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Supporting Information

Synthesis and Application of a Perfluorinated Ammoniumyl Radical Cation as a Very Strong Deelectronator

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Electronic Supporting Information

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Innocence is Bliss: Synthesis and Application of a very strong Perfluorinated Ammoniumyl Radical Cation in Deelectronation Chemistry.

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Contents

S-1 Experimental Details and Characterisation Techniques

All reactions and manipulations were carried out under an inert argon atmosphere, using standard Schlenk-line and glovebox techniques (box atmosphere kept below 1 ppm H_2O/O_2). Glassware has been stored over-night in an oven set to 180°C and flame dried under vacuum prior to use. Decamethyl ferrocene (Acros), Pyrazole (99%, ChemPUR), $LiNH_2$ (Acros), C_6F_6 (fluorochem) were used as received. *tert*-Butylisocyanide (Sigma/Aldrich) was stored of activated 3 Å molecular sieves and then vacuum transferred to new flask to prepare 1 M stock solution with *o*DFB. $Li[Al(OR^F)_4]$ was prepared following reported procedure[1]. Br_2 (99%, Acros) was vacuum transferred prior to use. I_2 (Acros) was sublimed under static vacuum. Pentane was collected from a solvent purification system (SPS) and oxygen removed by purging with Argon. PhF, *o*-DFB, CD_2Cl_2, hexane and heptane were refluxed/stirred over CaH_2 and distilled. All solvents were stored over activated 3 Å molecular sieves in gas tight ampoules.

Powder Diffraction. Powder diffractograms were recorded with the sample sealed with perfluoropolyalkylether oil (AB128330, abcr GmbH & Co. KG) in a 0.3 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) at 100(10) K in the 2θ range 2.0-40.0° with a STOE STADI P powder diffractometer with Mo-$K_{\alpha1}$ radiation (λ = 0.709300 Å) equipped with a Ge-(111) monochromator and Mythen 1K detector. Data acquiring, processing and the calculation of powder diffractograms from single-crystal data were performed using STOE WinXPOW® package. All powder diffractograms were background corrected.

ATR-IR Spectroscopy. ATR FT-IR spectra were recorded at ambient temperature on a ZnSe crystal on a FTIR Bruker ALPHA with a QuickSnap Platinum ATR sampling module inside an inert atmosphere glovebox. Spectra were recorded in a range from 4000-500 cm^{-1}. The spectra were recorded with either 64 or 128 scans and a resolution of 2 cm^{-1}. Data processing was carried out with the software package OPUS 7.5. For all spectra, signal intensity was normalised to one and the relative band intensities were described as follows: ≥ 0.8 = very very strong (vvs), ≥ 0.7 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.5 = medium strong (ms), ≥ 0.4 = medium (m), ≥ 0.3 = medium weak (mw), ≥ 0.2 = weak (w), ≥ 0.1 = very weak (vw), < 0.1 = very very weak (vvw).

Single crystal X-ray diffraction. Single crystal X-ray diffraction data were collected using either a Bruker SMART APEXII QUAZAR detector with fixed-Chi D8 Goniometer, INCOATEC Mo microsource or Bruker D8 VENTURE with PHOTONIII detector, fixed-Chi D8 Goniometer and INCOATEC Mo/Cu microsource. Crystals were selected under perfluoropolyether oil, mounted on 0.1 to 0.3 mm diameter CryoLoops and quench-cooled using an Oxford Cryostream 800 open flow N_2 cooling device.[2] Data were collected at 100 K using monochromated Cu Kα or Mo Kα radiation (λ = 1.5418/0.71073 Å). Data processing was done with SHELXS/XL and refined by least squares on weighted F^2 values for all reflections, disordering

of fragments was done with the help of the implemented DSR tool.[3] Graphical representations have been prepared using Olex2-1.2. Finalisation of gathered data was done using final cif tool.[4]

NMR spectroscopy. NMR samples were prepared inside an inert atmosphere glovebox in either flame sealable NMR tubes or NMR tubes equipped with a gas-tight J.Young valve. ^{1}H, ^{13}C, ^{19}F, ^{27}Al, ^{31}P-NMR spectra were acquired either on a Bruker Biospin Avance II+ 400 MHz WB, a Bruker Avance 200 MHz or a Bruker Avance III HD 300 MHz spectrometer. ^{1}H and ^{13}C NMR spectra are reported relative to TMS and were calibrated to residual solvent resonances.[5] Data analysis was performed using the Bruker TOPSPIN 3.5 software. The broad resonance at δ = 70 ppm observed in ^{27}Al-NMR spectra corresponds to a background from Al-nuclei in the probe head.

EPR spectroscopy. EPR spectroscopic measurements were carried out in the continuous wave (cw) mode at X-band frequency (9.7973 GHz), using a Bruker Elexsys E580 spectrometer equipped with a super-high-Q cavity (4119HS-W1). The experiment were performed at room temperature under liquid-state conditions (SO_2) by using a microwave power of 0.04743 mW and a modulation amplitude of 0.05 mT. A home-written anaylsis program, which is based on the EasySpin simulation package, were used to determine the g-factor, hyperfine couplings and the intrinsic line-width parameter.

Quantum Chemical Calculations. All quantum chemical calculations were carried out with the TURBOMOLE program package using the BP86 functionals with def-SV(P) basis sets and D3(BJ) dispersion correction.[6] Vibrational frequencies were calculated using the AOFORCE-module.[7] All calculated structures were checked for consistency in terms of geometric conversion, sensible electron occupations and the absence of imaginary vibrational frequencies. Thermal contributions to the enthalpy and free energy of the systems were calculated with the FREEH application based on the analysis of the vibrations obtained by BP86/def-SV(P)/D3(BJ) calculations.

S-2 Experimental

S-2.1 Synthesis of $[N(C_6H_4Br\text{-}4)_3][Al(OR^F)_4]$ **S1**

S-2.1.1 Synthesis of **S1** by salt metathesis

$[N(C_6H_4Br\text{-}4)_3][SbCl_6]$ (245 mg, 0.300 mmol) and $Li[Al(OR^F)_4]$ (307 mg, 0.315 mmol, 1.05 eq.) have been dissolved in CH_2Cl_2 (15 ml). The reaction mixture was stirred over night at ambient temperature. The supernatant deep blue solution has been filtered and CH_2Cl_2 was removed under reduced pressure to yield a deep blue precipitate (350 mg, 0.242 mmol, 81%). Crystals suitable for single crystal XRD experiments were obtained upon layering of a solution of **S1** (35 mg) in CH_2Cl_2 (3 ml) with hexane (15 ml).

^{19}F-NMR (282.45 MHz, CD_2Cl_2, 298 K): δ = −75.6 (s, 36F, $[Al\{OC(CF_3)\}_4]^-$) ppm. ^{27}Al-NMR (78.22 MHz, CD_2Cl_2, 298 K): δ = 34.6 (s, 1Al, $[Al\{OC(CF_3)\}_4]^-$) ppm. ESI-MS(source voltage: 20V) positive ion mode: m/z = 402.0 $[C_{36}H_{24}Br_4N_2]^{2+}$ (**S2^{2+}**), 480.8 $[C_{18}H_{12}Br_3N]^+$ (**S1**), 803.8 $[[C_{36}H_{24}Br_4N_2]^+$ (**S2$^+$**). negative ion mode: m/z = 966.9 $[F_{36}C_{16}O_4Al]^-$. ATR-FTIR: *v* = 3096 (vw), 2567 (vw), 1560 (w), 1547 (m), 1486 (vw), 1476 (vw), 1418 (vw), 1352 (vw), 1296 (w), 1273 (m), 1239 (s), 1208 (vs), 1165 (s), 1065 (s), 969 (vs), 969 (vs), 914 (w), 830 (s), 809 (m), 755 (vw), 726 (vs), 617 (vw), 568 (w), 559 (w) cm^{-1}

S-2.1.2 Synthesis of **S1** by oxidation with $Ag[Al(OR^F)_4]$

$N(C_6H_4Br\text{-}4)_3$ (1.45 g, 3.00 mmol) and $Ag[Al(OR^F)_4]$ (3.22 g, 3.00 mmol, 1eq.) have been dissolved in CH_2Cl_2 (6 ml). Upon addition of the solvent an intensive blue colour was observed. The reaction mixture was stirred over night at ambient temperature and then filtered *via* a G4 frit, the precipitate has been washed with CH_2Cl_2 (3 x 6 ml). The solvent was removed under reduced pressure to yield the title compound **1** as a dark blue powder (4.18 g, 2.89 mmol, 96.2%).

ESI-MS(source voltage: 20V) positive ion mode: m/z = 402.2 $[C_{36}H_{24}Br_4N_2]^{2+}$ (**S2^{2+}**), 481.2 $[C_{18}H_{12}Br_3N]^+$ (**S1**). negative ion mode: m/z = 967.7 $[F_{36}C_{16}O_4Al]^-$. ATR-FTIR: *v* = 3101 (vw), 2566 (vw), 1559 (w), 1548 (m), 1485 (vw), 1419 (vw), 1351 (vw), 1296 (w), 1273 (s), 1239 (s), 1209 (vs), 1168 (s), 1065 (s), 1010 (w), 1002 (w), 969 (vs), 914 (w), 830 (s), 810 (m), 755 (vw), 726 (vs), 617 (w), 559 (w) cm^{-1}

S-2.1.3 Synthesis of **S1** by oxidation with Br_2

Perfluorohexane (10 ml) has been added to a mixture of $N(C_6H_4Br\text{-}4)_3$ (0.339 g, 0.705 mmol) and $Li[Al(OR^F)_4]$ (0.686 g, 0.705 mmol, 1eq.). The reaction mixture was degassed by three freeze-pump-thaw cycles and Br_2 (0.0563 g, 0.352 mmol, 0.5 eq.) was condensed onto the reaction mixture at −196 °C. The reaction mixture was allowed to warm to −78 °C and stirred for 30 min. As no colour change was observable the reaction mixture was allowed to warm to room temperature. Slow colour change from the starting orange solution to dark green was observed after 30 min. The reaction mix was stirred over night to yield dark blue precipitate with supernatant colourless solution, which was filtered away *via* a G4 frit. The precipitate was washed with perfluorohexane (3 x 5 ml) and dissolved in CH_2Cl_2 (6 ml). The dark blue solution was filtered and the solvent removed under reduced pressure to yield a dark blue powder contaminated with colourless powder. The powder was again washed with perfluorohexane (3x 5ml) dissolved in CH_2Cl_2 (5 ml) stirred over-night and filtered. The solvent was removed under reduced pressure to yield the title compound **1** as a dark blue powder (0.520 g, 0.358 mmol, 50.9%).

ESI-MS(source voltage: 20V) positive ion mode: m/z = 402.0 $[C_{36}H_{24}Br_4N_2]^{2+}$ (**S2^{2+}**), 480.9 $[C_{18}H_{12}Br_3N]^+$ (**S1**), 803.8 $[[C_{36}H_{24}Br_4N_2]^+$ (**S2$^+$**). negative ion mode: m/z = 967.0 $[F_{36}C_{16}O_4Al]^-$. ATR-FTIR: *v* = 3088 (w), 1897 (vw), 1579 (w), 1560 (w), 1548 (m), 1485 (s), 1424 (w), 1418 (w), 1352 (w), 1311 (m), 1282 (s),

1240 (vs), 1211 (vs), 1177 (s), 1169 (s), 1105 (w), 1066 (vs), 1002 (s), 971 (vs), 914 (w), 831 (m), 812 (vs), 755 (w), 726 (vs), 711 (m), 698 (w), 666 (m), 617 (w), 606 (w), 568 (w), 560 (m) cm^{-1}

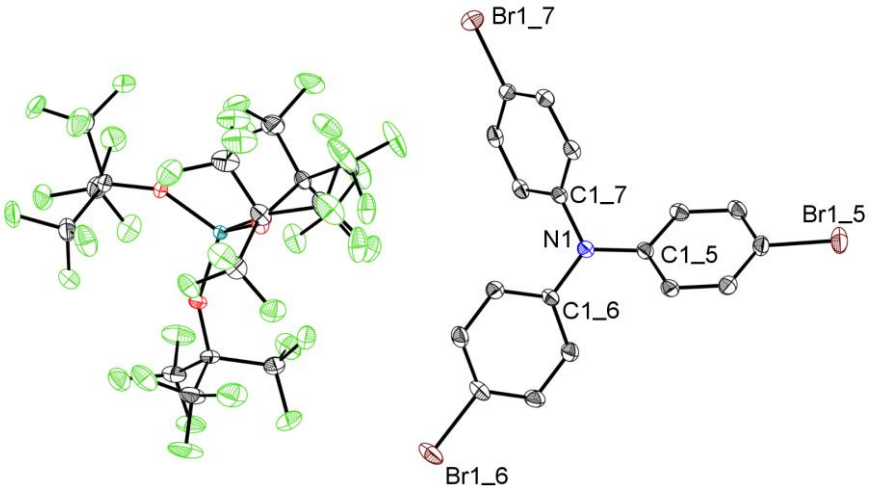


Figure S 1: Molecular structure of $[N(ArBr\text{-}4)_3][Al(OR^F)_4]$ **S1**. Thermal displacement ellipsoids set at 50 % probability. Protons omitted for clarity.

Table S 1: Selected interatomic distances and bond angles found in **S1** compared to bond metrics reported by Quiroz-Guzman *et al.*[8]

Interatomic distances [Å]			
$[N(ArBr\text{-}4)_3][Al(OR^F)_4]$ **1**		$[N(ArBr\text{-}4)_3][SbCl_6]$	$N(ArBr\text{-}4)_3$
N1–C1_5	1.401(3)	1.409(6)	1.416(4)
N1–C1_6	1.406(3)	1.410(6)	1.419(4)
N1–C1_7	1.425(3)	1.414(6)	1.420(4)

Bond angles			
$[N(ArBr\text{-}4)_3][Al(OR^F)_4]$ **1**		$[N(ArBr\text{-}4)_3][SbCl_6]$	$N(ArBr\text{-}4)_3$
C1_5–N1–C1_6	123.2(2)	121.1(4)	122.4(3)
C1_5–N1–C1_7	118.2(2)	119.3(4)	119.3(3)
C1_6–N1–C1_7	118.3(2)	119.6(4)	118.2(3)

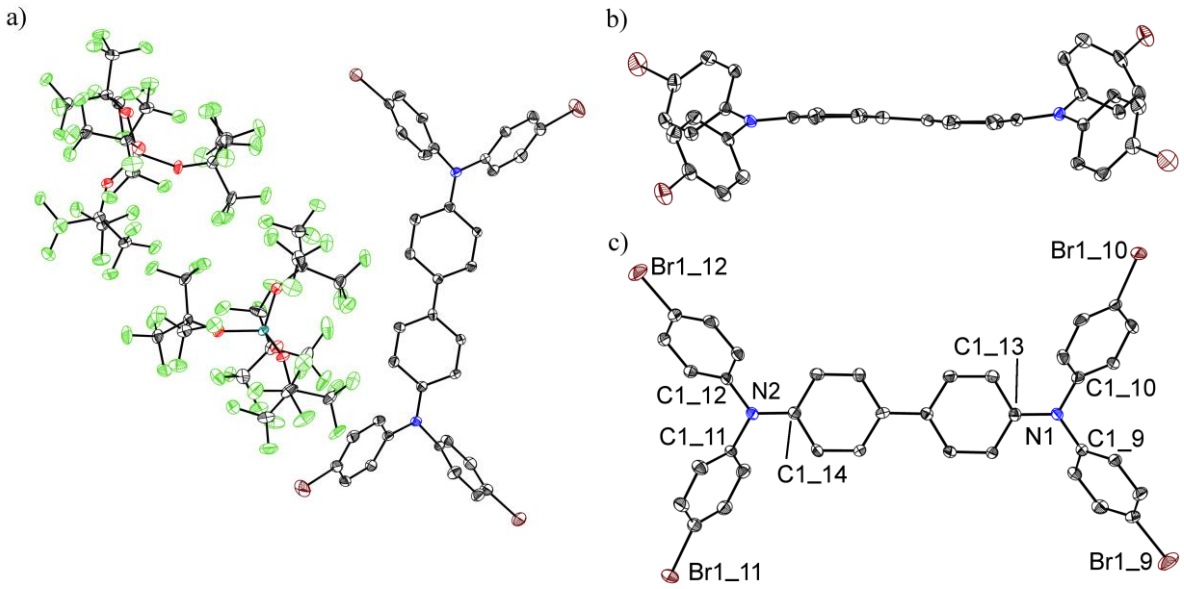


Figure S 2: Molecular structure of a) $[(\mu\text{-}C_{12}H_8)\{N(ArBr\text{-}4)_2\}_2]\{[Al(OR^F)_4]\}_2$ **S2** and molecular structure of the cation in b) side-on and c) top-down view. Thermal displacement ellipsoids set at 50 % probability. Protons omitted for clarity.

Table S 2: Selected interatomic distances and bond angles found in **S2**.

Interatomic distances [Å]		Bond angles	
N2–C1_12	1.425(5)	C1_14–N2–C1_11	119.1(3)
N2–C1_11	1.445(5)	C1_14–N2–C1_12	124.0(3)
N2–C1_14	1.353(5)	C1_12–N2–C1_11	116.8(3)
N1–C1_10	1.426(5)	C1_13–N1–C1_10	122.2(3)
N1–C1_9	1.427(5)	C1_13–N1–C1_9	119.7(4)
N1–C1_13	1.356(5)	C1_10–N1–C1_9	118.0(3)

S-2.2 Reactions between **S1** and σ-Donor Ligands

S-2.2.1 Reaction between **S1** and DMAP

DMAP (25 mg, 205 mmol, 1.12 eq.) dissolved in *o*-DFB (3 ml) was added to a stirred solution of **S1** (267 mg, 0.184 mmol) in *o*-DFB (3 ml). A quick colour change from opaque dark blue to translucent orange-red was observed after completed addition. The solvent was removed under reduced pressure and pentane (10 ml) was added to the dark red-brown residual oil. The mixture was stirred over-night. The supernatant pentane solution was filtered. The beige brown precipitate was washed with pentane (5 ml) and redissolved in *o*-DFB (3 ml) to give a cloudy orange-red solution. Colourless single crystals suitable for single crystal X-ray diffraction analysis were grown by layering of a solution of the washed products with hexanes (15 ml).

