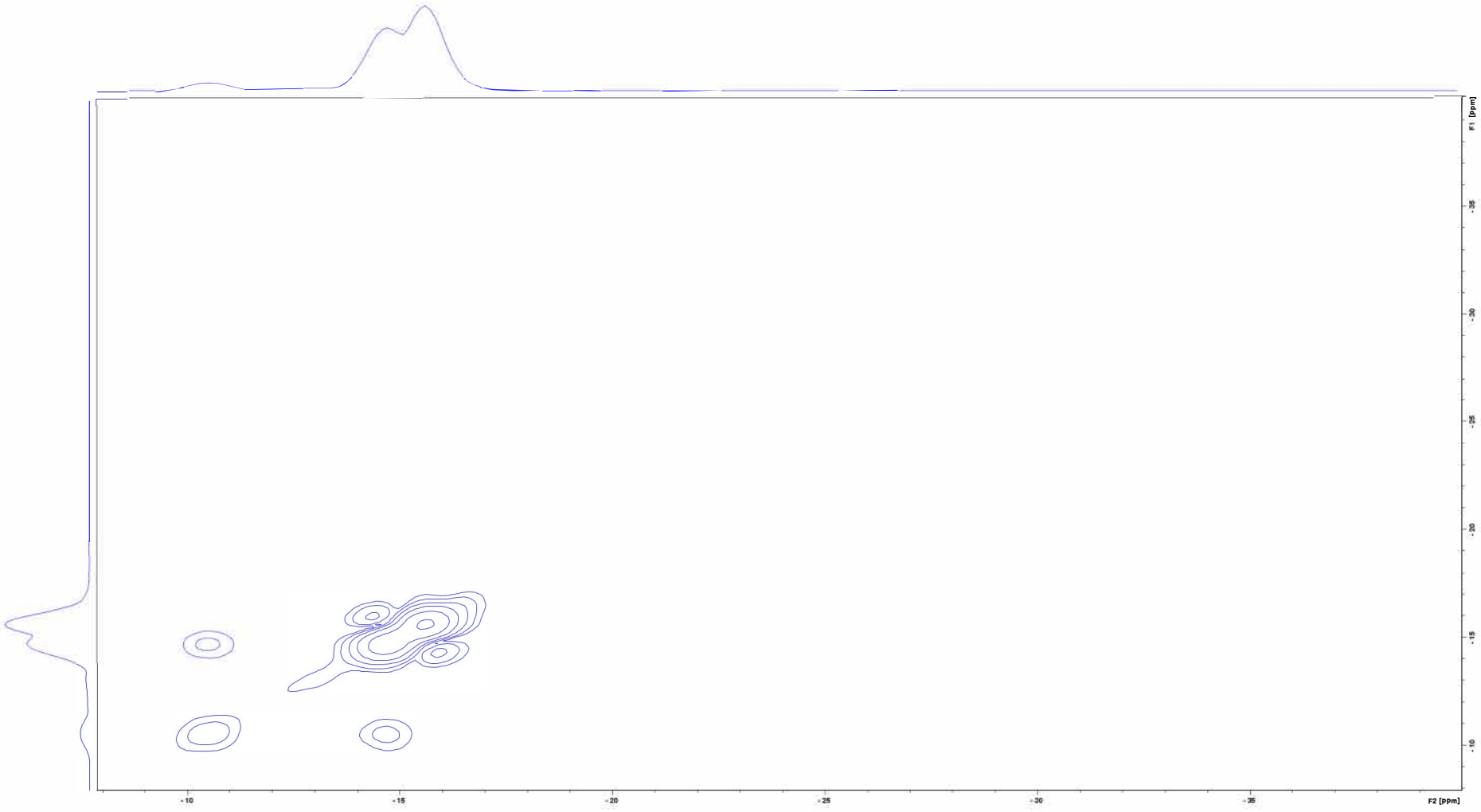
Current Data Parameters
NAME Jan12-2018
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180112
Time 14.23
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CD3CN
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 94.6
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

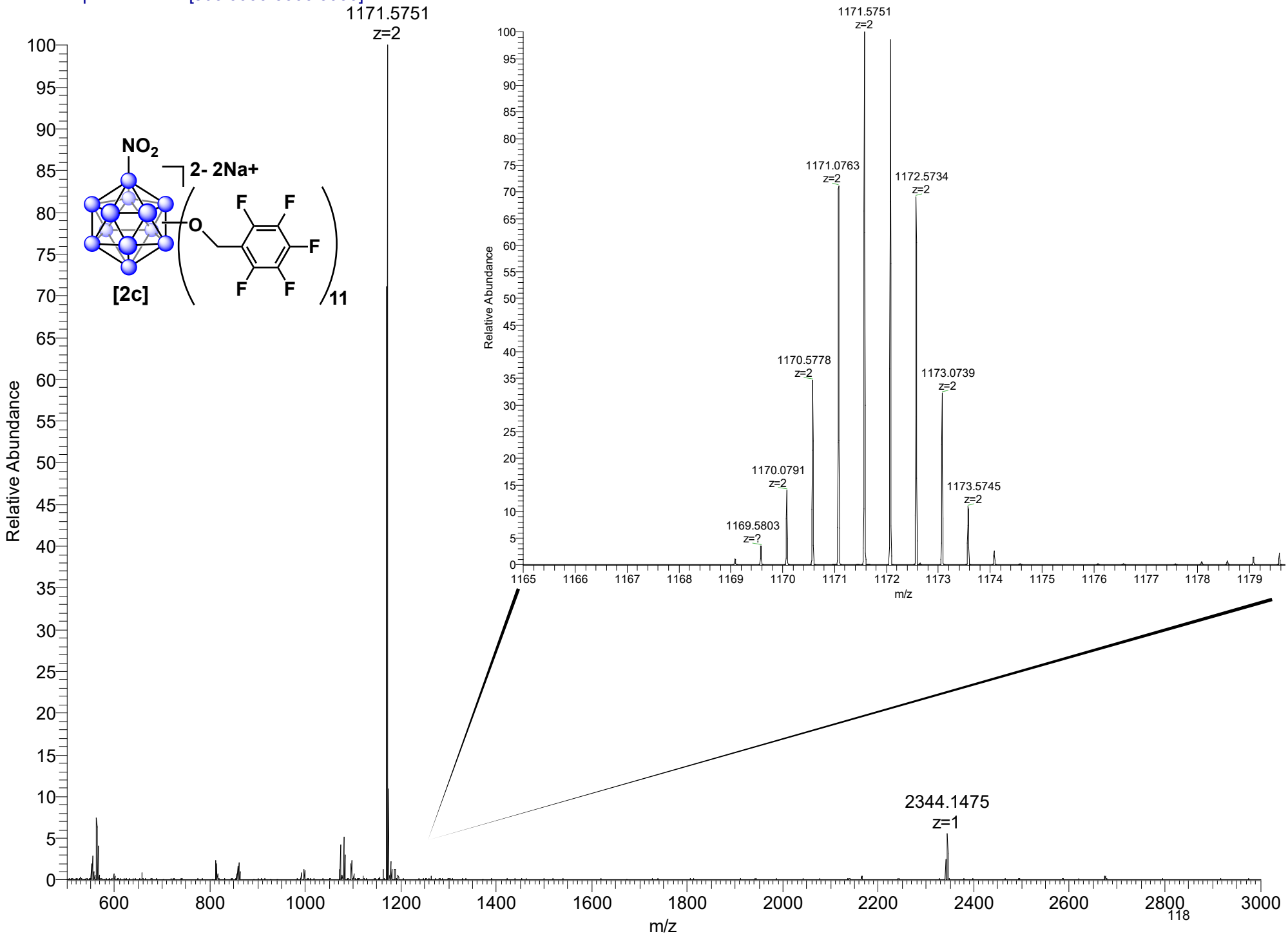
^{11}B-^{11}B COSY NMR Spectra of **[2c]**