^{1}H-NMR (400.16 MHz, CD_2Cl_2, 298 K): unknown comp. 1 δ = 7,94 (m, AA´BB´, Pyr–*H*), 6.764 (m, AA´BB´, Pyr–*H*), 3.22 (s, N(C*H*$_3$)$_2$) ppm. unknown comp. 2 δ = 8.363 (m, AA´BB´, Pyr–*H*), 6.758 (m, AA´BB´, Pyr–*H*), 3.22 (s, N(C*H*$_3$)$_2$) ppm. unknown comp 3 δ = 7.75 (m, AA´BB´, 6.79 (m, AA´BB´, Pyr–*H*), 3.25 (s, N(C*H*$_3$)$_2$) ppm. unknown comp 4 δ = 7.48 (m, AA´BB´, Pyr–*H*), 6.55 (m, AA´BB´, Pyr–*H*), 5.60 (s, N(CH$_3$)C*H*$_n$X$_{3-n}$ (n = 1,2)), 3.22 (s, N(C*H*$_3$)CH$_n$X$_{3-n}$ (n = 1,2)), unknown comp 5 δ = 7.34 (m, AA´BB´), 6.73 (m, AA´BB´) ppm. ^{13}C-NMR (100.62 MHz, CD_2Cl_2, 298 K): unknown comp. 1 δ = 139.9 (Pyr), 107.6 (Pyr), 40.1 (N(*C*H$_3$)$_2$) ppm. unknown compound 2 δ = 149.9 (Pyr), 107.6 (Pyr) ppm. unknown compound 3 δ = 137.9 (Pyr), 108.5 (Pyr), 40.43 (N(*C*H$_3$)$_2$) ppm. unknown compound 4 δ = 141.79 (Pyr), 107.5 (Pyr), 72.43 (N(CH$_3$)(*C*H$_n$X$_{3-n}$ (n = 1,2)), 37.86 ((N(*C*H$_3$)(CH$_n$X$_{3-n}$ (n = 1,2)) ppm. unknown compound 5 δ = 132.82 (Ar–H), 124.25 (Ar–H) ppm. ^{19}F-NMR (282.45 MHz, CD_2Cl_2, 298 K): δ = −75.8 (s, 36F, [Al{OC(C*F*$_3$)}$_4$]$^-$) ppm. ^{27}Al-NMR (78.22 MHz, CD_2Cl_2, 298 K): δ = 34.6 (s, 1Al, [Al{OC(C*F*$_3$)}$_4$]$^-$) ppm. ESI-MS(source voltage: 20V) positive ion mode: m/z = 123.1 [$C_7H_{11}N_2$]$^+$, 164.1 [$C_9H_{14}N_3$]$^+$, 243.2 [$C_{14}H_{19}N_4$]$^+$, 604.0 [$C_{25}H_{21}Br_3N_3$]$^+$ (**2a**). negative ion mode: m/z = 967.0 [$F_{36}C_{16}O_4Al$]$^-$.

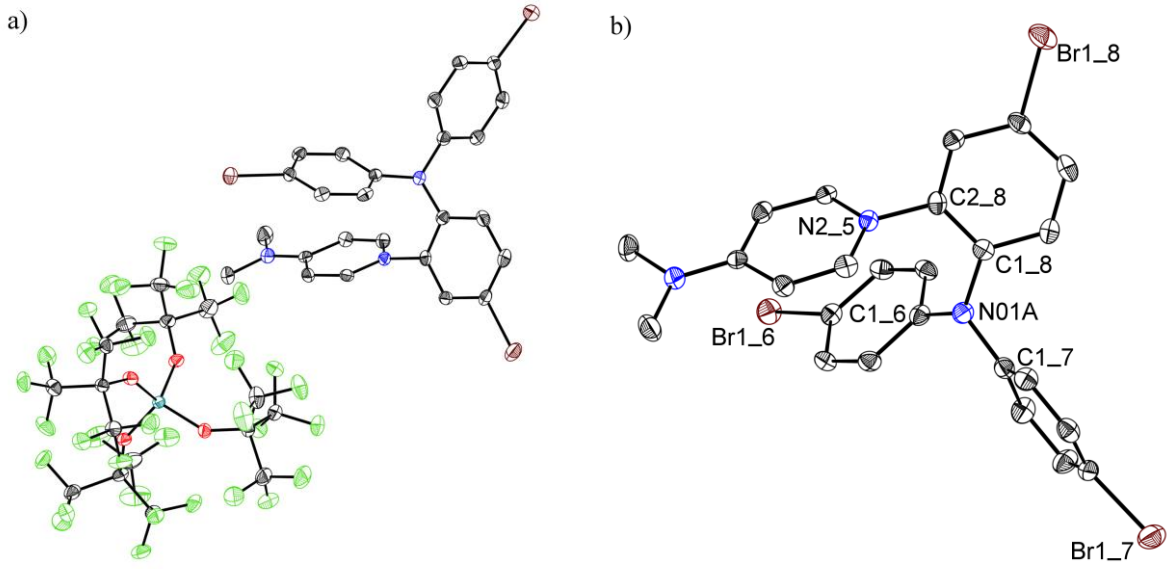


Figure S 3: Molecular structure of a) DMAP magic blue substitution product **S3** and b) structure of the cation. Thermal displacement ellipsoids set at 50 % probability. Protons omitted for clarity.

Table S 3 Selected interatomic distances and bond angles in **S3**.

Bond distances [Å]	
N01A–C1_8	1.418(4)
N01A–C1_6	1.429(4)
N01A–C1_7	1.432(4)
N2_5–C2_8	1.443(4)

Bond angles	
C1_8–N01A–C1_6	116.7(2)
C1_8–N01A–C1_7	118.8(2)
C1_6–N01A–C1_7	119.1(2)

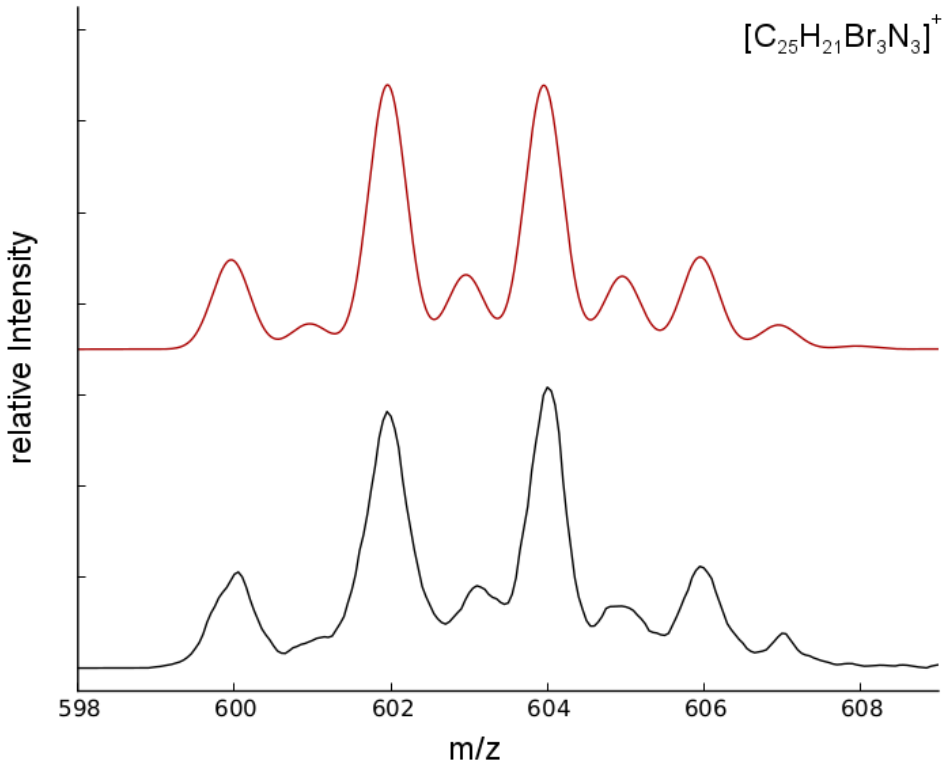


Figure S 4: Simulated (red) and found (black) isotope pattern of the DMAP magic blue substitution product **S3**.

S-2.2.2 Reaction between **S1** and IPr.

IPr (78 mg, 0.200 mmol) and **S1** (272 mg, 0.188 mmol, 0.94 eq.) have been dissolved in Et_2O under stirring at ambient temperature. A quick colour change from opaque dark blue to translucent orange-red was observed upon addition of the solvent. The solvent was removed under reduced pressure and the resulting dark brown oil was washed with pentane (3 x 5 ml) and dried under vacuum. The dark brown oil was dissolved in *o*-DFB (3 ml) and layered with pentane (10 ml). The product oiled out over-night. After inverting the layer tube light orange crystals suitable for X-ray diffraction analysis were obtained.

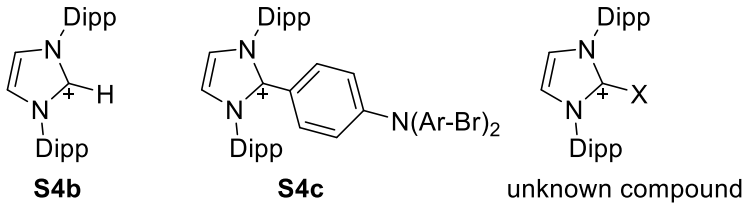


Figure S 5: Major products assignable by NMR spectroscopy.

^{1}H-NMR (400.16 MHz, CD_2Cl_2, 298 K): comp. **S4b** δ = 8.30 (t, ^4J = 1.6 Hz, 1H, –N–C*H*–N–), 7.68 (t, ^3J = 7.9 Hz, 4H, *p*(Dipp)–C*H*), 7.62 (d, ^4J = 1.6 Hz, 2H, –N–(C*H*)$_2$–N–), 7.46 (d, ^3J = 7.9 Hz, 8H, *m*(Dipp)–C*H*), 2.38 (sept, ^3J = 6.9 Hz, 4H, –C*H*(CH_3)$_2$), 1.32 (d, ^3J = 6.9 Hz, 12H, –CH(C*H*$_3$)$_2$), 1.24 (d, ^3J = 6.9 Hz,

12H, –CH(CH_3)$_2$) ppm. comp. **S4c** δ = 7.63 (t, ^3J = 7.9 Hz, 4H, *p*(Dipp)–C*H*), 7.46 (s, 2H, –N–(C*H*)$_2$–N–),7.42 (m, AA´BB´, 4H, *m*(N(ArBr-4)$_2$)–C*H*), 7.40 (d, ^3J = 7.9 Hz, 8H, *m*(Dipp)–C*H*), 6.84 (m, AA´BB´, 4H, *o*(N(ArBr-4)$_2$–C*H*), 6.71 (m, AA´BB´, 2H, *m*(IPr–C_4H_4–N–)–C*H*), 6.67 (m, AA´BB´, 2H, *o*(IPr–C_4H_4–N–)–C*H*)), 2.43 (sept, ^3J = 6.8 Hz, 4H, –C*H*(CH$_3$)$_2$), 1.26 (d, ^3J = 6.8 Hz, 12H, –CH(CH_3)$_2$), 1.06 (d, ^3J = 6.8 Hz, 12H, –CH(CH_3)$_2$) ppm. unknown comp. δ = 7.732 (t, ^3J = 7.9 Hz, 4H, *p*(Dipp)–C*H*), 7.730 (s, 2H, –N–(C*H*)$_2$–N–), 7.49 (d, ^3J = 7.9 Hz), 2.27 (sept, 4H, ^3J = 6.9 Hz, –C*H*(CH$_3$), 1.29 (d, 12H, ^3J = 6.9 Hz, –CH(CH_3), 1.29 (d, 12H, ^3J = 6.9 Hz, –CH(CH_3) ppm. ^{13}C-NMR (100.62 MHz, CD_2Cl_2, 298 K): comp. **S4b** δ = 144.9 (*o*(Dipp)–*C*–CH(CH$_3$)), 136.6 (–N–*C*H–N–), 133.52 (*p*(Dipp)–*C*H), 126.2 (–N–(*C*H)$_2$–N–), 125.5 (*m*(Dipp)–*C*H), 29.4 (–*C*(CH$_3$)$_2$),24.3 (–C(*C*H$_3$)$_2$), 23.3 (–C(*C*H$_3$)$_2$) ppm. comp **S4c** δ = 150.9 (*p*(IPr–C_6H_4N–)–*C*), 145.9 (–N–*C*(C_6H_4N(ArBr-4)$_2$)–N–), 144.5 (*o*(Dipp)–*C*–CH(CH$_3$)), 143.9 (*ipso*(–N(C_6H_4Br))–*C*Br), 133.6 (*m*(–N(C_6H_4Br))–*C*H), 132.9 (*p*(Dipp)–*C*H), 130.2 (*m*(IPr–C_6H_4N–)–*C*H), 127.7 (*o*(–N(C_6H_4Br))–*C*H), 126.0 (*m*(Dipp)–*C*H), 125.2 (–N–(*C*H)$_2$–N–), 119.0 (*o*(IPr–C_6H_4N–)–*C*H), 118.9 (*p*(–N(C_6H_4Br)–*C*N–), 110.9 (*ipso*(IPr–C_6H_4N–)–*C*N–), 29.4 (–*C*(CH$_3$)$_2$), 24.7 (–C(*C*H$_3$)$_2$), 22.1 (–C(*C*H$_3$)$_2$) ppm. unknown compound δ = 144.9 (*o*(Dipp)–*C*–CH(CH$_3$)$_2$), 133.8 (*p*(Dipp)–*C*H), 127.2 (–N–(*C*H)$_2$–N–), 125.8 (*m*(Dipp)–*C*H), 29.7 (–*C*H(CH$_3$)$_2$), 23.9 (–CH(*C*H$_3$)$_2$), 22.8 (–CH(*C*H$_3$)$_2$) ppm. ^{15}N-NMR (40.54 MHz, CD_2Cl_2, 273 K): comp **S4b** δ = 185.5 (–*N*–(CH)$_2$–*N*–) ppm. comp **S4c** δ = 176.4 (–*N*–(CH)$_2$–*N*–), 104.7 (IPr–(C_6H_4)–*N*(ArBr-4)$_2$) ppm. unknown compound δ = 188.9 (–*N*–(CH)$_2$–*N*–) ppm. ^{19}F-NMR (376.54 MHz, CD_2Cl_2, 298 K): δ = −75.7 (s, 36F, [Al{OC(CF_3)}$_4$]$^-$) ppm. ^{27}Al-NMR (104.27 MHz, CD_2Cl_2, 298 K): δ = 34.6 (s, 1Al, [Al{OC(CF_3)}$_4$]$^-$) ppm. ESI-MS(source voltage: 20V) positive ion mode: m/z = 389.4 $[C_{27}H_{37}N_2]^+$ (**S4b**), 467.2 $[C_{27}H_{36}BrN_2]^+$, 628.7 $[C_{72}H_{82}Br_3N_5]^{2+}$, 790.2 $[C_{45}H_{48}Br_2N_3]^+$ (**3c**), 868.1 $[C_{45}H_{47}Br_3N_3]^+$ (**S4**). negative ion mode: m/z = 967.0 $[F_{36}C_{16}O_4Al]^-$ m/z

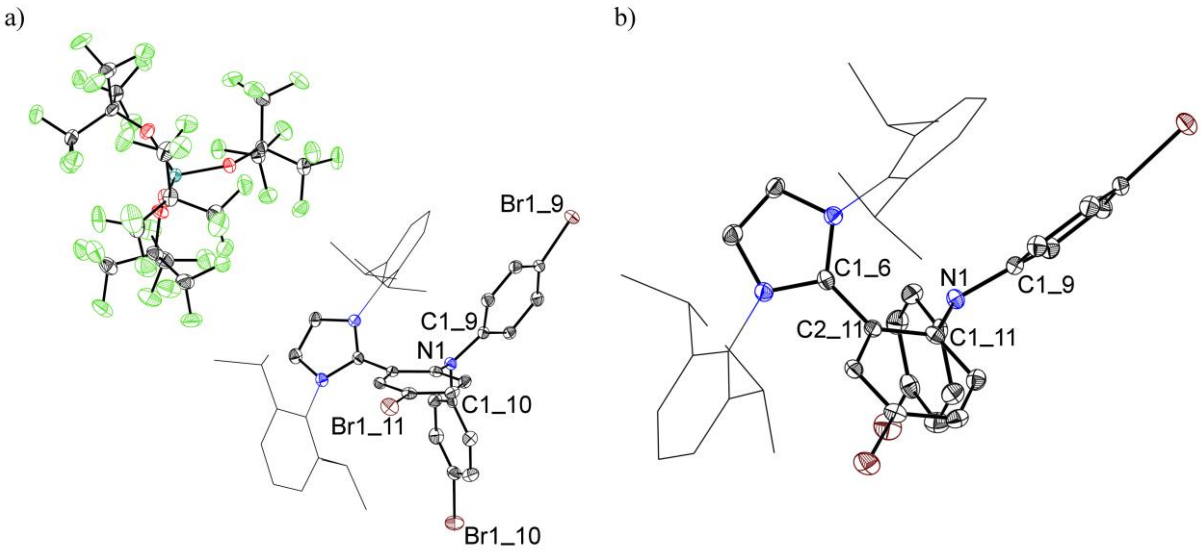


Figure S 6: Molecular structure of a) IPr magic blue substitution product **S4** and b) structure of the cation. Thermal displacement ellipsoids set at 50 % probability. Dipp groups drawn as wireframe and Protons omitted for clarity.

Table S 4: Selected interatomic distances and bond angles in **S4**.

Interatomic distances [Å]	
N1–C1_9	1.430(3)
N1–C1_11	1.431(3)
N1–C1_10	1.449(3)
C1_6–C2_11	1.478(3)

Bond angles	
C1_9–N1–C1_11	117.31(17)
C1_9–N1–C1_10	118.33(17)
C1_11–N1–C1_10	113.26(17)

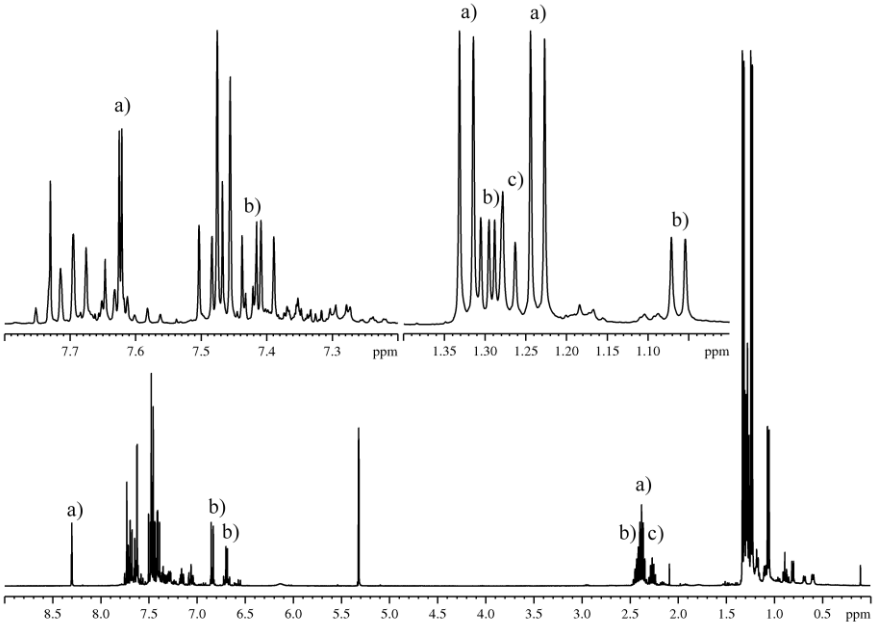


Figure S 7: ^{1}H-NMR (400.17 MHz, CD_2Cl_2,298 K) spectrum of isolated crystals. Selected resonances have been assigned to the three major products a), b) and c) (**Fehler! Verweisquelle konnte nicht gefunden werden.**) for clarification.