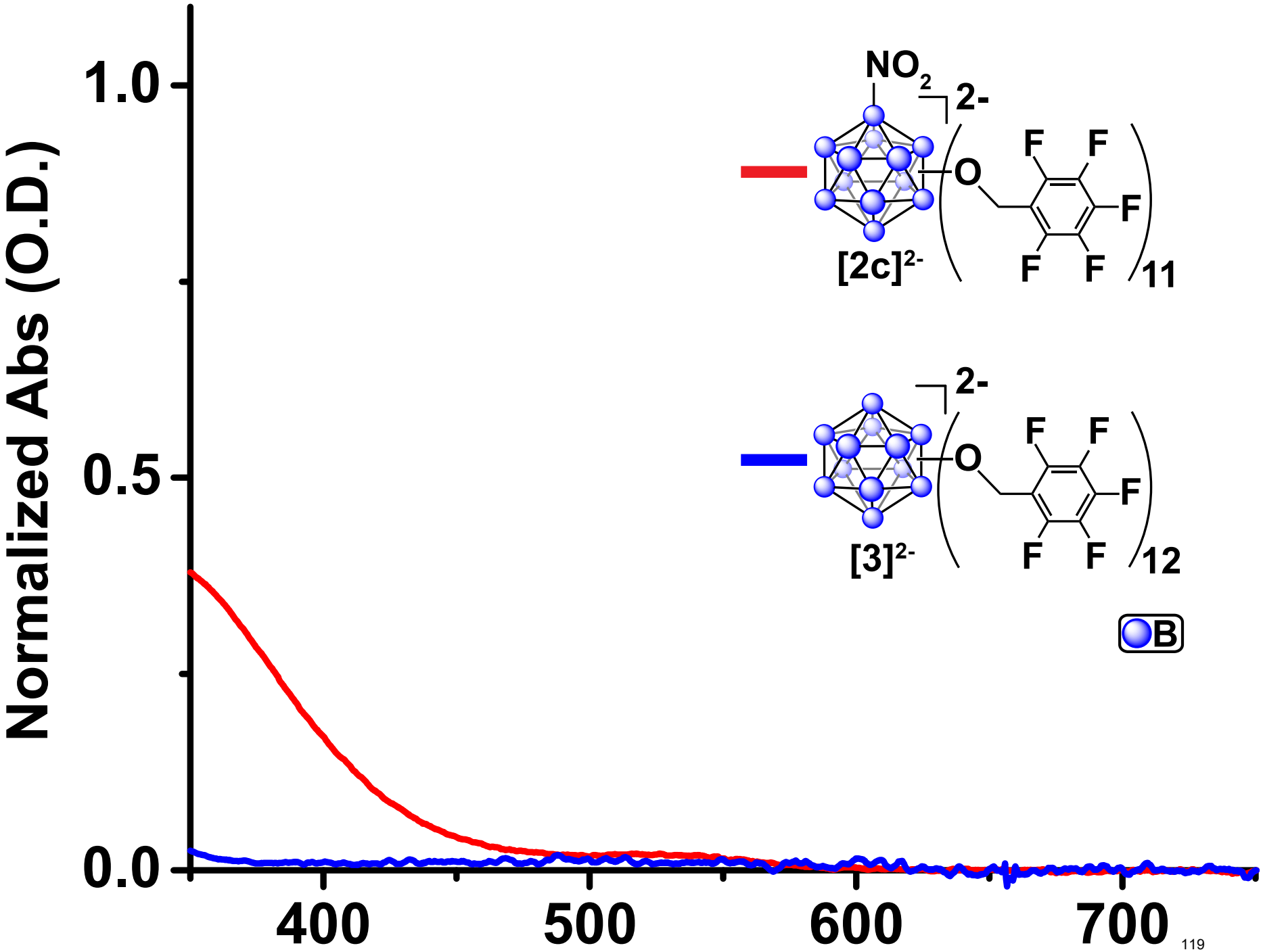
180329 B12NO2PFB11 2- #1 RT: 0.01 AV: 1 NL: 6.29E6
T: FTMS - p ESI Full ms [500.0000-3000.0000]

HRMS of **[2c]**

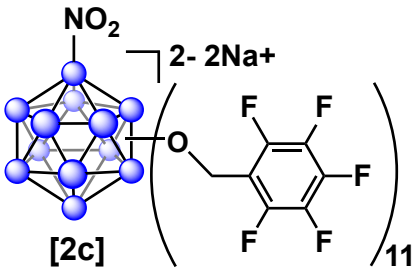
[2c]

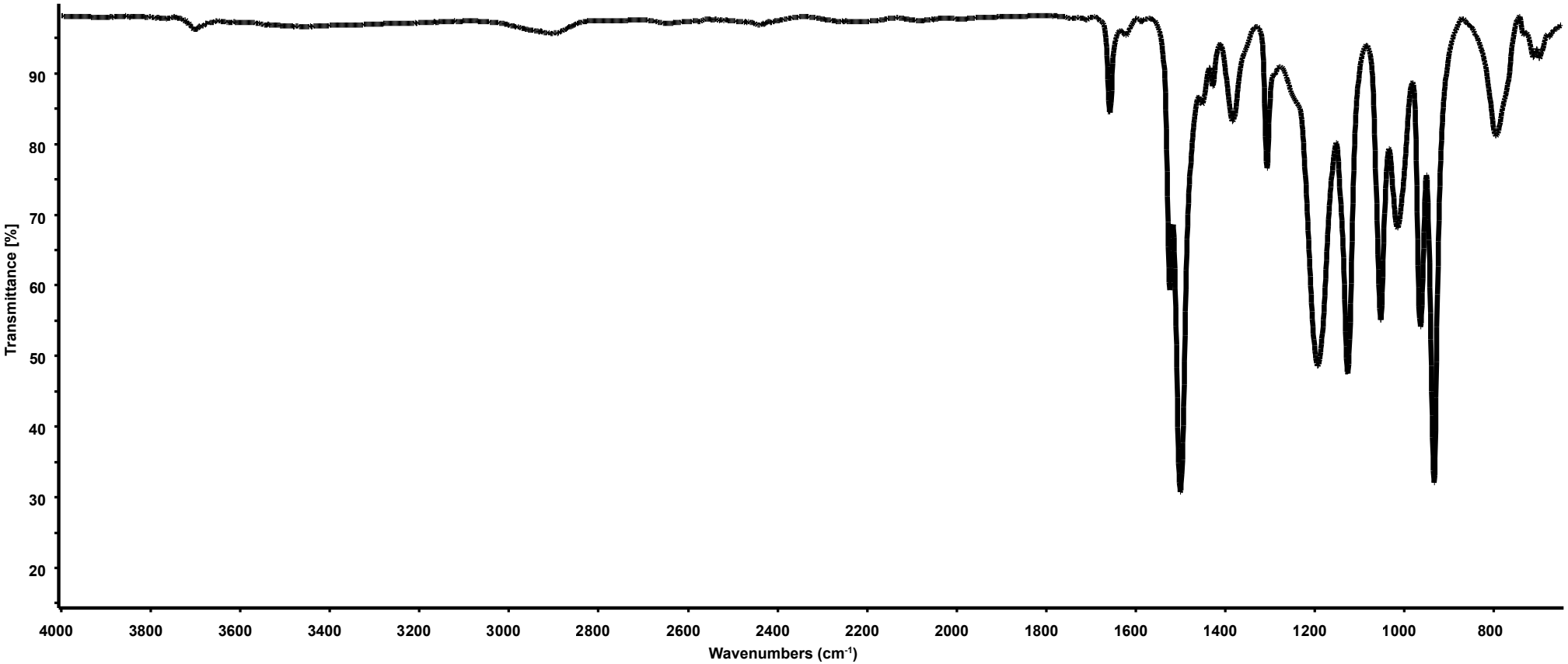


UV-vis spectra of **[2c]$^{2-}$** and **[3]$^{2-}$**

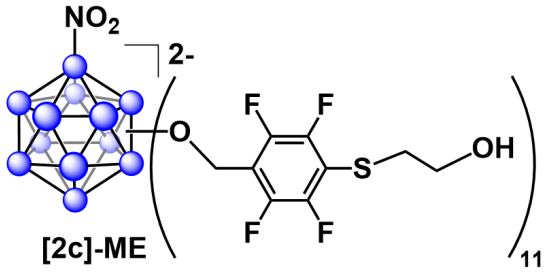


IR Spectra of **[2c]**

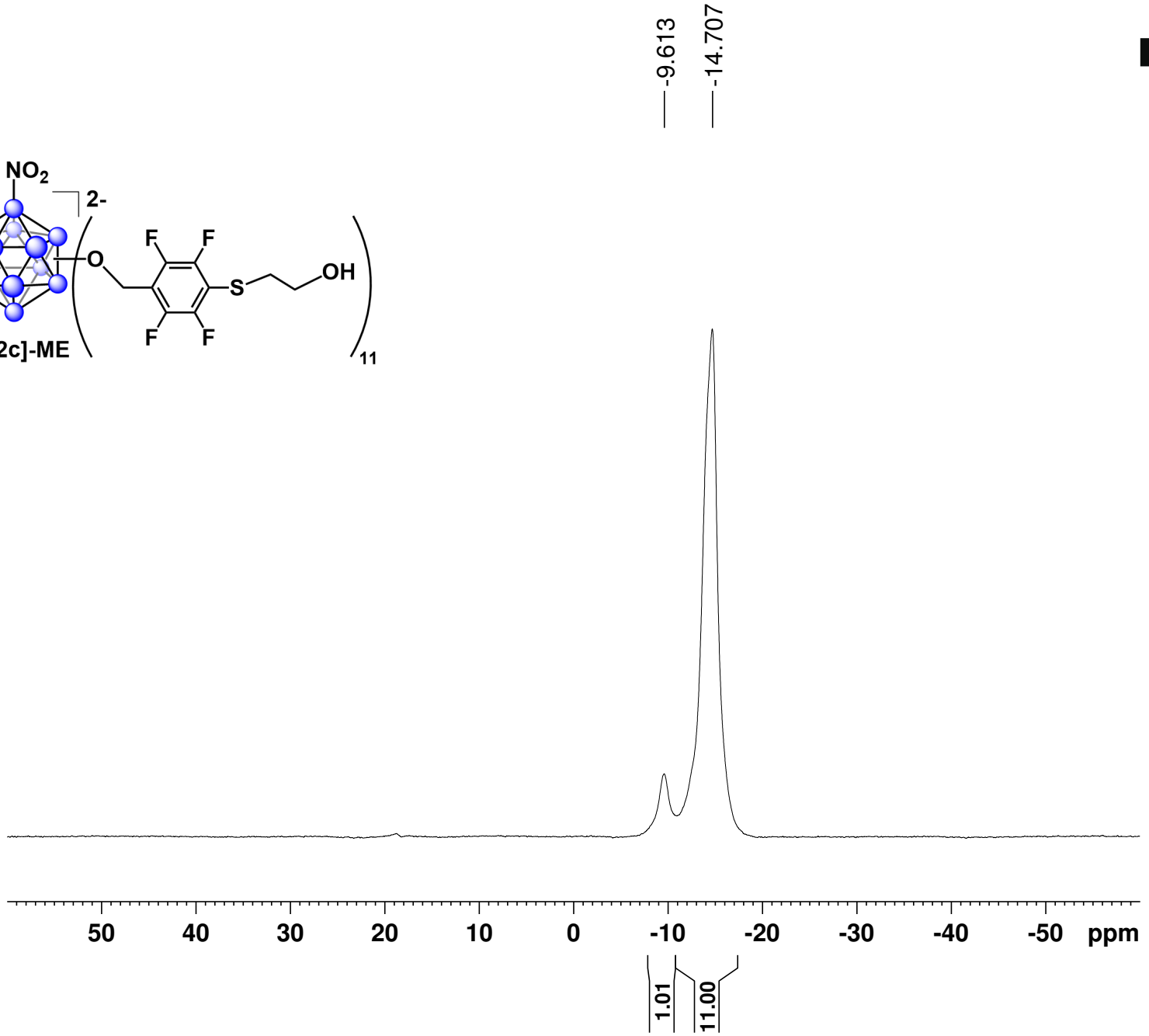




^{11}B NMR Spectra of **[2c]-ME**



[2c]-ME



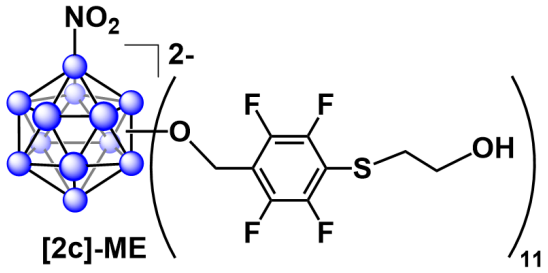
Current Data Parameters
NAME Feb28-2018
EXPNO 80
PROCNO 1