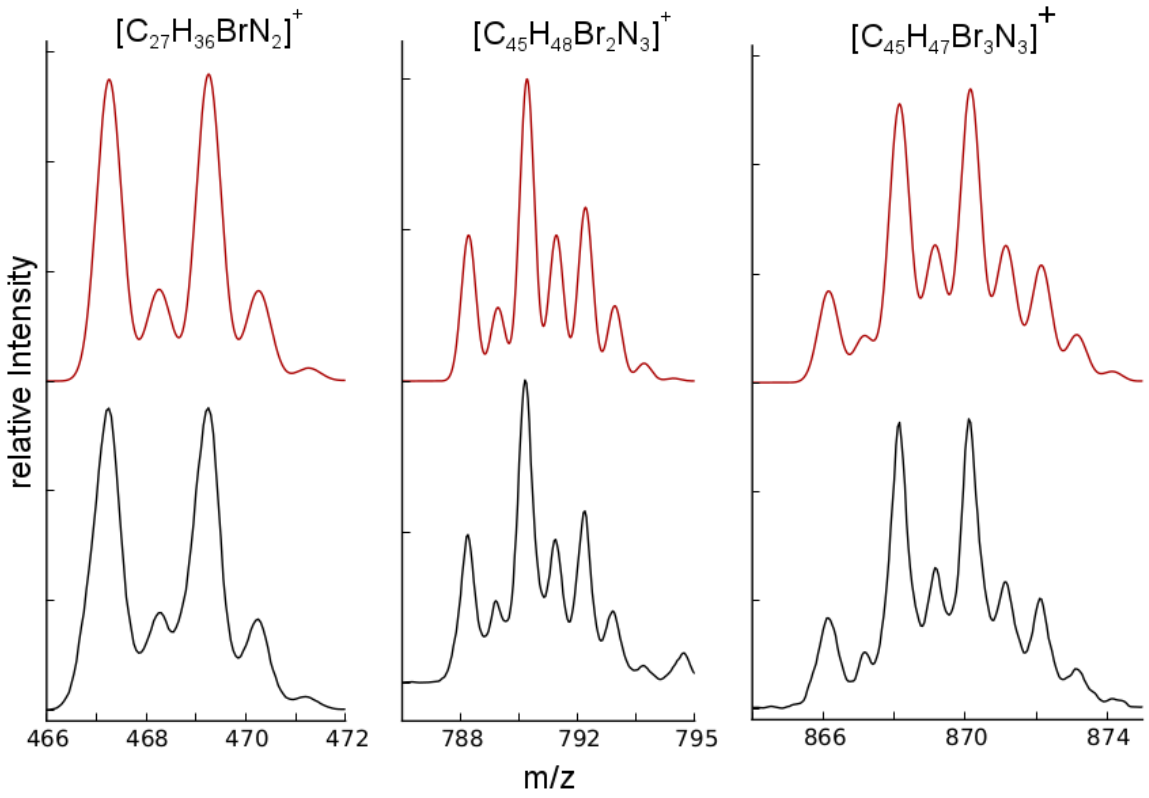


Figure S 8: Selected simulated (red) and found (black) isotopic distribution patterns for $[IPr\text{-}Br]^+$ (left), **S4c** (middle), and **S4** (right).

S-2.2.3 Reaction between **S1** and PPh_3

PPh_3 (52 mg, 0.200 mmol) and **S1** (278 mg, 0.192 mmol, 0.96 eq.) have been weighed into a H-cell equipped with a G4 frit, and dissolved in CH_2Cl_2 (4 ml) under stirring at ambient temperature. Upon addition of the solvent a rapid colour change from dark opague blue to bright yellow was observed within a minute. After complete colour change the solvent was removed under reduced pressure. The bright yellow residue was washed with pentane (3 x 5 ml). The collected pentane extract was freed from volatiles under reduced pressure to yield a colourless powder, which was shown by ^1H and ^{31}P-NMR to consist of PPh_3 and $N(ArBr\text{-}4)_3$. The bright yellow residue was redissolved in CH_2Cl_2 to yield a cloudy bright yellow solution, which was filtered into another vessel and concentrated under reduced pressure. Crystals suitable for scXRD were grown from the concentrated solution at −40 °C.

$^1H\{^{31}P\}$-NMR (400.16 MHz, CD_2Cl_2, 298 K): $[Ph_3POEt]^+$ δ = 7.78 (m, Ph–*H*), 7.75 (m, Ph–*H*), 7.69 (m, Ph–*H*), 4.29 (q, ^3J = 7.1 Hz, 2H, –OC*H*$_2$–), 1.50 (t, ^3J = 7.1 Hz, 3H, –OCH$_2$–C*H*$_3$) ppm. $N(ArBr\text{-}4)_3$ δ = 7.37 (m, AA´BB´, 6H, N(C$_6$*H*$_4$Br), 6.94 (m, AA´BB´, 6H, N(C$_6$*H*$_4$Br) ppm. unknown compound δ = 7.88 (m, Ph–H), 7.72 (m, Ph), 7.53 (br. s, AA´BB´), 7.29 (m, Ph), 7.12 (m, AA´BB´, 1,2-X$_2$C$_6$*H*$_4$) ppm. ^{31}P-NMR (161.99 MHz, CD_2Cl_2, 273 K): $[Ph_3POEt]^+$ δ = 62.1 (s, $[Ph_3POEt]^+$) ppm. unknown compound δ = 22.1 (s) ppm. not assignable resonances δ = 43.5 (br.s), 22.9 (s), 22.7 (s), 21.4 (s), 8.8 (br. s), 7.6 (br. s) ppm ^{19}F-NMR (376.54 MHz, CD_2Cl_2, 298 K): δ = −75.7 (s, 36F, $[Al\{OC(CF_3)\}_4]^-$) ppm. ^{27}Al-NMR (104.27 MHz, CD_2Cl_2, 298 K): δ = 34.6 (s, 1Al, $[Al\{OC(CF_3)\}_4]^-$) ppm. ESI-MS(source voltage: 20V) positive ion mode:

m/z = 263.1 $[C_{18}H_{16}P]^+$, 279.1 $[C_{18}H_{16}OP]^+$, 307.1 $[C_{20}H_{20}OP]^+$, 557.2 $[C_{36}H_{31}O_2P_2]^+$, 664.0 $[C_{36}H_{27}Br_2NP]^+$. negative ion mode: m/z = 967.0 $[F_{36}C_{16}O_4Al]^-$.

S-2.3 Synthesis of starting materials

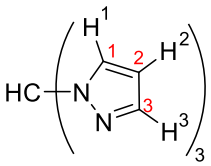
S-2.3.1 Synthesis of $Ag[Al(OR^F)_4]$

$Li[Al(OR^F)_4]$ (10.7 g, 11.0 mmol) and AgF (2.79 g, 22.0 mmol, 2.00 eq.) have been weighed into an H-cell equipped with a G4 frit. SO_2 (~10 ml) has been condensed at −78 °C onto the reaction mixture. The coffee brown solution was stirred for 9 days at ambient temperature, until the colour noticeably brightened. The mixture was allowed to settle and the supernatant solution filtered over the G4 frit. The filter residue was washed by recondensing SO_2 at −78 °C and filtering away from the residue. After three washing cycles the solvent has been condensed back into to the stock bottle, residual solvent was removed under reduced pressure and the title compound was received as a colourless powder (10.4 g, 9.69 mmol, 88.1%).

^{19}F-NMR (282.45 MHz, CD_2Cl_2/Et_2O, 298 K): δ = −75.6 (s, 36F, $[Al\{OC(CF_3)\}_4]^-$) ppm. ^{27}Al-NMR (78.22 MHz, CD_2Cl_2/Et_2O, 298 K): δ = 34.6 (s, 1Al, $[Al\{OC(CF_3)\}_4]^-$) ppm.

S-2.3.2 Synthesis of trispyrazolylmethane $CHpz_3$

Pyrazole (12 g, 176 mmol) and NBu_4Br (2.8, 8.8 mmol, 5 mol %) were suspended in H_2O (300 ml). Na_2CO_3 (114 g, 1075 mmol, 6.1 eq.) were added under vigorous stirring. The reaction mixture was stirred for 1 h at ambient temperature. Then $CHCl_3$ (90 ml) was added and the mixture refluxed at 70°C for 3 d. The reaction mixture was filtered and Et_2O (300 ml) added to the filtrate. The aqeuos phase was separated, extracted with Et_2O (3 x 50 ml). The combined organic phases were washed with water (3 x 100 ml), brine (100 ml), dried over $MgSO_4$ and charcoal. The solvent of the filtered colourless solution was removed at reduced pressure and leftover pyrazole removed by sublimation at 80°C. $CHpz_3$ was obtained as colourless solid (7.31 g, 58.8 mmol, 58 %).



^{1}H-NMR (300.18 MHz, CD_3CN, 298 K): δ = 8.54 (s, 1 H, *H*Cpz_3), 7.68 (m, 3 H, pz H^3), 7.63 (m, 3 H, pz H^1), 6.39 (m, 3 H, pz H^2) ppm. ^{13}C-NMR (75.48 MHz, CD_3CN, 298 K): δ = 141.6 (s, pz C^3), 129.8 (s, pz C^1), 107.0 (s, pz C^2), 82.7 (s, H*C*pz_3).

S-2.3.3 Synthesis of $[FeCp^*_2][Al(OR^F)_4]$ **S5**

$FeCp^*_2$ (0.23 g, 0.70 mmol) was dissolved in CH_2Cl_2 (4 ml) and added to a solution of $NO[Al(OR^F)_4]$ (0.70 g, 0.70 mmol) in CH_2Cl_2 (8 ml) at ambient temperature and stirred for 3 h. The solvent was

removed under reduced pressure and the dark green precipitate washed with n-pentane (3 x 6 ml). $[FeCp^*_2][Al(OR^F)_4]$ was received as green solid (0.89 g, 0.69 mmol, 98 %). Crystals suitable for X-ray diffraction analysis were grown from concentrated CH_2Cl_2 solutions by layering with n-pentane (see Figure S 9).

The obtained crystals showed severe super structure as visible by large cell containing in total 24 formula units. Because of the poor quality of the obtained structure ($wR_2 = 0.38$) we decided to not upload the data to the CCDC. The obtained model was only used for simulation powder XRD pattern for phase purity analysis of **S5**.

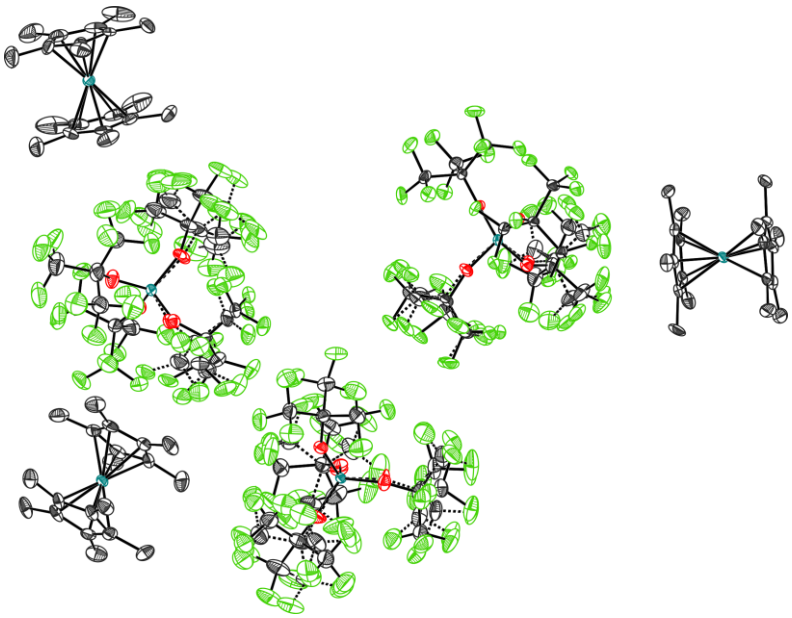


Figure S 9 asymmetric unit of crystals of $[FeCp^*_2][Al(OR^F)_4]$. H-atoms omitted for clarity. All disordered components shown. Thermal displacement ellipsoids set at 50% probability. Please note that collected crystals most likely contains a super structure as visible by large cell, poor refinement quality ($wR_2 = 0.38$) and residual electron density mostly in the anionic part which can not easily be modelled by additional disorder.

S-2.4 Synthesis of Phenazin^F **3**

S-2.4.1 Synthesis of $HNAr^F_2$ ($Ar^F = C_6F_5$) **1**

$$3\ LiNH_2 + 2\ C_6F_6 \xrightarrow[\text{THF, 80°C}]{\text{- 2 NH}_3\ \text{- 2 LiF}} HN(C_6F_5)_2$$

$LiNH_2$ (10.0 g, 436 mmol) was suspended in THF (100 ml). C_6F_6 (42.2 ml, 366 mmol, 0.84 eq.) were slowly added at 0 °C and the reaction mixture stirred for 30 min at this temperature and then heated for reflux for 9 h. First Et_2O (100 ml) and then HCl (10%, 100ml) were added to the dark brown reaction mixture. The organic layer was separated and the aqeous layer extracted with Et_2O (3 x 50 ml). The combined organic phases were washed with H_2O (50 ml) and brine (50 ml) and dried over $MgSO_4$.

Solvent was removed under reduced pressure and the crude product purified by sublimation at 70 °C under dynamic vacuum to yield **1** as a colourless solid (44.5 g, 127.5 mmol, 87.8 %).

^{1}H-NMR (200.12 MHz, CD_3CN, 298 K) δ = 6.58 (s, 1 H, *H*-N(C_6F_5)$_2$) ppm. ^{19}F-NMR (188.31 MHz, CD_3CN, 298 K) δ = −155.3 (m, 4 F, *ortho*-F, **1**), −165.9 (m, 4 F, *meta*-F, **1**), −166.5 (m, 2 F, *para*-F, **1**) ppm.

S-2.4.2 Synthesis of solvent free LiNAr$^{F}_2$ **2**

1 (20.0 g, 57.3 mmol) was dissolved in *o*DFB (50 ml) and slowly added to a stirred solution of LiHMDS (10.5 g, 63.0 mmol, 1.1 eq.) in *o*DFB (100 ml) at 0°C. After complete addition a colourless precipitate is rapidly formed solidifying the reaction mixture. Additional *o*DFB (30 ml) was added and the reaction mixture stirred for 12 h at ambient temperature and then stored for 1 d at −28°C. The solvent was filtered off and the precipitate washed with n-pentane (3 x 30 ml) and dried under reduced pressure to yield **2** as colourless powder (18.48 g, 52.0 mmol, 91 %). Single crystals of the respective difluorobenzene adduct **2**·*o*DFB were grown from concentrated *o*DFB solution (see Figure S 10). NMR of isolated dried **2** in proteo-THF revealed 3% *o*DFB in respect to **2** ensuring complete removal of *o*DFB from the adduct.

^{19}F-NMR (188.31 MHz, *o*DFB, 298 K) δ = −162.3 (d, 4 F, *ortho*-F, **2**), −166.6 (dd, 4 F, *meta*-F, **2**), −173.7 (m, 2 F, *para*-F, **1**) ppm. ^{7}Li-NMR (188.31 MHz, *o*DFB, 298 K) δ = 1.45 ppm.

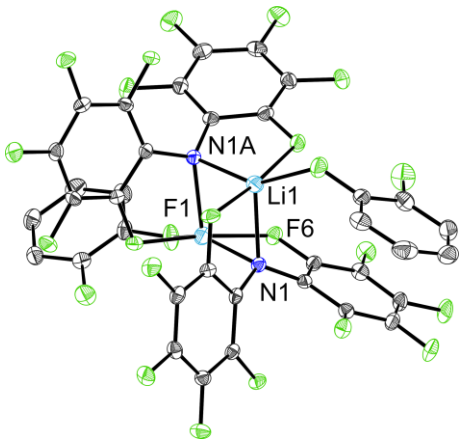


*Figure S 10 molecular structure of **2**·**oDFB**. Protons omitted for clarity. Thermal displacement ellipsoids set at 50 % probability.*

S-2.4.3 Synthesis of perfluoro-5,10-bis(perfluorophenyl)-5,10-dihydrophenazine **3** (phenazine^{F})

2 (8.0 g, 23 mmol) was placed in a Schlenktube and under slow stirring and dynamic vacuum heated to 180 °C and then 200 °C on a fitted aluminium block. When the set point was reached, the tap to the vacuum manifold was closed. After 1 h hour the reaction proceeded instantaneous forming a white precipitate on the walls of the schlenktube together with a highly viscous black oil in the bottom of the

tube. The combined residue was dissolved in hot MeCN (200 ml) and filtered hot. H_2O was added to the MeCN solution to precipitate crude **3** (3.9 g, 5.92 mmol, 52.6 %) free of **1** & **2** but contaminated with an unknown impurity by less than 20 % as determined by NMR. Crude **3** was further purified by sublimation under dynamic vacuum at 170 °C to yield **3** as off-white solid (2.83 g, 4.29 mmol,38 %). Note that impurities in crude **3** form a highly viscous oil during sublimation limiting the liberation of pure **3**. Crystals suitable for X-ray diffraction analysis were grown from concentrated CH_2Cl_2 solution (see Figure S 11 right).

^{19}F-NMR (282.45 MHz, $CDCl_3$, 298 K): δ = −141.6 (m, AA´BB´C, 4F, F^5), −150.4 (m, AA´BB´C, 2F, F^7), −154.3 (m, AA´BB´, 4F, F^1), −160.3 (m, AA´BB´, 4F, F^2), −161.2 (m, AA´BB´C, 4F, F^6) ppm. ^{13}C-NMR (100.62 MHz, CD_2Cl_2, 298 K): δ = 147.4 (s, 4C, C^3), 142.7 (s, 2C, C^5), 139.0 (s, 4C, C^2), 138.5 (s, 4C, C^1), 137.8 (s, 4C, C^4), 122.1 (s, 4C, C^6), 117.5 (s, 2C, C^7) ppm.