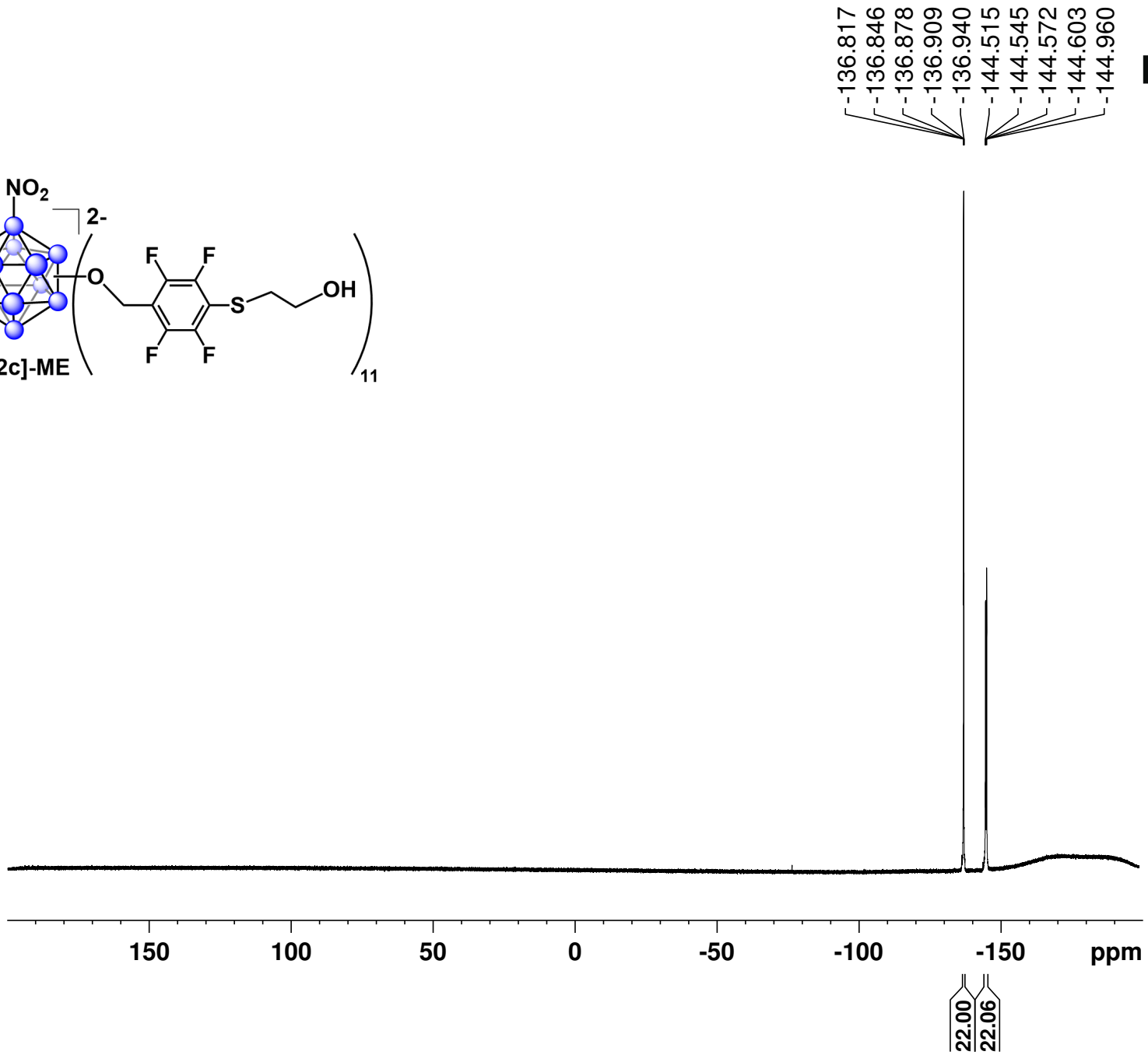
F2 - Acquisition Parameters
Date_ 20180228
Time 11.43
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 5096
SOLVENT MeOD
NS 1024
DS 0
SWH 51020.406 Hz
FIDRES 10.011854 Hz
AQ 0.0499408 sec
RG 189.85
DW 9.800 usec
DE 6.50 usec
TE 297.3 K
D1 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 128.3776052 MHz
NUC1 11B
P1 10.00 usec
PLW1 52.00000000 W