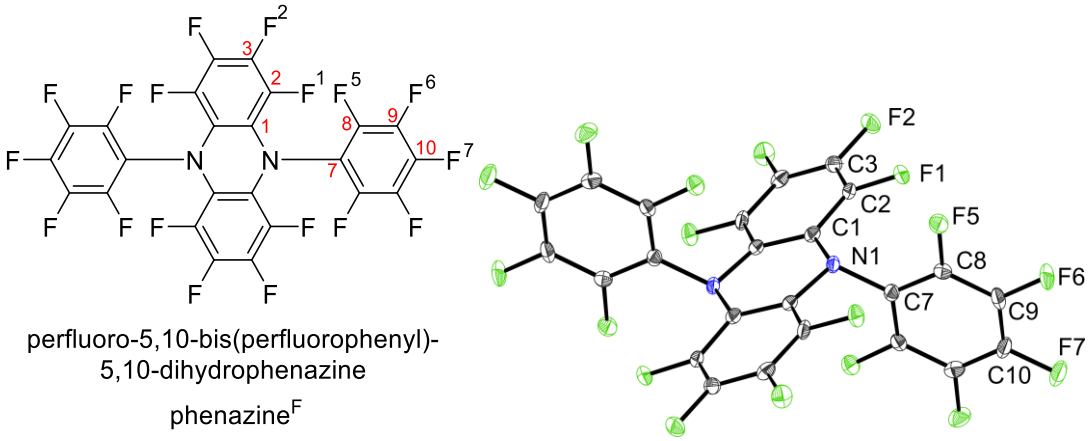


*Figure S 11 (left) numbering scheme of fluorine (black) and carbon (red) atoms for NMR analysis. (right) Molecular structure of **3**. Thermal ellipsoids set at 50% probability.*

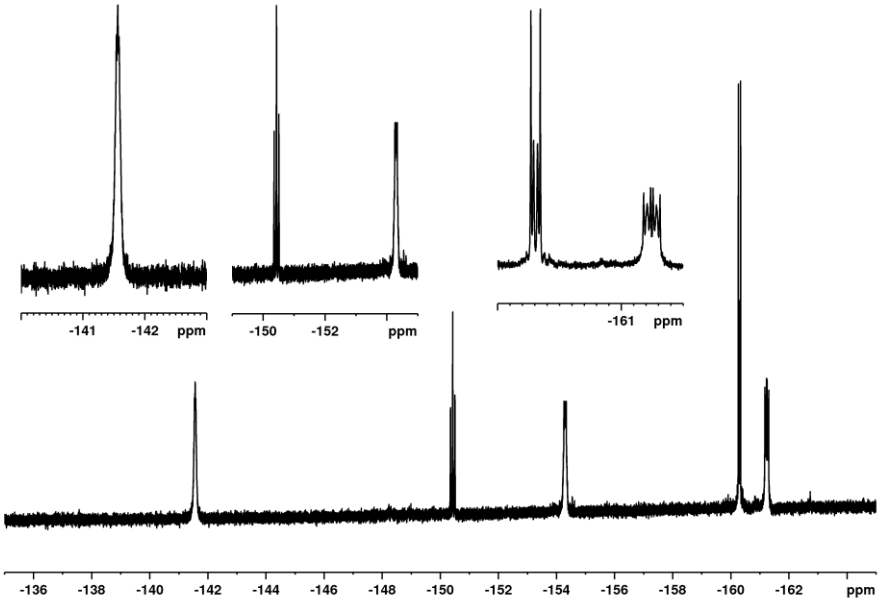


*Figure S 12 ^{19}F-NMR (282.45 MHz, CDCl3, 298 K) of **3**.*

Cyclovoltammetric measurements: For collection of CV measurements a three electrode set up, consisting of a Pt-net working electrode a Pt-wire counterelectrode and a Pt/Pt^+ quasi-reference electrode was chosen. Blank measurements were collected with a 100 mMol solution of conducting salt $[NBu_4][Al(OR_F)_4]$ in the respective solvent. After that the analyte **3** was added to a concentration of 10 mMol. For referencing of the obtained oxidation waves, $FeCp_2$ was added to the mixture. In the case of *o*DFB the oxidation wave of **3** vanished upon addition of $FeCp_2$. **3** in *o*DFB was therefore by the same method referenced against $N(C_6H_4Br)_3$ ("magic blue"), which itself was separately referenced against $FeCp_2$. Analysis of the collected fully reversible oxidation waves gave a half-wave potential for **3** of 1.21 V in MeCN and 1.29 V in *o*DFB against Fc^+/Fc (see Figure S 13).

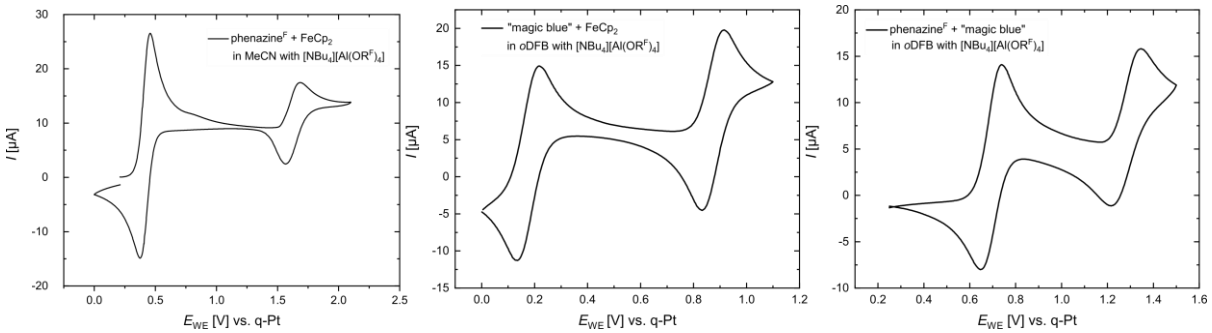


*Figure S 13 cyclovoltammetric measurements of (left) **3** and $FeCp_2$ in MeCN, (middle) "magic blue" and $FeCp_2$ in oDFB and (right) **3** and "magic blue" in oDFB.*

S-2.5 Synthesis of [phenazine^F][Al(OR^F)$_4$] **4**

3 (0.900 g, 1.367 mmol) and Ag[Al(OR^F)$_4$] (1.47 g, 1.367 mmol, 1 eq.) were placed in one arm of an H-cell equipped with a G4 frit. Br_2 (0.3 ml, 5.9 mmol, 4.3 eq.) was dissolved in SO_2 (5 ml) and the mixture condensed into the empty arm of the H-cell. The Br_2/SO_2 solution was then poured onto the reaction mixture through the frit, which resulted in immediate colour change to deep purple. The reaction mixture was stirred for 12 h at ambient temperature. The Br_2/SO_2 solution was condensed into the empty arm of the H-cell to allow for complete precipitation of AgBr and poured back onto the reaction mixture. The deep purple solution was then filtered via the internal frit and extracted three times by back condensing the SO_2 until no purple tint of the solution was visible. The Br_2/SO_2 solution was removed under reduced pressure and the precipitate dried under vacuum. **4** was obtained as deep purple to black solid (2.15 g, 1.32 mmol, 96.7 %). Crystals suitable for X-ray diffraction analysis were grown by layering of solutions of **4** in CH_2Cl_2 or *o*DFB with n-pentane.

ESI-MS positive ion mode: m/z = 491.08 $[N_2C_{18}F_{13}]^+$ (4%), 658.08 $[N_2C_{24}F_{18}]^+$ (**4**). negative ion mode: m/z = 967.00 $[AlO_4C_{16}F_{36}]^-$.

Crystals obtained from *o*DFB solution show a superstructure, which could be collected at 80 K the asymmetric unit of which is show in Figure S 14. The obtained structure shows a very large cell (a = 22.30, b = 58.21, c = 26.45) containing 24 formula units and stops refinement at $wR_2 = 0.27$, with residual electron density, which could not be modelled with additional disorder. However, the structure of the radical cation [phenazine^F]$^{\cdot+}$ is identical to the structure collected from crystals grown from CH_2Cl_2 solution. Because of the poor quality of the obtained structure (numerous unresolvable A/B/C alerts in checkcif) the data was not uploaded to the CCDC.

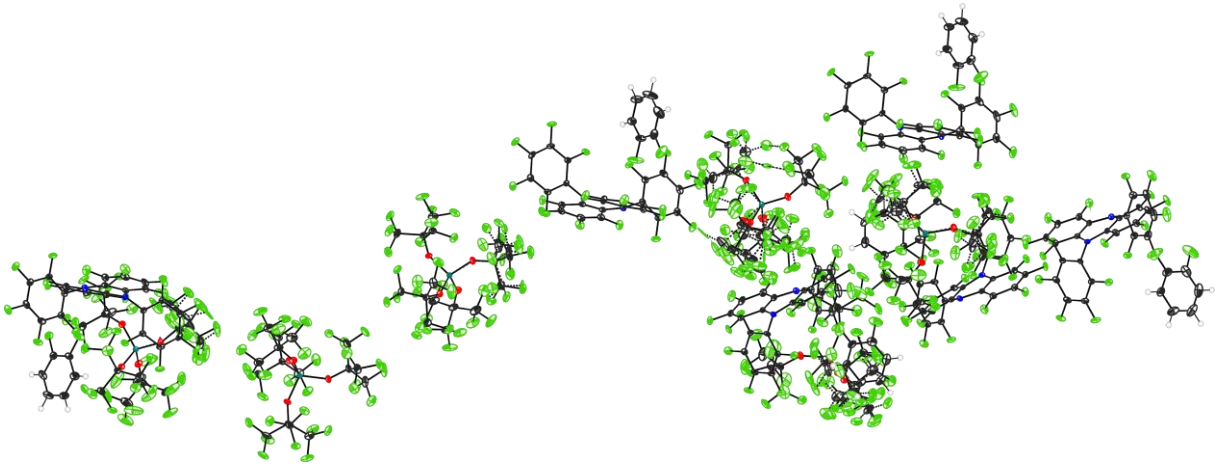


*Figure S 14. Asymetric unit of crystals of **4** grown from oDFB solution.*

The structure of **4** obtained from CH_2Cl_2 solution contains two crystallographically inequivalent moieties of **4** in the asymmetric unit, where the C_6F_4 residues of the dihydrophenazin backbone are slightly U-bent to 17.2 resp. 14.2° whereas the C_6F_5-groups show a tilt of 10.6 resp. 17.1° against each

other. Furthermore the C_6F_5 moieties are bend downwards to allow for two relatively short N,F distances to the *ortho*-fluorine substituents. The central nitrogen atoms are almost perfectly planar coordinated with an angle sum of 358.2° compared to more pyramidal neutral **3** with an angle sum of 342.2° and show two identical N–C bond lengths to the dihydrophenazine backbone (avg. $d_{N\text{-}C}$ = 1.393(4) Å); which are by 0.05 Å significantly shorter than the N–C bonds to the *ipso*-carbon on the C_6F_5 residue (avg. $d_{N\text{-}C}$ = 1.444(4) Å). Similar but slightly longer bond distances are found in neutral **3** ($d_{N\text{-}C\ backbone}$ = 1.422(3) Å, $d_{N\text{-}C\ ipso\text{-}C6F5}$ = 1.447(3) Å).

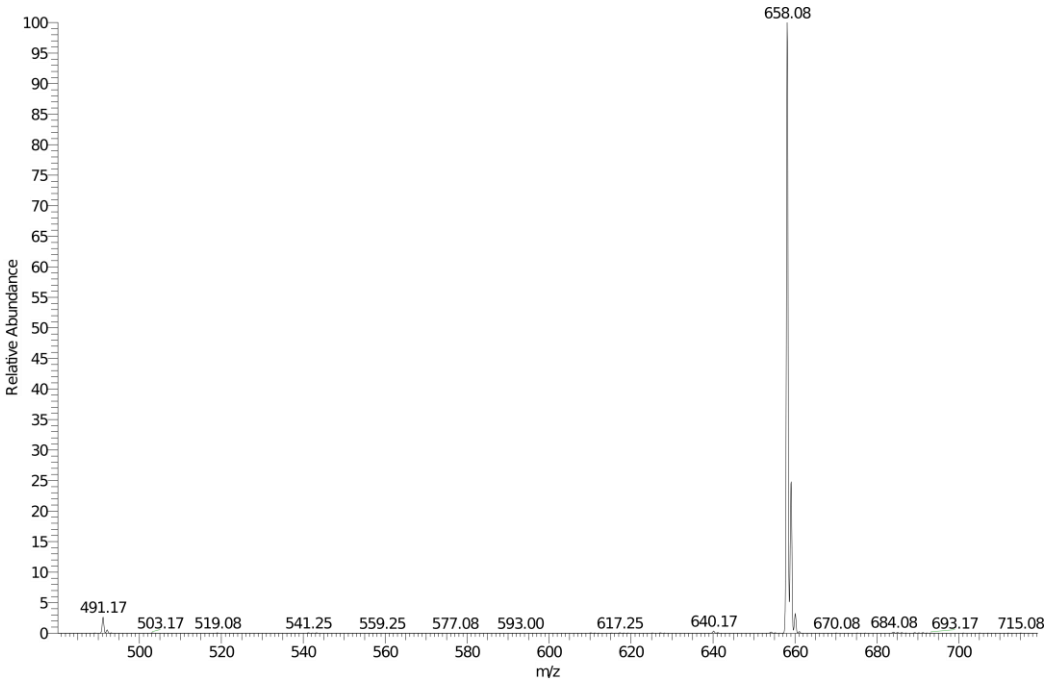


*Figure S 15 positive ion mode ESI-MS spectrum of **4**.*

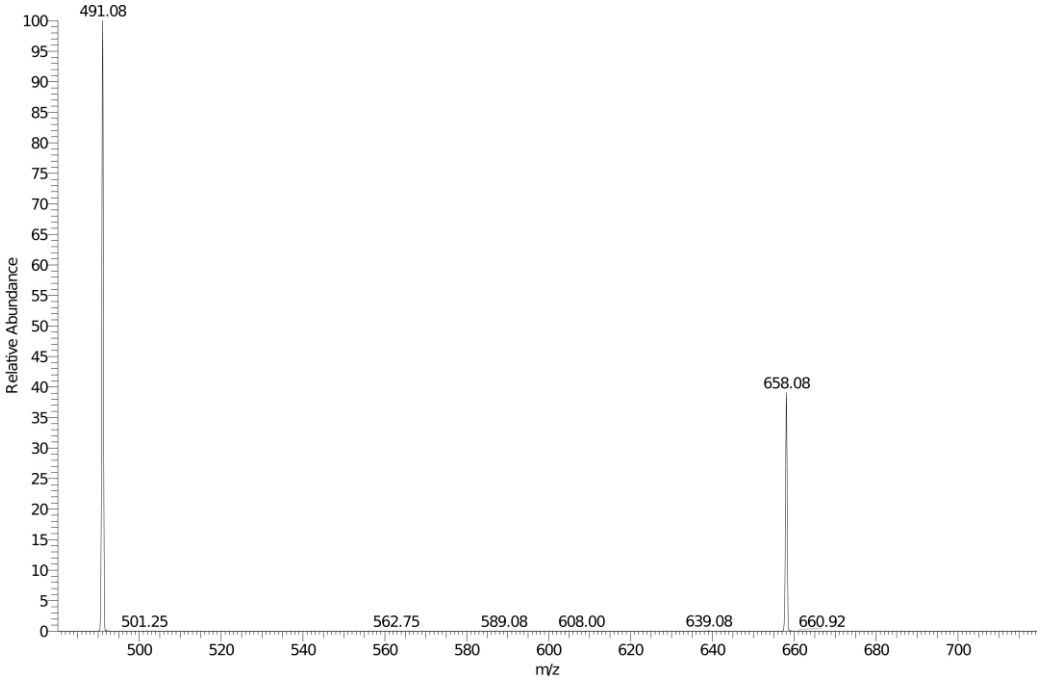


*Figure S 16 postive ion mode ESI-MS spectrum of **4** with CID on mass envelope at 658.08 m/z at with normalized collision energy of 40.*

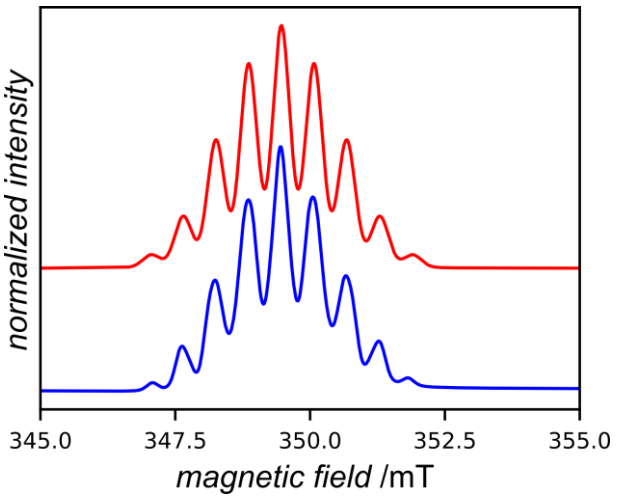


*Figure S 17 (blue trace) integrated field modulated liquid state cw-EPR of **4** in SO_2 at ambient temperature with corresponding fit (red trace).*

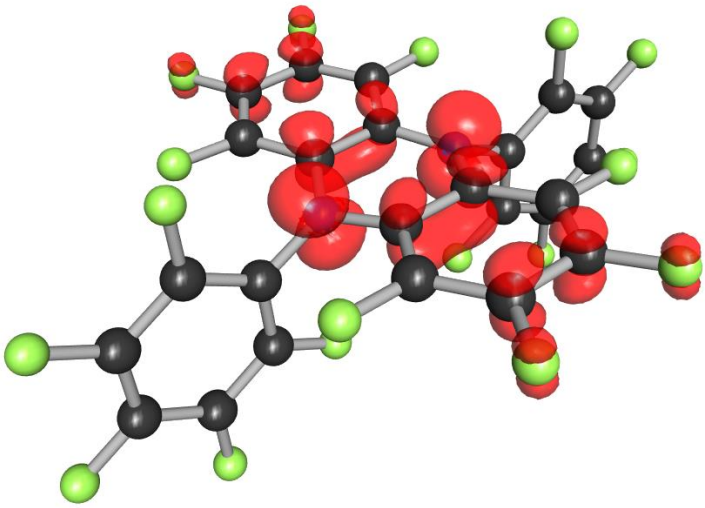


*Figure S 18 spin density plot of [phenazine^F]$^{+}$ **4**$^{\cdot+}$. The spin density shows delocalisation of unpaired electron over the dihydrophenazine backbone with biggest occupancy on central pyrazine subunit as well as positions para in respect to the nitrogen atoms.*

S-2.6 Reaction between **4** and different substrates

S-2.6.1 Reaction between **4** and Sn in MeCN. Synthesis of [Sn(MeCN)$_5$][Al(OR^F)]$_2$ **5**.