F2 - Processing parameters
SI 32768
SF 128.3775591 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

^{19}F NMR Spectra of **[2c]-ME**





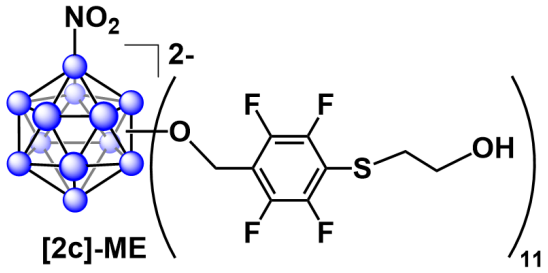
Current Data Parameters
NAME Feb28-2018
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180228
Time 11.48
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgflqn30
TD 262144
SOLVENT MeOD
NS 64
DS 0
SWH 150000.000 Hz
FIDRES 0.572205 Hz
AQ 0.8738133 sec
RG 189.85
DW 3.333 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1

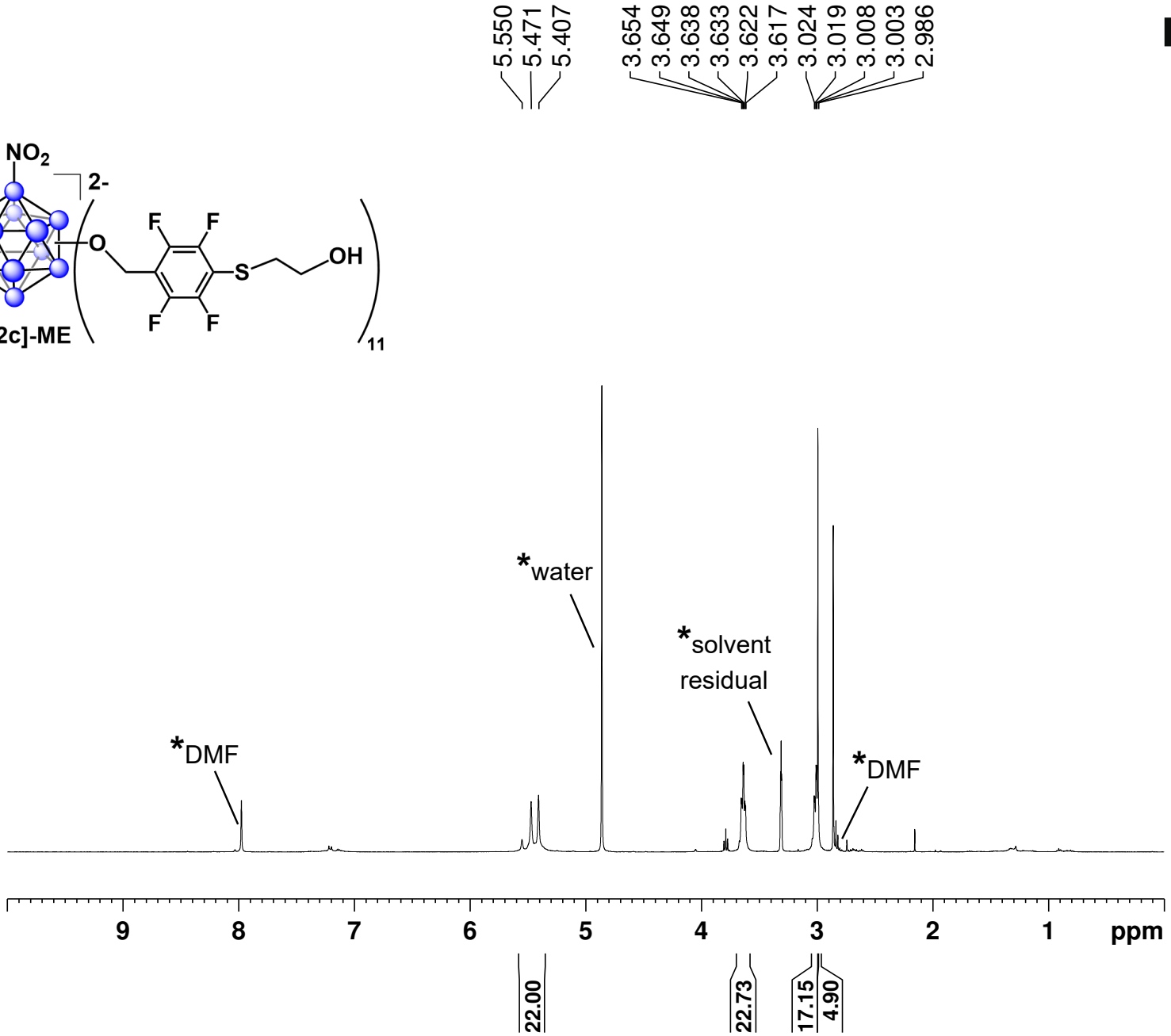
======== CHANNEL f1 ========
SFO1 376.4983660 MHz
NUC1 19F
P1 14.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 262144
SF 376.4981771 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

^{1}H NMR Spectra of **[2c]-ME**



[2c]-ME



Current Data Parameters
NAME Feb28-2018
EXPNO 82
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180228
Time 11.51
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT MeOD
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 155.85
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1

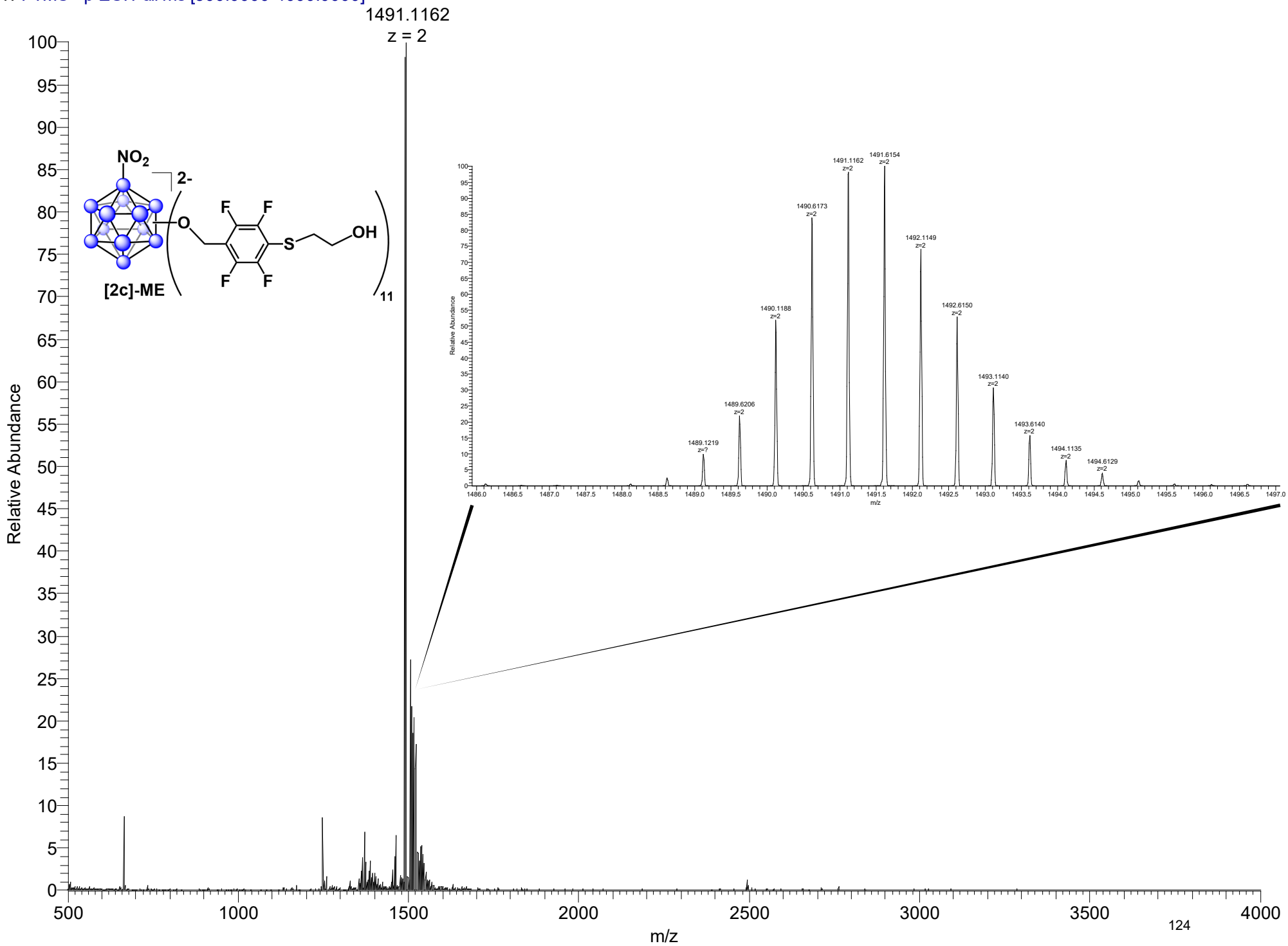
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