4 (90.0 mg, 0.0553 mmol) and Sn (52.0 mg, 0.443 mmol, 8 eq. were weighed in a Schlenk tube. MeCN (4 ml) was added and the reaction mixture stirred for 2 h at ambient temperature, during which a colour change from dark purple to faint yellow was observed. The solvent was removed under reduced pressure and the residue dissolved in *o*DFB (0.8 ml) and filtered into an NMR tube equipped with J.Young Teflon valve. After completed NMR measurement the solution was layered with n-pentane to yield crystals of **5** suitable for X-ray diffraction analysis (see Figure S 19).

NMR analysis revealed intact anion in 1 : 1 ration to neutral **3** underlining purity of employed **4**. Furthermore ratio between the anion and MeCN is 2 : 6 by referencing to oDFB as internal standard. ^{119}Sn-NMR revealed no tin resonances probably due to low sample concentration.

^{1}H-NMR (400.17 MHz, *o*DFB, 298 K) δ = 2.04 (s, 3 H, NCC*H*$_3$) ppm. ^{19}F-NMR (376.54 MHz, *o*DFB, 298 K) δ = −74.9 (s, 9 F, OC(C*F*$_3$)$_3$), −75.4 (S, 36 F, [Al(OC(C*F*$_3$)$_3$)$_4$]$^-$), −142.4 (m, AA´BB´C, 4F, F^5, **3**), −152.4 (m, AA´BB´C, 2F, F^7, **3**), −156.0 (m, AA´BB´, 4F, F^1, **3**), −162.3 (m, AA´BB´, 4F, F^2, **3**), −163.3 (m, AA´BB´C, 4F, F^6, **3**). ^{27}Al-NMR (104.27 MHz, *o*DFB, 298 K) δ = 36.4 (s, [*Al*(OC(CF$_3$)$_3$)$_4$]$^-$) ppm.

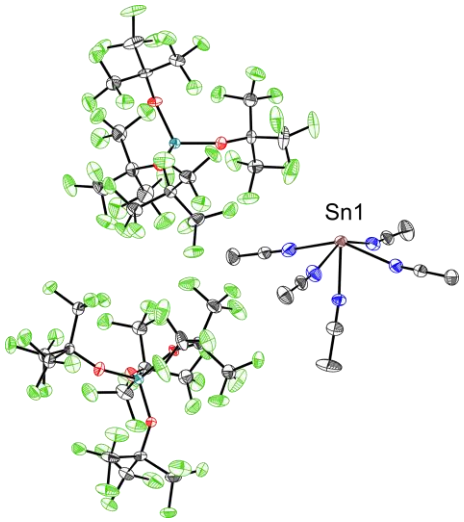


*Figure S 19 molecular structure of $[Sn(MeCN)_5][Al(OR^F)_4]_2$ **5***

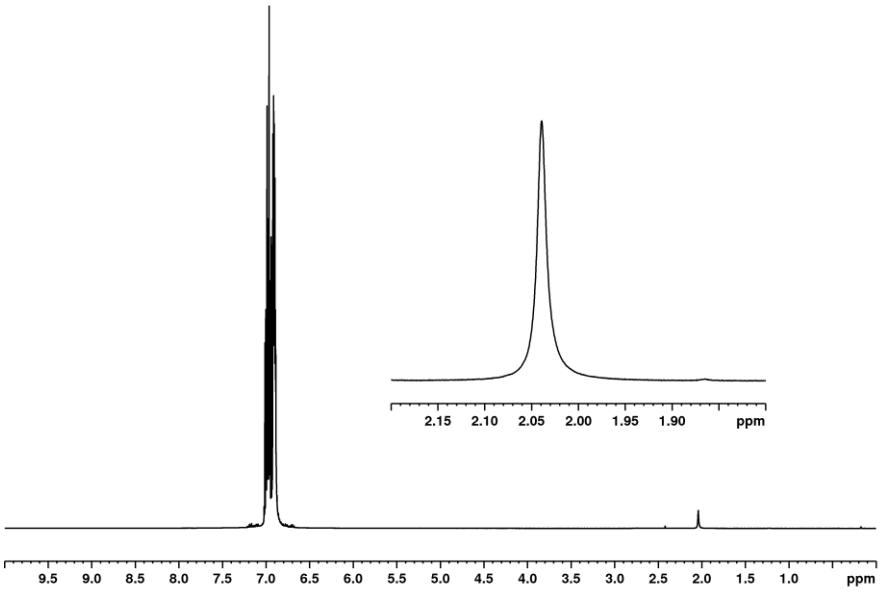


*Figure S 20:^{1}H-NMR (400.17 MHz, oDFB, 298 K) of dried reaction mixture between **4** and Sn in MeCN.*

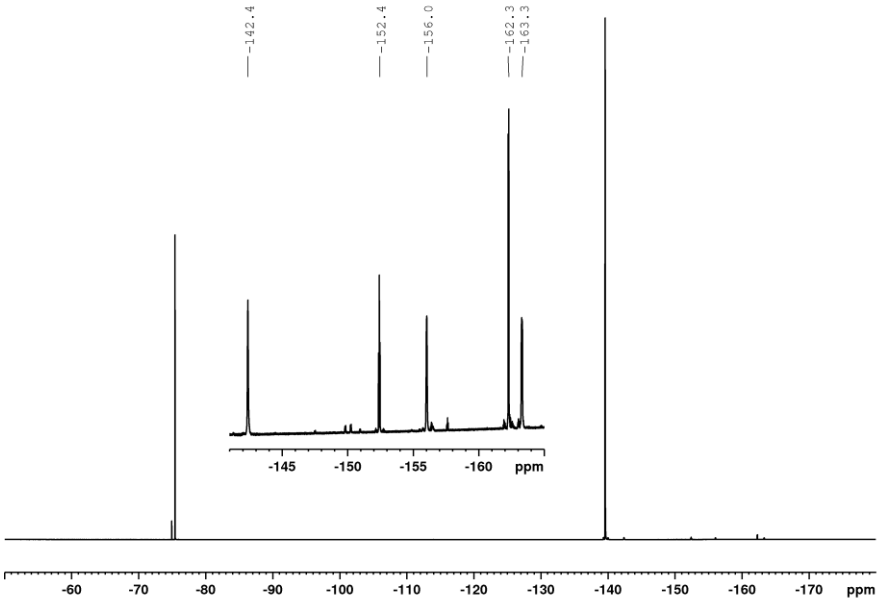


*Figure S 21: ^{19}F-NMR (376.54 MHz, oDFB, 298 K) of dried reaction mixture between **4** and Sn in MeCN.*

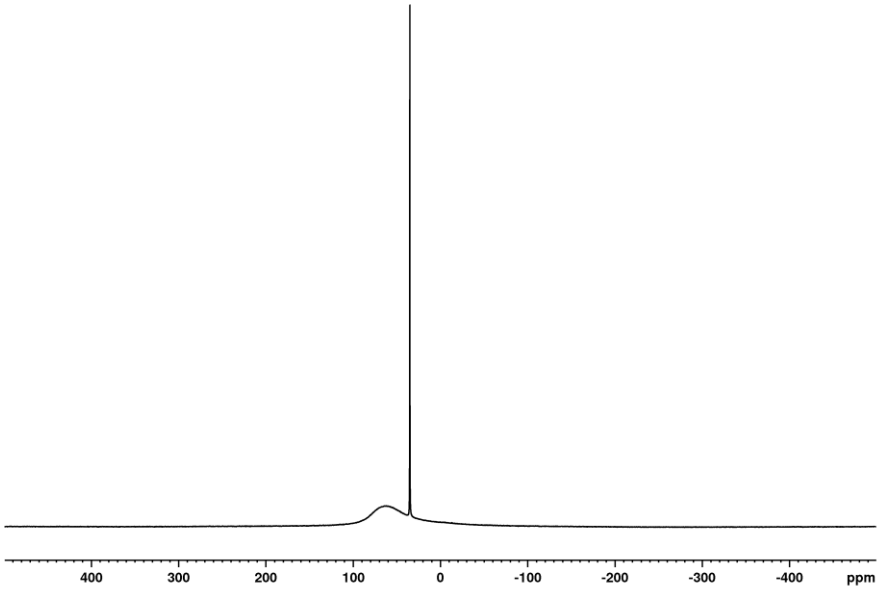


*Figure S 22: ^{27}Al-NMR (104.27 MHz, oDFB, 298 K) of dried reaction mixture between **4** and Sn in MeCN.*

S-2.6.2 Reaction between **4** and Sn in presence of trispyrazolylmethane ($CHpz_3$). Synthesis of $[Sn(CHpz_3)_2][Al(OR^F)_4]_2$ **6**.

4 (150 mg, 0.0923 mmol) and $CHpz_3$ (22 mg, 0.10 mmol, 1.1 eq.) were dissolved in *o*DFB (3 ml). Sn grains (110 mg, 0.923 mmol, 10 eq.) were added in a positive stream of argon and the reaction mixture

stirred for 12 h at ambient temperature. The faint yellow reaction mixture was filtered and layered with n-pentane. **6** was obtained as colourless crystals (110 mg, 0.046 mmol, 88 % crystalline yield).

NMR analysis revealed intact anion in 2 : 2 ratio to the employed $CHpz_3$. ^{119}Sn-NMR revealed no tin resonances probably due to low sample concentration.

^{1}H-NMR (300.18 MHz, *o*DFB, 298 K) δ = 8.73 (s, 1 H, *H*C(pz)$_3$), 8.24 (m, 3 H, pz H^1), 7.71 (m, 3 H, pz H^3), 6.54 (m, 3 H, pz H^2) ppm. ^{13}C-NMR (75.48 MHz, *o*DFB, 298 K) δ = 143.8 (s, pz C^1), 133.1 (s, pz C^3), 108.7 (s, pz C^2), 78.7 (s, H*C*pz$_3$) ppm. ^{19}F-NMR (376.54 MHz, *o*DFB, 298 K) δ = −75.3 (S, 36 F, [Al(OC(C*F*$_3$)$_3$)$_4$]$^-$) ppm. ^{27}Al-NMR (104.27 MHz, *o*DFB, 298 K) δ = 35.0 (s, [*Al*(OC(CF$_3$)$_3$)$_4$]$^-$) ppm. ATR-FTIR: *v* = 3163 (vvw) 3146 (vvw) 1525 (vvw) 1511 (vvw) 1438 (vvw) 1407 (vvw) 1351 (vw) 1297 (mw) 1273 (ms) 1240 (vvs) 1212 (vvs) 1169 (m) 1098 (vw) 1063 (vw) 969 (vvs) 850 (vw) 831 (vw) 792 (m) 765 (m) 755 (mw) 726 (vvs).

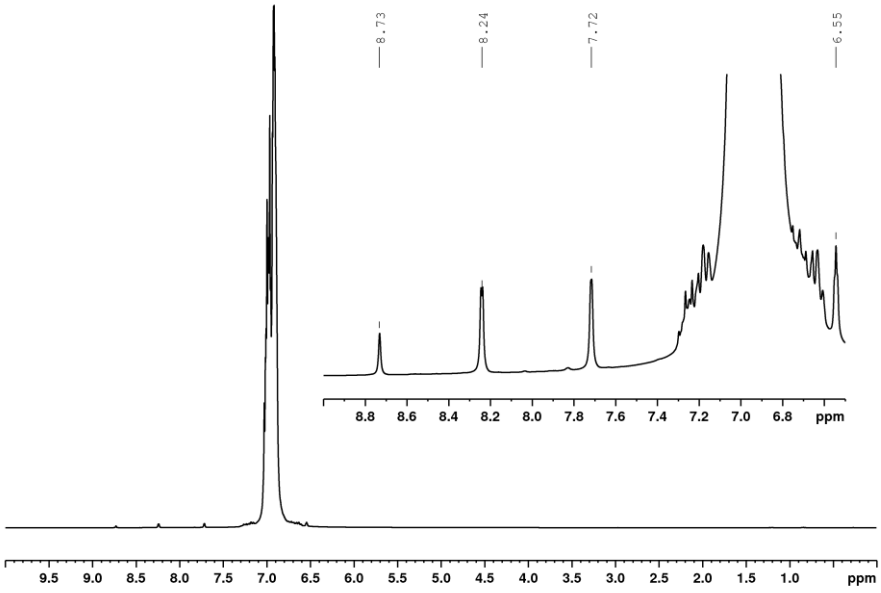


*Figure S 23 ^{1}H-NMR (300.18 MHz, oDFB, 298 K) of isolated crystalline **6**.*

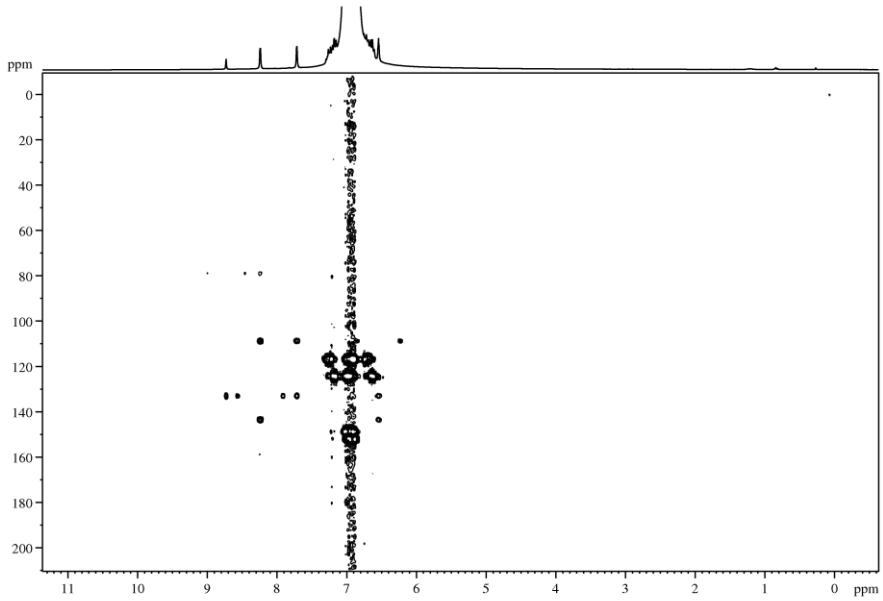


*Figure S 24 ^{1}H-^{13}C-HMBC NMR (75.48 MHz, oDFB, 298 K) of isolated crystalline **6**.*

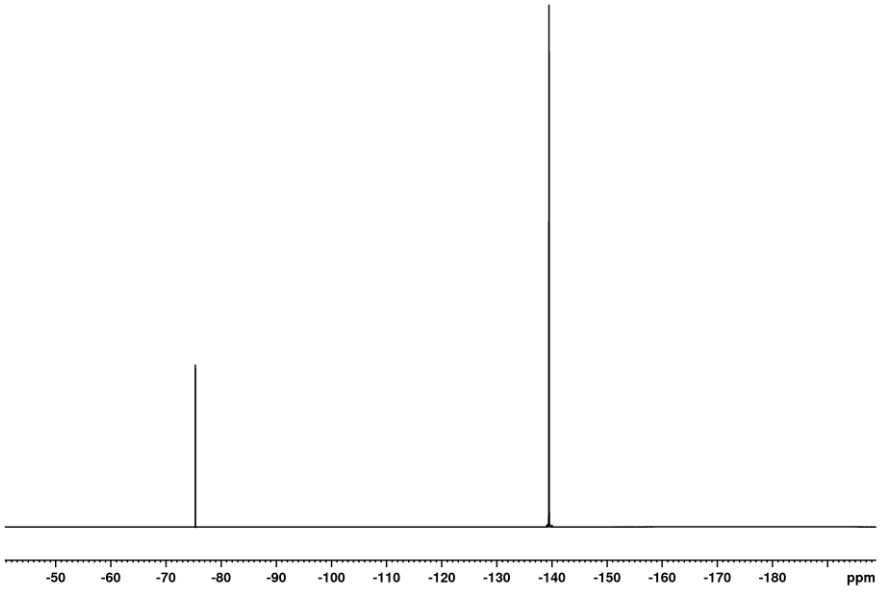


*Figure S 25 . ^{19}F-NMR (376.54 MHz, oDFB, 298 K) of isolated crystalline **6**.*

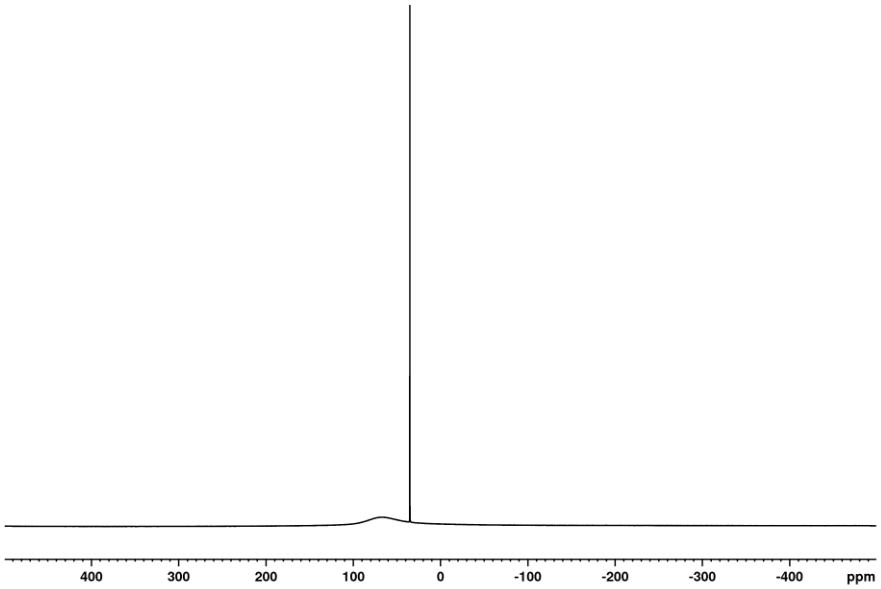


*Figure S 26 ^{27}Al-NMR (104.27 MHz, oDFB, 298 K) of isolated crystalline **6**.*