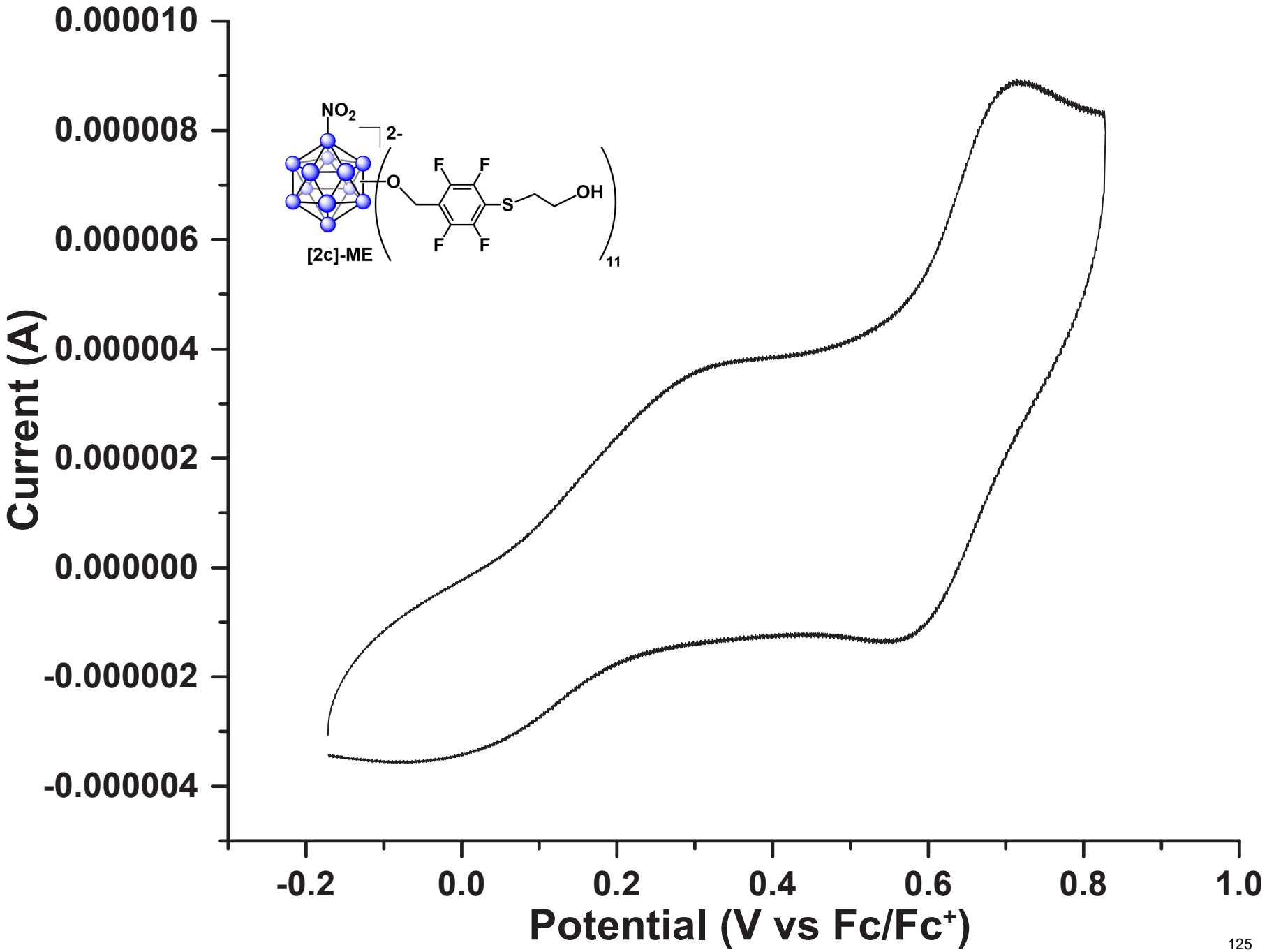
EQ_022618 B12NO2(PFB)11 2ME #1 RT: 0.01 AV: 1 NL: 4.55E6
T: FTMS - p ESI Full ms [500.0000-4000.0000]

HRMS of **[2c]-ME**

[2c]-ME



CV of **[2c]-ME**


0.000010
0.000008
0.000006
0.000004
0.000002
0.000000
-0.000002
-0.000004
Current (A)
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
Potential (V vs Fc/Fc+)
NO2
2-
O
F
F
F
F
S
OH
11
[2c]-ME