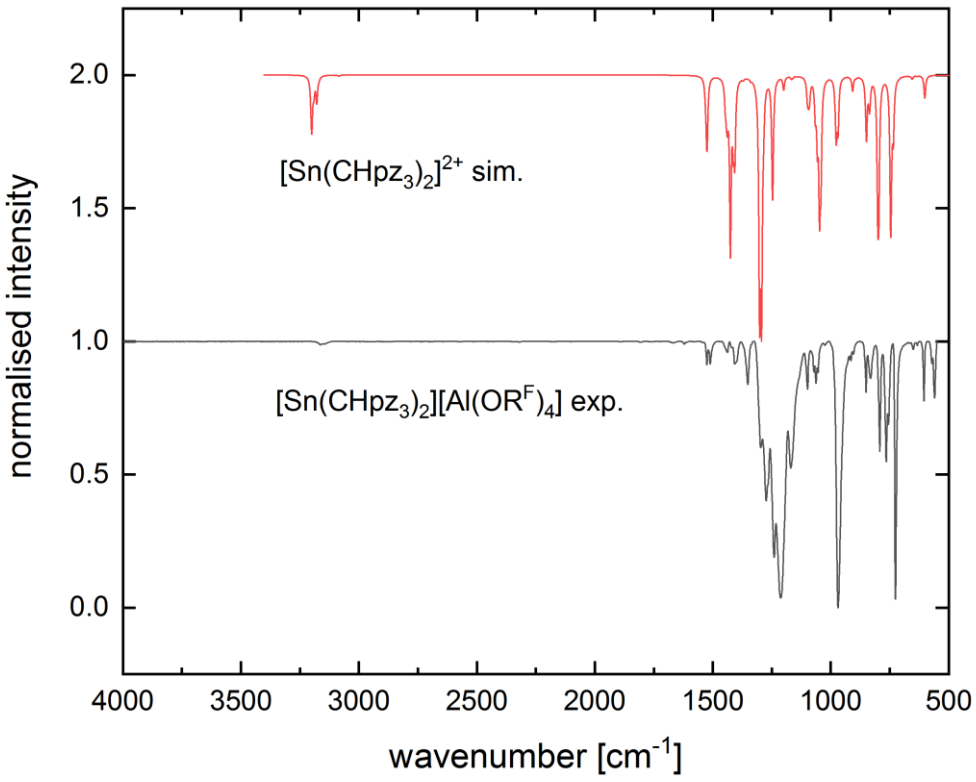


*Figure S 27 (black) ATR-FTIR spectrum of **6** together with simulated IR spectrum.*

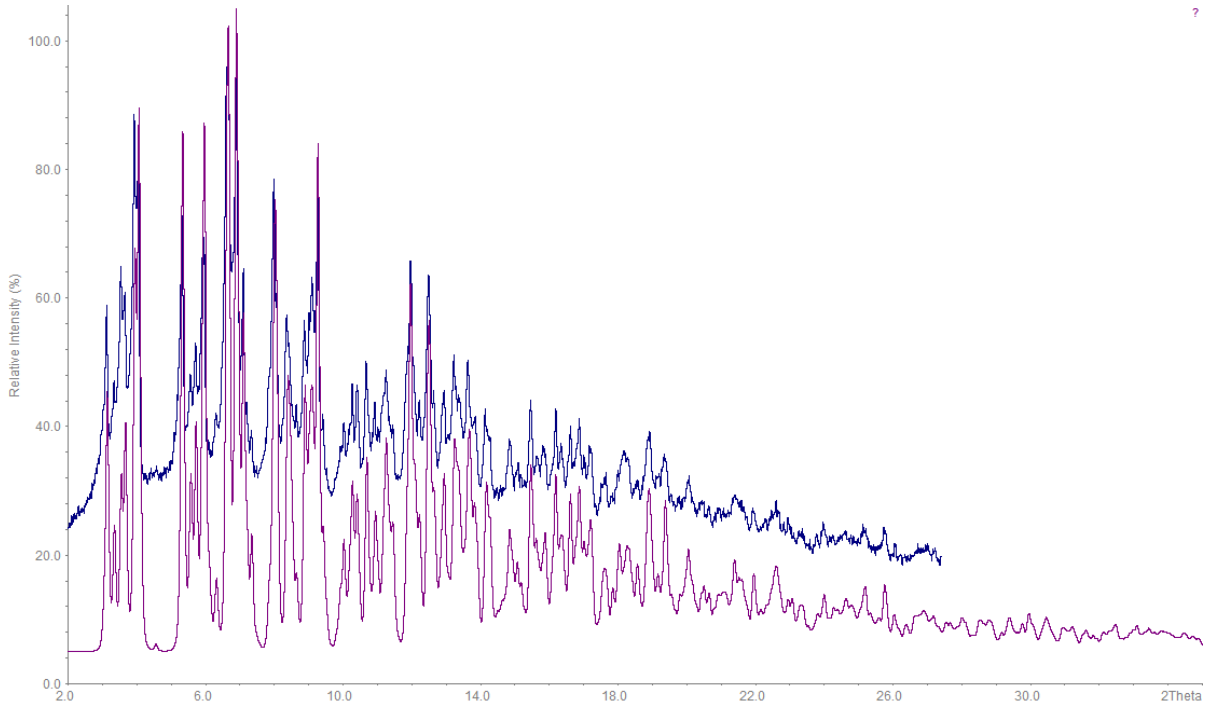


*Figure S 28 (blue trace) pwd-XRD analysis of bulk material of **6**. (purple trace) simulated powder diffraction pattern from obtained crystalline **6**.*

S-2.6.3 Reaction between **4** and $[FeCp^*_2][Al(OR^F)_4]$ in oDFB under 3 atm of CO. Synthesis of $[Fe(CO)Cp^*_2][Al(OR^F)_4]_2$ **7.**

4 (150 mg, 0.0923 mmol) and $[FeCp^*_2][Al(OR^F)_4]$ (119 mg, 0.0923 mmol, 1 eq.) were weighed into an H-cell equipped with a G4 frit and dissolved in *o*DFB (5 ml). The solution was degassed by three freeze pump thaw cycles. CO (3 bar) was added onto the H-cell and the reaction mixture stirred for 2 h at ambient temperature. The vessel was vented via the argon manifold and n-pentane (15 ml) was added to the empty arm of the H-cell and 1 atmosphere of CO was added onto the H-cell. Dark red crystals of **7** were grown by vapour diffusion (132 mg, 0.0577 mmol, 62.5 % crystalline yield).

^{1}H-NMR (200.13 MHz, *o*DFB, 298 K) δ = 2.24 (s, 15 H, $[C_5(CH_3)_5]^-$) ppm. ^{13}C-NMR (50.32 MHz, *o*DFB, 298 K) δ = 215.5 (s, *C*O), 111.6 (s, $[C_5(CH_3)_5]^-$), 8.2 (s, $[C_5(CH_3)_5]^-$) ppm. ^{19}F-NMR (188.31 MHz, *o*DFB, 298 K) δ = −75.4 (S, 36 F, $[Al(OC(CF_3)_3)_4]^-$) ppm. ATR-FTIR: *v* = 2930 (vvw) 2057 (w) 1507 (vvw) 1458 (vvw) 1390 (vvw) 1352 (vw) 1297 (mw) 1274 (ms) 1266 (ms) 1241 (vvs) 1209 (vvs) 1177 (ms) 1077 (vvw) 969 (vvs) 832 (w) 756 (vvw) 727 (vvs) 617 (vvw) 560 (vw).

NMR analysis revealed intact anion in 2 : 2 ratio to Cp* by referencing with *o*DFB as internal standard, underlining purity of the collected sample. This is in line with the single vibrational band of bound CO at 2057 cm^{-1} observed.

Crystals grown by vapour diffusion show super structured data, which was refineable by employing huge amounts of disorder in both cationic and anionic part. The collected crystal shows pseudo trigonal geometry with best solution in trigonal space group $R\bar{3}$ (No. 148). The rather poorly described model of the molecular structure of **7** is shown in Figure S 29. The asymmetric unit contains 1 1/6 formula units in the cationic part and 2 1/3 formula units in the anionic part giving an overall charge of the cation of +2. The first cationic moiety was described by disorder of each of the two Cp* fragments over two positions while the single CO molecule is disordered over three positions. The second cationic moiety lies on a special position with 6-fold symmetry. Here the Cp* moiety was disordered over two positions while CO is duplicated by symmetry over six positions to give occupancy of 1/6. Refinement was stopped at wR_2 = 0.23, with much residual electron density in the anionic part, while the highest q-peaks are located around Fe probably due to absorption. The obtained molecular structure was used for simulation of powder diffraction patterns for phase purity analysis. Bond metric data is not discussed because of the poor quality of the obtained data set/model and structure was not uploaded to CCDC (numerous unresolvable A/B/C alerts in checkcif). The authors want to make clear the obtained structure is by no means good. While the structure does support the presence of **7** the other analytical data collected from the same sample strongly confirmes presence and purity of **7**. Recrystallisation of bulk material by layering of concentrated oDFB solution with n-pentane gave block shaped crystals which again showed underlying superstructure. However the obtained data set was satisfyingly refinable.

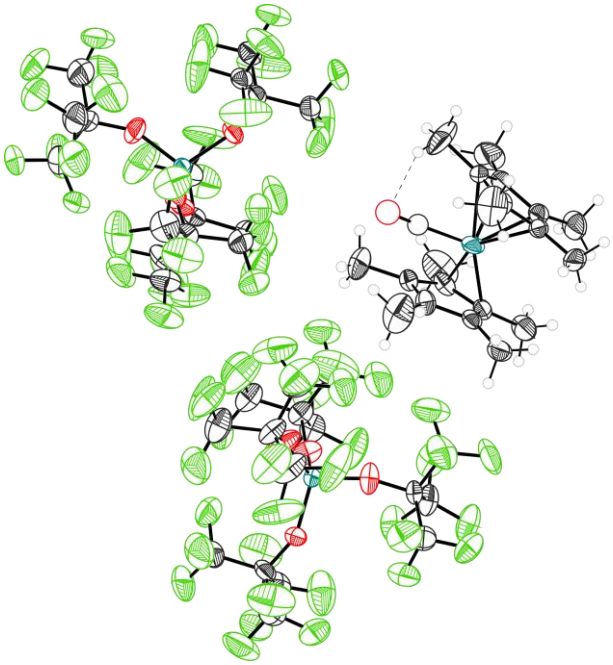


*Figure S 29: Molecular structure of **7**. Thermal displacement ellipsoids set 50% probability. Only majority part of disordered components shown for clarity.*

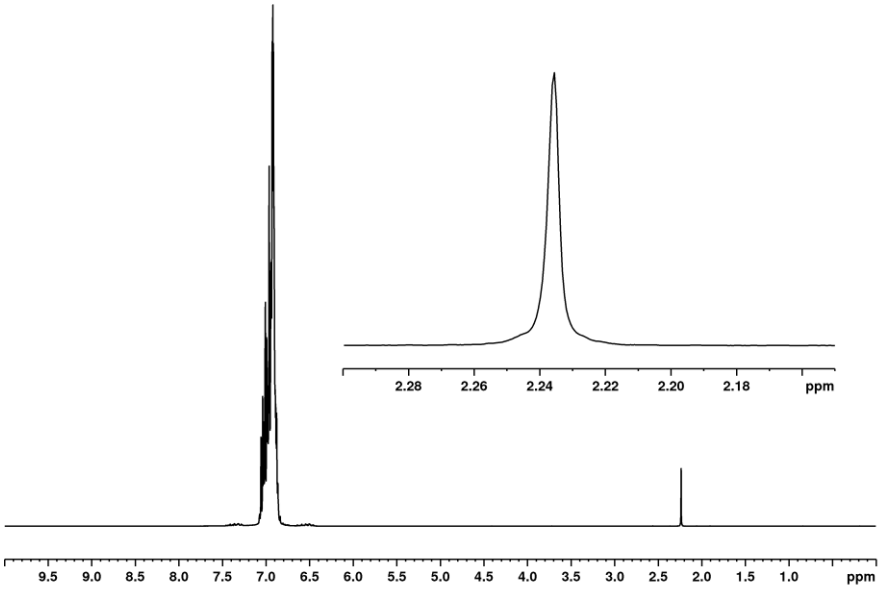


*Figure S 30 ^{1}H-NMR (200.13 MHz, oDFB, 298 K) of isolated crystalline **7**.*

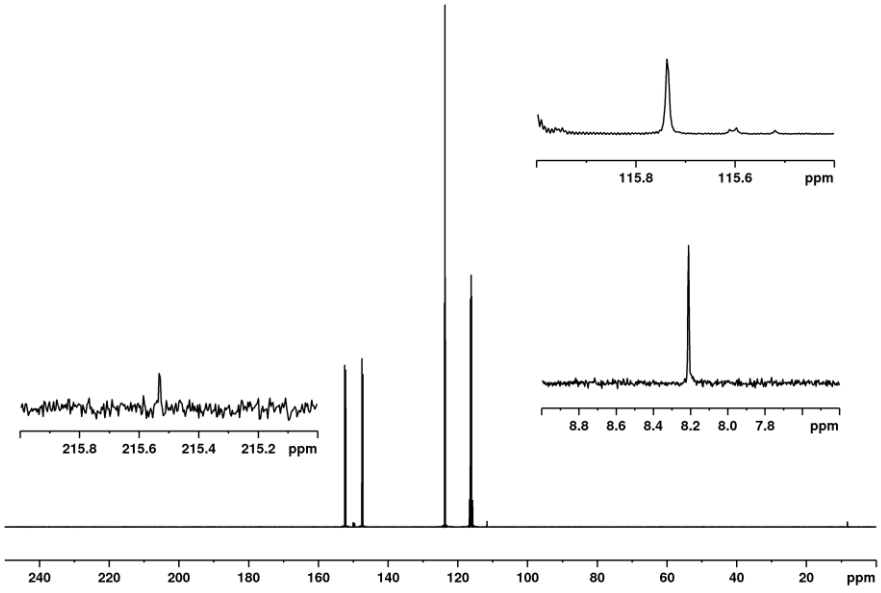


*Figure S 31 ^{13}C-NMR (50.32 MHz, oDFB, 298 K) of isolated crystalline **7**.*

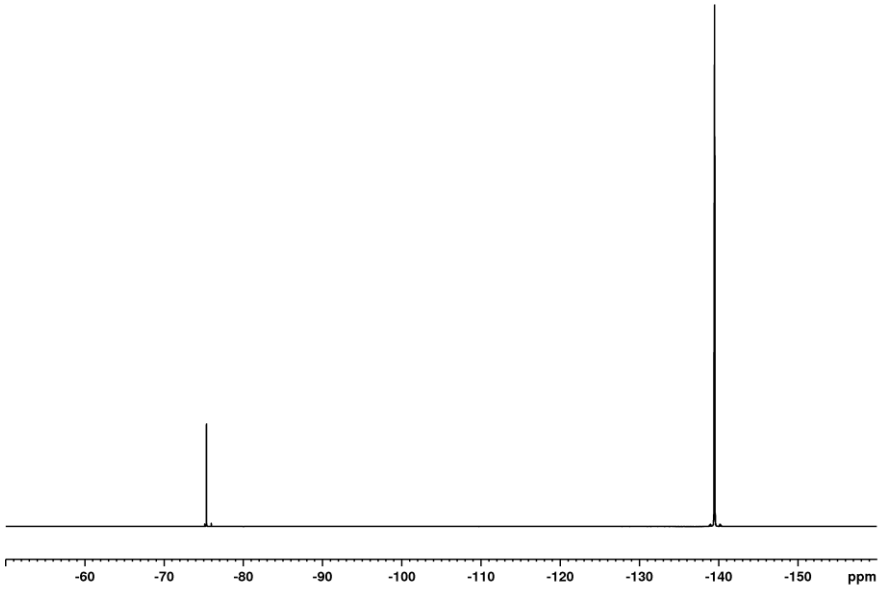


*Figure S 32 ^{19}F-NMR (188.31 MHz, oDFB, 298 K) of isolated crystalline **7**.*

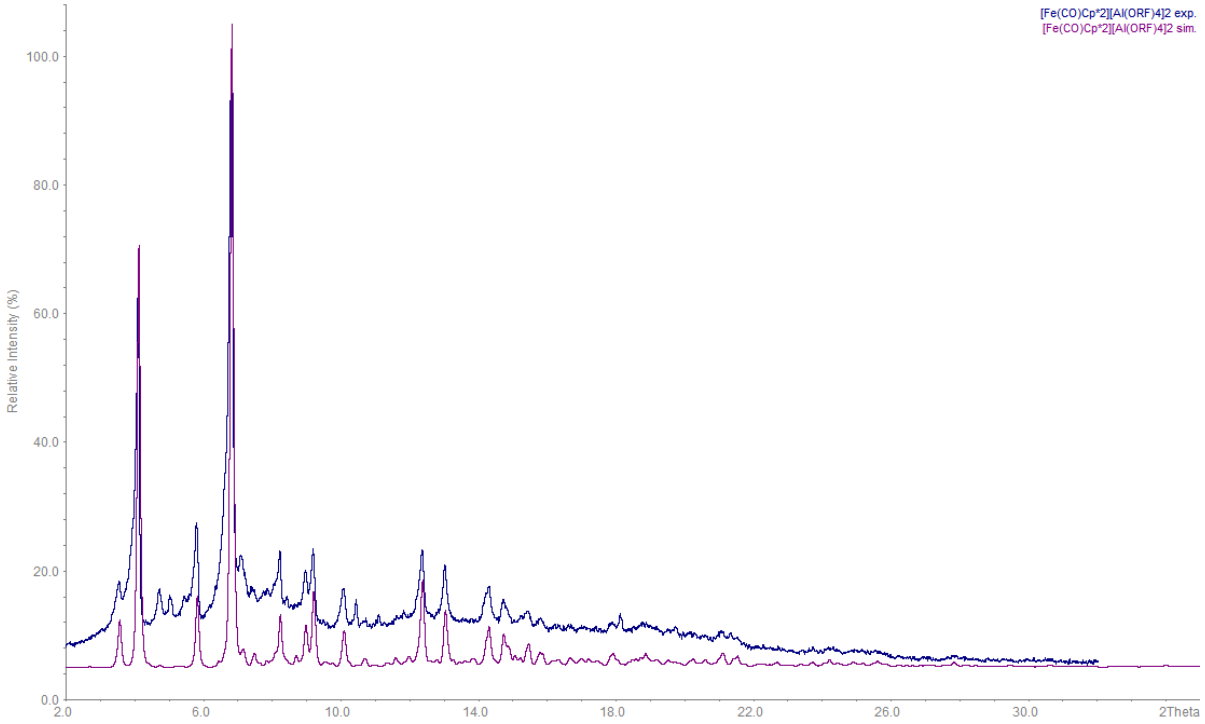


*Figure S 33 (blue trace) pwd-XRD analysis of bulk material of **7**. (purple trace) simulated powder diffraction pattern from obtained crystalline **7.***

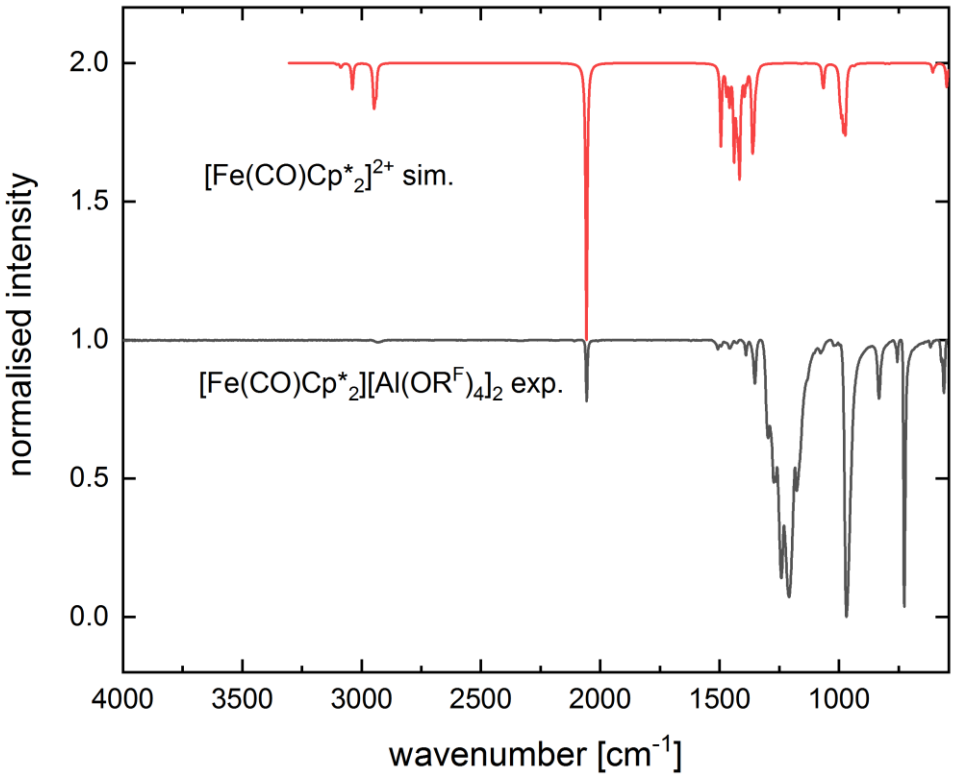


*Figure S 34 (black) ATR-FTIR spectrum of **7** together with simulated IR spectrum of the dication only.*

S-2.6.4 Reaction between **4** and $[FeCp^*_2][Al(OR^F)_4]$ in oDFB in presence of excess ^{t}Bu-NC. Synthesis of $[Fe(CN\text{-}^t Bu)Cp^*_2]^{2+}$ **8**.

4 (200 mg, 0.123 mmol) and $[FeCp^*_2][Al(OR^F)_4]$ (0.152 mg, 0.117 mmol, 0.95 eq.) were dissolved in *o*DFB (4 ml). Under stirring at ambient temperature a solution of ^{t}Bu-NC in *o*DFB (1Mol, 0.3 ml, 0.3 mmol) was added to the reaction mixture. After 1 h at ambient temperature the deep purple colour of **4** vanished to give a dark brown solution. The reaction mixture was layered with n-pentane to yield **8** as dark red crystals (210 mg, 0.089 mmol, 76.6 % crystalline yield).

^{1}H-NMR (400.17 MHz, *o*DFB, 298 K) δ = 1.99 (shoulder, 9 H, CN-(C*H*$_3$)$_3$), 1.98 (s, 30 H, 2 x {C$_5$(C*H*$_3$)$_5$}) ppm. ^{13}C-NMR (50.32 MHz, *o*DFB, 298 K) δ = 108.4 (s, [*C*$_5$(CH$_3$)$_5$]$^-$), 65.1 (s, *C*N-(CH$_3$)$_3$), 29.6 (s, CN-(*C*H$_3$)$_3$) 9.1 (s, [C$_5$(*C*H$_3$)$_5$]$^-$) ppm. ^{14}N-NMR (28.908 MHz, *o*DFB, 298 K) δ = 177.4 (s, C*N*-(CH$_3$)$_3$) ppm. ^{19}F-NMR (376.54 MHz, *o*DFB, 298 K) δ = −75.4 (S, 36 F, [Al(OC(C*F*$_3$)$_3$)$_4$]$^-$) ppm. ^{27}Al-NMR (104.27 MHz, *o*DFB, 298 K) δ = 35.4 (s, [*Al*(OC(CF$_3$)$_3$)$_4$]$^-$) ppm. ATR-FTIR: *v* = 2198 (vvw) 2176 (vvw) 2129 (vvw) 1509 (vvw) 1458 (vvw) 1390 (vvw) 1352 (vw) 1297 (mw) 1274 (ms) 1239 (vvs) 1213 (vvs) 1172 (ms) 1102 (vvw) 1078 (vvw) 970 (vvs) 831 (vw) 750 (vw) 726 (vvs) 612 (vvw) 560 (vw).

NMR analysis revealed intact anion in 2.23 : 2 ratio to {(NC-^{t}Bu)Cp*$_2$} by referencing to *o*DFB. This is probably due to < 20 % contamination by paramagnetic starting material [FeCp*$_2$][Al(OR^F)$_4$]. (NC-^{t}Bu) is not stable towards **4** and forms a plethora of degradation products over time. This also explains the two additional small bands around 2170 cm^{-1} in collected IR spectra.

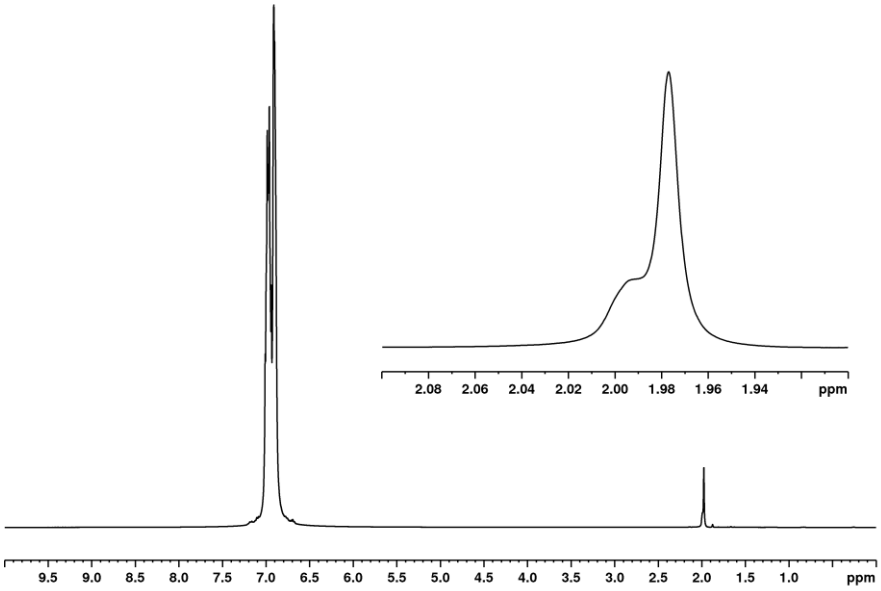


*Figure S 35 ^{1}H-NMR (400.17 MHz, oDFB, 298 K) of isolated crystalline **8**.*

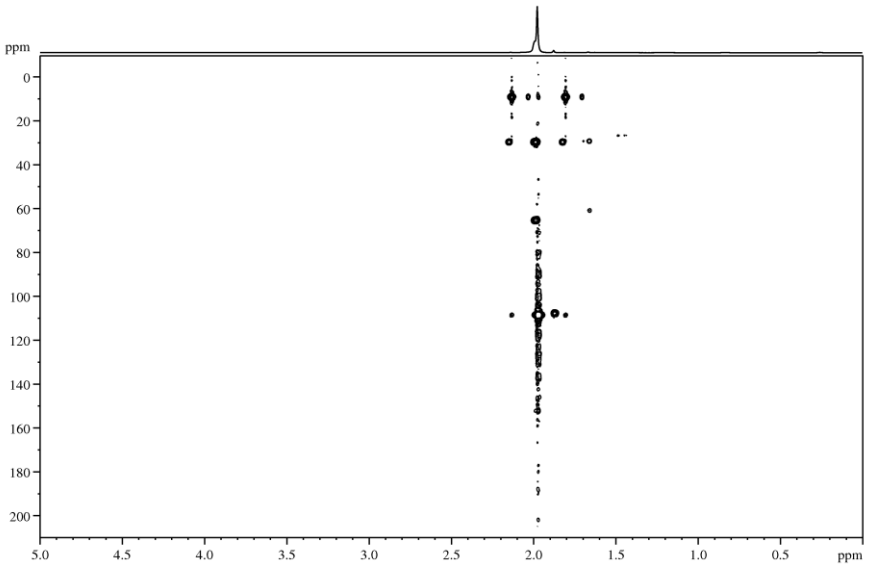


*Figure S 36 ^{1}H-^{13}C-HMBC NMR (400.17 MHz, oDFB, 298 K) of isolated crystalline **8**.*

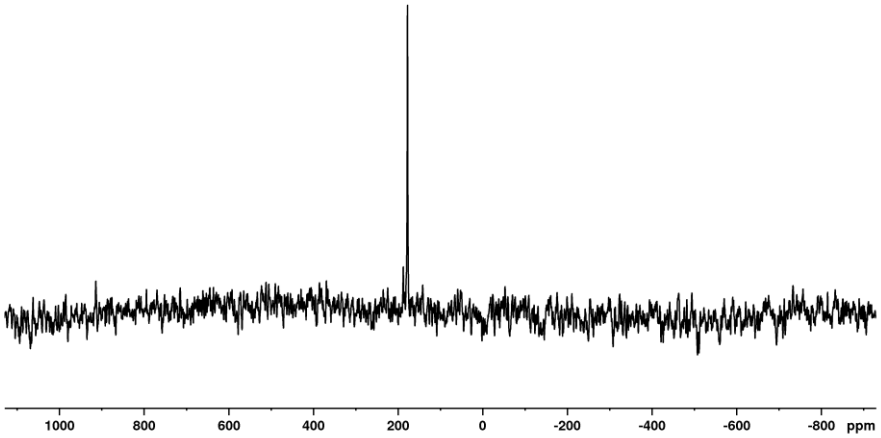


*Figure S 37 ^{14}N-NMR (28.908 MHz, o*DFB*, 298 K) of isolated crystalline **8.***

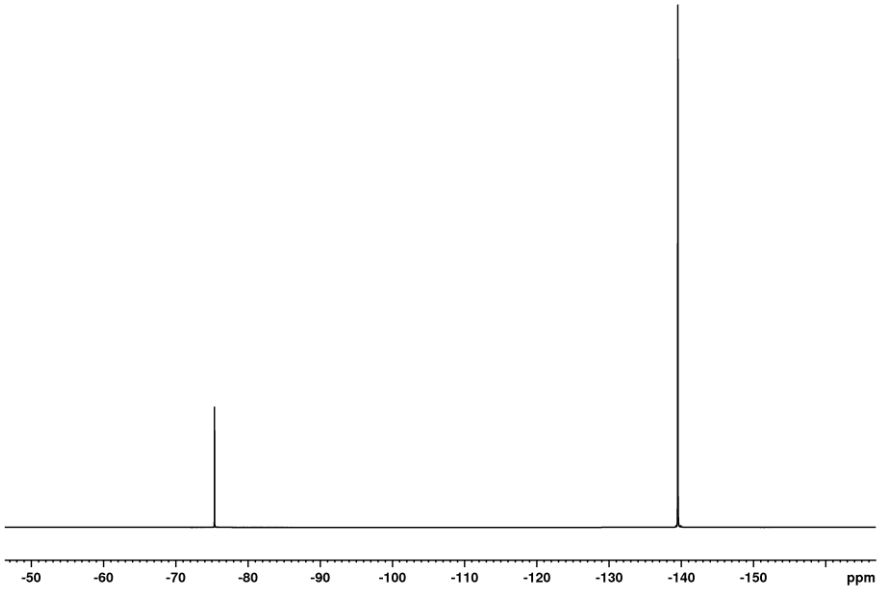


*Figure S 38 ^{19}F-NMR (376.54 MHz, o*DFB*, 298 K) of isolated crystalline **8.***

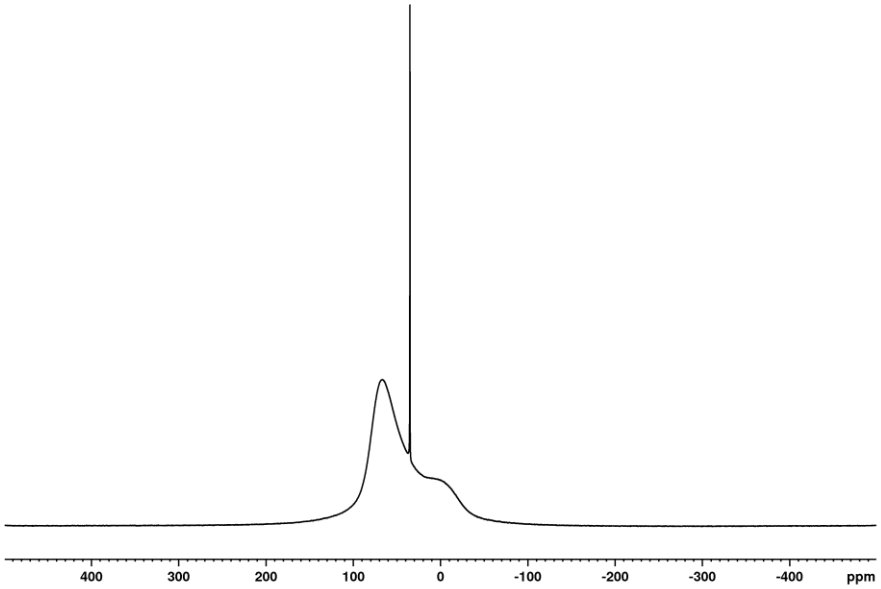


*Figure S 39 ^{27}Al-NMR (104.27 MHz, oDFB, 298 K) of isolated crystalline **8**.*

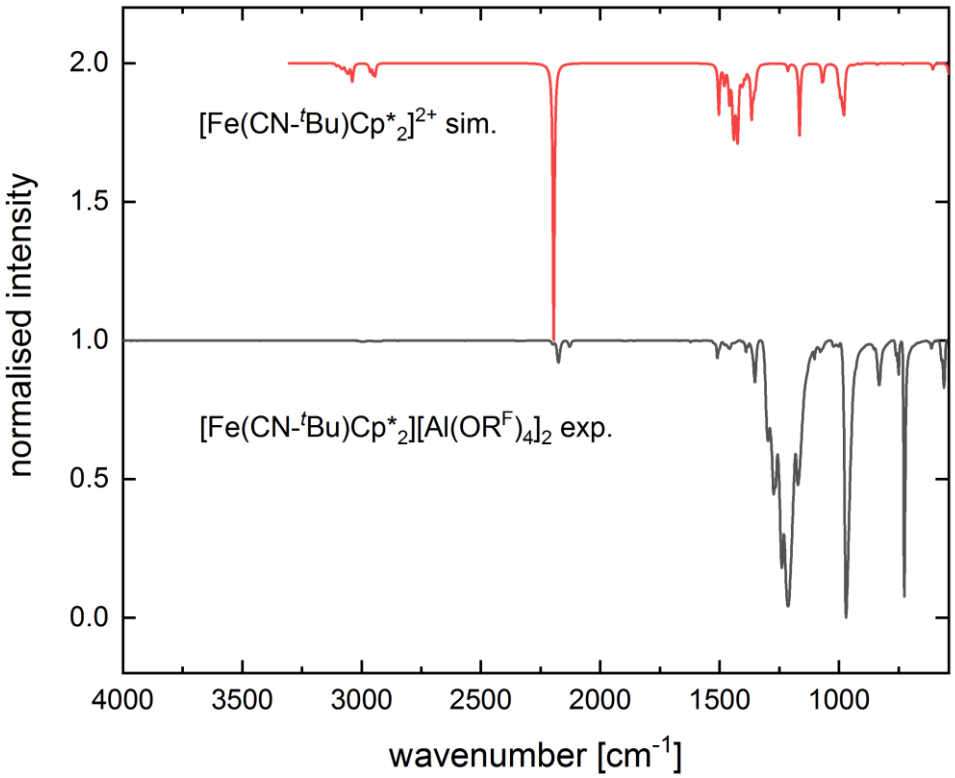


*Figure S 40 (black) ATR-FTIR spectrum of **8** together with simulated IR spectrum.*

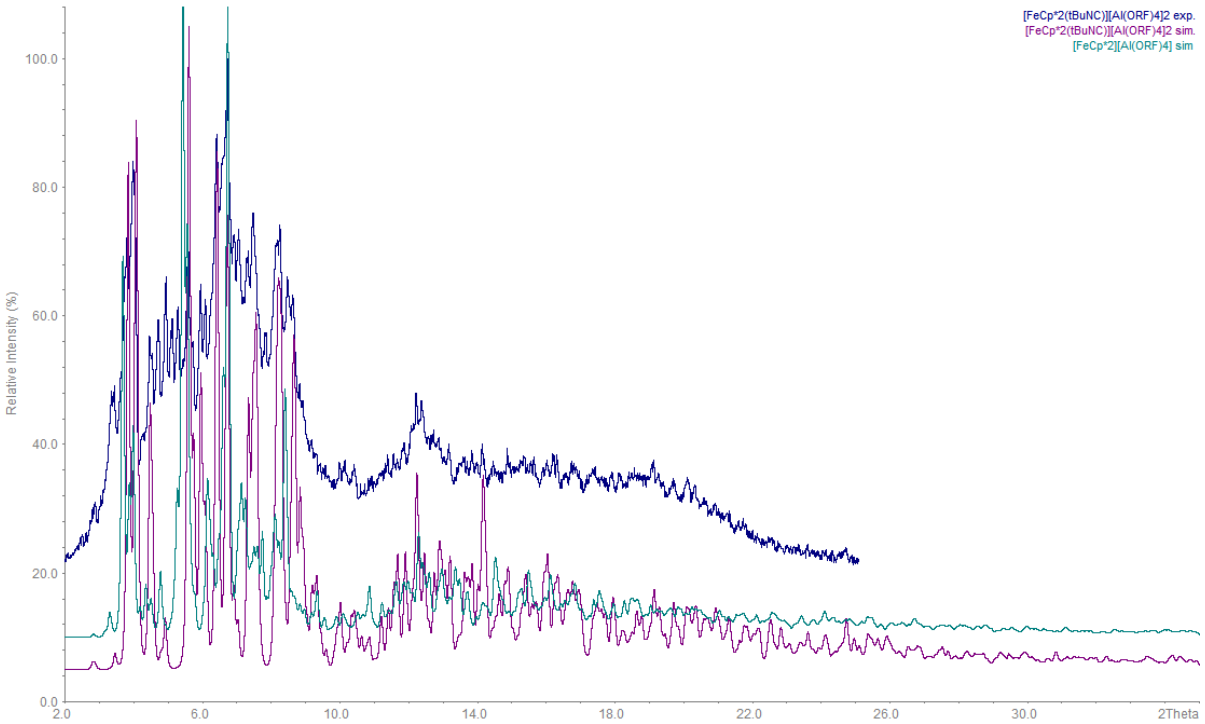


*Figure S 41 (blue trace) pwd-XRD analysis of bulk material of **8**. (purple trace) simulated powder diffraction pattern from obtained crystalline **8** and (green trace) simulated powder diffraction pattern from obtained crystalline [FeCp*$_2$][Al(OR^F)$_4$]. Experimental pattern is in good agreement with superposition of the two simulated diffraction patterns.*

S-3 Crystallographic data

	2·oDFB	**3**	**4 (CH_2Cl_2)**	**4 (oDFB)**
Empirical formula	$C_{36}H_8F_{24}Li_2N_2$	$C_{24}F_{18}N_2$	$C_{41}H_2AlCl_2F_{54}N_2O_4$	$C_{46}H_4AlF_{56}N_2O_4$
Formula weight	938.32	658.26	1710.33	1739.49
Temperature/K	100(2)	100(2)	100(2)	85(2)
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	$C2/c$ (15)	$P\bar{1}$ (2)	$P2_1/c$ (14)	$P2_1/c$ (14)
a/Å	33.4501(18)	6.2273(12)	14.8323(5)	22.3031(14)
b/Å	7.4054(4)	9.1591(17)	32.8612(10)	58.214(4)
c/Å	27.2418(16)	9.3845(17)	21.9601(7)	26.4508(17)
α/°	90	99.223(4)	90	90
β/°	96.611(2)	95.085(4)	96.729(2)	105.964(2)
γ/°	90	100.059(4)	90	90
Volume/Å^3	6703.2(6)	516.46(17)	10629.8(6)	33018(4)
Z	8	1	8	24
ρ_{calc}g/cm^3	1.860	2.116	2.137	2.100
μ/mm^{-1}	0.203	0.241	0.377	0.277
F(000)	3680	320	6616	20232
Crystal size/mm^3	0.500×0.130×0.120	0.35×0.1×0.08	0.25×0.1×0.1	0.35×0.26×0.18
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range /°	4.10 to 52.84	4.43 to 52.85	2.24 to 52.81	3.76 to 60.77
Index ranges	twinned	twinned	-18 ≤ h ≤ 18; -41 ≤ k ≤ 41; -27 ≤ l ≤ 27	-31 ≤ h ≤ 31, -82 ≤ k ≤ 82,-37 ≤ l ≤ 37
Reflections collected	6865	2126	129612	1932167
Independent reflections	6865 [R_{int} = 0.0762, R_{sigma} = 0.0338]	2126 [R_{int} = 0.0319,R_{sigma} = 0.0306]	21795 [R_{int} = 0.0332,R_{sigma} = 0.0262]	99511 [R_{int} = 0.1082, R_{sigma} = 0.0400]
Data/restraints/parameters	6865/380/577	2126/0/199	21795/38145/2890	99511/170559/7158
Goodness-of-fit on F^2	1.114	1.039	1.058	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0394, wR_2 = 0.0894	R_1 = 0.0376, wR_2 = 0.0864	R_1 = 0.0530, wR_2 = 0.1394	R_1 = 0.0927, wR_2 = 0.2423
Final R indexes [all data]	R_1 = 0.0468, wR_2 = 0.0921	R_1 = 0.0547, wR_2 = 0.0926	R_1 = 0.0698, wR_2 = 0.1508	R_1 = 0.1324, wR_2 = 0.2667
Largest diff. peak/hole / e Å^{-3}	0.35/-0.36	0.36/-0.24	0.74/-0.45	2.20/-0.90
CCDC ref.	1985540	1985541	1985545	poor quality not uploaded

	5	**6**	**7 (vap. dif.)**	**7 (layer)**
Empirical formula	$C_{48}H_{19}Al_2F_{74}N_5O_8Sn$	$C_{58}H_{24}Al_2F_{74}N_{12}O_8Sn$	$C_{369}H_{210}Al_{14}F_{504}Fe_7O_{61}$	$C_{660}H_{376}Al_{24}F_{872}Fe_{12}O_{108}$
Formula weight	2372.33	2595.54	15976.82	27919.31
Temperature/K	100(2)	100(2)	130(2)	100(2)
Crystal system	monoclinic	triclinic	trigonal	orthorhombic
Space group	Cc (9)	$P\overline{1}$ (2)	$R\overline{3}$ (148)	$P\mathrm{na}2_1$ (33)
a/Å	15.4929(8)	13.7648(9)	36.874(2)	22.605(6)
b/Å	23.5408(12)	15.3404(10)	36.874(2)	26.708(6)
c/Å	20.7908(12)	23.5287(15)	34.387(2)	38.782(11)
α/°	90	107.663(2)	90	90
β/°	91.140(2)	90.055(2)	90	90
γ/°	90	116.361(2)	120	90
Volume/Å^3	7581.2(7)	4187.9(5)	40492(5)	23414(10)
Z	4	2	3	1
ρ_{calc}g/cm^3	2.078	2.058	1.966	1.980
μ/mm^{-1}	0.596	0.552	0.444	0.443
F(000)	4592	2524	23455	13672
Crystal size/mm^3	0.250×0.200×0.080	0.3×0.25×0.21	0.3×0.28×0.12	0.442×0.422×0.246
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range /°	3.74 to 52.83	4.07 to 52.88	3.83 to 52.76	2.36 to 52.67
Index ranges	-19 ≤ h ≤ 19, -29 ≤ k ≤ 29, -26 ≤ l ≤ 26	-17 ≤ h ≤ 17, -19 ≤ k ≤ 19, -29 ≤ l ≤ 29	-46 ≤ h ≤ 46, -46 ≤ k ≤ 46, -42 ≤ l ≤ 42	-28 ≤ h ≤ 28, -33 ≤ k ≤ 33, -48 ≤ l ≤ 48
Reflections collected	148647	232532	802398	834680
Independent reflections	15550 [R_{int} = 0.0922, R_{sigma} = 0.0442]	17170 [R_{int} = 0.0337, R_{sigma} = 0.0126]	18400 [R_{int} = 0.0666, R_{sigma} = 0.0178]	47582, [R_{int} = 0.1567, R_{sigma} = 0.0642]
Data/restraints/parameters	15550/26468/1877	17170/25656/2033	18400/64070/3153	47582/196847/5436
Goodness-of-fit on F^2	0.966	0.759	1.017	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0189, wR_2 = 0.0371	R_1 = 0.0371, wR_2 = 0.0993	R_1 = 0.0828, wR_2 = 0.2172	R_1 = 0.0906, wR_2 = 0.2502
Final R indexes [all data]	R_1 = 0.0258, wR_2 = 0.0377	R_1 = 0.0407, wR_2 = 0.1028	R_1 = 0.0934, wR_2 = 0.2285	R_1 = 0.1152, wR_2 = 0.2687
Largest diff. peak/hole / e Å^{-3}	0.27/-0.21	0.97/-0.93	1.28/-0.96	1.36/-1.22
CCDC ref.	1985536	1985542	not uploaded due to poor quality	1985548

	8
Empirical formula	$C_{63}H_{43}Al_2F_{74}FeNO_8$
Formula weight	2457.79
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	$Pna2_1$ (33)
a/Å	20.1226(10)
b/Å	19.8877(7)
c/Å	21.1779(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	8475.2(6)
Z	4
ρ_{calc}g/cm^3	1.926
μ/mm^{-1}	0.415
F(000)	4840
Crystal size/mm^3	0.300×0.200×0.180
Radiation	MoK_α (λ=0.71073 Å)
2Θ range /°	2.79 to 54.26
Index ranges	-25 ≤ h ≤ 25, -25 ≤ k ≤ 25, -27 ≤ l ≤ 27
Reflections collected	378183
Independent reflections	18753 [R_{int} = 0.0381, R_{sigma} = 0.0144]
Data/restraints/parameters	18753/15526/1604
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0399, wR_2 = 0.1099
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.1113
Largest diff. peak/hole / e Å^{-3}	0.81/-0.33
CCDC ref.	1985548

	S1	**S2**	**S3**	**S4**
Empirical formula	$C_{34}H_{12}AlBr_3F_{36}NO_4$	$C_{68}H_{24}Al_2Br_4F_{72}N_2O_8$	$C_{41}H_{21}AlBr_3F_{36}N_3O_4$	$C_{61}H_{47}AlBr_3F_{36}N_3O_4$
Formula weight	1449.16	2738.49	1570.32	1836.72
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	monoclinic	orthorhombic
Space group	$P2_1/c$ (14)	$P1$ (1)	$P2_1/c$ (14)	$Pbca$ (61)
a/Å	10.5826(3)	10.4545(10)	14.1201(18)	16.8899(7)
b/Å	21.3372(7)	14.7987(13)	15.8932(19)	24.2873(11)
c/Å	20.6368(6)	15.4823(13)	23.462(3)	33.5884(14)
α/°	90	93.013(5)	90	90
β/°	100.820(2)	101.553(5)	100.597(6)	90
γ/°	90	109.273(5)	90	90
Volume/Å^3	4577.0(2)	2196.9(3)	5175.5(11)	13778.3(10)
Z	4	1	4	8
ρ_{calc}g/cm^3	2.103	2.070	2.015	1.771
μ/mm^{-1}	2.852	2.060	2.532	1.916
F(000)	2788	1324	3048	7264
Crystal size/mm^3	0.250×0.250×0.230	0.330×0.110×0.050	0.360×0.130×0.050	0.500×0.350×0.160
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range /°	2.77 to 52.86	2.71 to 52.98	2.93 to 52.98	2.42 to 53.02
Index ranges	-13 ≤ h ≤ 13, -25 ≤ k ≤ 26, -25 ≤ l ≤ 25	-12 ≤ h ≤ 13, -18 ≤ k ≤ 18, -19 ≤ l ≤ 19	-17 ≤ h ≤ 17, -19 ≤ k ≤ 19, -27 ≤ l ≤ 29	-21 ≤ h ≤ 21, -29 ≤ k ≤ 30,-42 ≤ l ≤ 42
Reflections collected	112640	52847	109470	218939
Independent reflections	9412 [R_{int} = 0.0298,R_{sigma} = 0.0154]	16534 [R_{int} = 0.0269,R_{sigma} = 0.0322]	10591 [R_{int} = 0.0338,R_{sigma} = 0.0223]	14222 [R_{int} = 0.0704, R_{sigma} = 0.0281]
Data/restraints/parameters	9412/2850/712	16534/12437/1463	10591/2850/795	14222/4322/1108
Goodness-of-fit on F^2	1.032	1.053	1.033	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0270, wR_2 = 0.0664	R_1 = 0.0380, wR_2 = 0.1021	R_1 = 0.0357, wR_2 = 0.0936	R_1 = 0.0304, wR_2 = 0.0652
Final R indexes [all data]	R_1 = 0.0328, wR_2 = 0.0690	R_1 = 0.0437, wR_2 = 0.1056	R_1 = 0.0461, wR_2 = 0.0986	R_1 = 0.0492, wR_2 = 0.0727
Largest diff. peak/hole / e Å^{-3}	0.75/-0.66	1.22/-0.49	0.91/-0.59	0.62/-0.33
CCDC ref.	1985543	1985539	1985547	1985546

	$[FeCp^*_2][Al(OR^F)_4]$ S5
Empirical formula	$C_{36}H_{30}AlF_{36}FeO_4$
Formula weight	1293.43
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$ (14)
a/Å	34.420(2)
b/Å	20.3939(14)
c/Å	21.0218(15)
α/°	90
β/°	106.022(2)
γ/°	90
Volume/Å^3	14183.0(17)
Z	12
ρ_{calc}g/cm^3	1.817
μ/mm^{-1}	0.519
F(000)	7692
Crystal size/mm^3	0.42×0.35×0.1
Radiation	MoK_α (λ=0.71073 Å)
2Θ range /°	1.23 to 52.79
Index ranges	-43 ≤ h ≤ 42, -25 ≤ k ≤ 25, -26 ≤ l ≤ 26
Reflections collected	188228
Independent reflections	29000 [R_{int} = 0.0741, R_{sigma} = 0.0549]
Data/restraints/parameters	29000/52737/3027
Goodness-of-fit on F^2	1.088
Final R indexes [I>=2σ (I)]	R_1 = 0.1379, wR_2 = 0.3690
Final R indexes [all data]	R_1 = 0.1563, wR_2 = 0.3797
Largest diff. peak/hole / e Å^{-3}	1.72/-1.04
CCDC ref.	Not uploaded due to poor quality

*Table S 5 Atomic coordinates and U_{eq} [Å^2] for **2**·o**DFB***

Atom	*x*	*y*	*z*	U_{eq}
C1	0.42163(5)	0.4277(2)	0.31554(6)	0.0149(3)
F1	0.44023(3)	0.73381(14)	0.31315(4)	0.0208(2)
F2	0.51820(3)	0.65127(15)	0.30690(4)	0.0263(2)
C2	0.45159(5)	0.5579(2)	0.31216(6)	0.0161(3)
F3	0.54237(3)	0.29886(16)	0.30853(4)	0.0253(2)
C3	0.49141(5)	0.5187(2)	0.30987(6)	0.0185(4)
F4	0.48688(3)	0.03331(14)	0.31299(4)	0.0225(2)
C4	0.50349(5)	0.3403(3)	0.31000(6)	0.0184(4)
F5	0.40874(3)	0.11295(13)	0.31760(3)	0.0173(2)
C5	0.47507(5)	0.2062(2)	0.31184(6)	0.0169(3)
F6	0.32157(3)	0.48717(14)	0.37791(3)	0.0195(2)
C6	0.43520(5)	0.2493(2)	0.31399(6)	0.0150(3)
F8	0.23681(3)	0.18755(17)	0.25375(4)	0.0285(3)
C8	0.31622(5)	0.4074(2)	0.33241(6)	0.0165(3)
C7	0.34959(5)	0.3989(2)	0.30610(6)	0.0153(3)
F7	0.24855(3)	0.35776(15)	0.34384(4)	0.0231(2)
F9	0.29999(3)	0.15440(17)	0.19960(4)	0.0286(3)
C9	0.27896(5)	0.3405(2)	0.31598(6)	0.0185(4)
N1A	0.38617(4)	0.8355(2)	0.39865(5)	0.0145(3)
N1	0.38414(4)	0.4886(2)	0.32553(5)	0.0154(3)
C11	0.30530(6)	0.2381(3)	0.24347(6)	0.0200(4)
C10	0.27310(5)	0.2538(3)	0.27087(7)	0.0201(4)
F10	0.37188(3)	0.29847(16)	0.23099(4)	0.0230(2)
C12	0.34222(5)	0.3107(2)	0.26040(6)	0.0176(3)
Li1A	0.38122(9)	0.7707(4)	0.32250(11)	0.0205(6)
C1A	0.42432(5)	0.8957(2)	0.41698(6)	0.0146(3)
F1A	0.44328(3)	0.58921(14)	0.42119(4)	0.0194(2)
C2A	0.45460(5)	0.7658(2)	0.42569(6)	0.0157(3)
F2A	0.52196(3)	0.67078(15)	0.44469(4)	0.0240(2)
C3A	0.49476(5)	0.8038(2)	0.43763(6)	0.0176(3)
F3A	0.54565(3)	1.02415(15)	0.45497(4)	0.0224(2)
C4A	0.50668(5)	0.9822(3)	0.44285(6)	0.0175(4)
F4A	0.48963(3)	1.28900(14)	0.44171(4)	0.0227(2)
C5A	0.47807(5)	1.1163(2)	0.43633(6)	0.0170(3)
F5A	0.41162(3)	1.21246(13)	0.41614(3)	0.0177(2)
C6A	0.43798(5)	1.0737(2)	0.42367(6)	0.0151(3)
F6A	0.32036(3)	0.83439(15)	0.33276(3)	0.0191(2)
C7A	0.35236(5)	0.9276(2)	0.41022(6)	0.0145(3)
F7A	0.24849(3)	0.96554(16)	0.35212(4)	0.0240(2)
C8A	0.31750(5)	0.9172(2)	0.37692(6)	0.0156(3)
F8A	0.24230(3)	1.14525(17)	0.43883(4)	0.0283(3)
C9A	0.28078(5)	0.9846(2)	0.38593(6)	0.0180(4)
F9A	0.30886(3)	1.17985(16)	0.50607(4)	0.0266(3)
C10A	0.27744(5)	1.0756(3)	0.42948(7)	0.0204(4)
F10A	0.37863(3)	1.03113(15)	0.48986(3)	0.0197(2)
C11A	0.31135(5)	1.0934(3)	0.46331(6)	0.0189(4)
C12A	0.34750(5)	1.0190(2)	0.45415(6)	0.0160(3)
Li1	0.38224(9)	0.5548(4)	0.39961(10)	0.0199(6)
C1_1	0.36057(6)	0.5796(2)	0.50782(6)	0.0204(4)
C2_1	0.32203(6)	0.6371(3)	0.51035(7)	0.0247(4)
C3_1	0.31258(7)	0.7335(3)	0.55062(8)	0.0310(5)
H3_1	0.285867	0.774391	0.552424	0.037
C4_1	0.34282(7)	0.7697(3)	0.58850(8)	0.0344(5)

H4_1	0.336775	0.835372	0.616675	0.041
C5_1	0.38159(7)	0.7113(3)	0.58565(8)	0.0344(5)
H5_1	0.402067	0.737059	0.611859	0.041
C6_1	0.39096(6)	0.6151(3)	0.54475(7)	0.0263(4)
H6_1	0.417653	0.575024	0.542424	0.032
F1_1	0.36882(3)	0.48229(16)	0.46725(4)	0.0265(3)
F2_1	0.29346(4)	0.5991(2)	0.47259(4)	0.0374(3)
C1_2	0.36924(5)	0.8125(3)	0.20499(6)	0.0197(4)
C2_2	0.40454(5)	0.8856(2)	0.19289(6)	0.0187(4)
C3_2	0.41357(6)	0.8779(3)	0.14492(6)	0.0206(4)
H3_2	0.437896	0.928452	0.136227	0.025
C4_2	0.38659(6)	0.7952(3)	0.10953(6)	0.0235(4)
H4_2	0.392349	0.790022	0.076211	0.028
C5_2	0.35136(6)	0.7203(3)	0.12224(7)	0.0252(4)
H5_2	0.333176	0.663273	0.097676	0.030
C6_2	0.34240(6)	0.7278(3)	0.17077(7)	0.0227(4)
H6_2	0.318377	0.675816	0.179928	0.027
F1_2	0.36079(3)	0.82809(17)	0.25291(4)	0.0279(3)
F2_2	0.43013(3)	0.96366(16)	0.22823(4)	0.0278(3)

*Table S 6 Atomic coordinates and U_{eq} [Å^2] for **3***

Atom	***x***	***y***	***z***	U_{eq}
F1	0.9481(2)	0.42111(14)	0.79210(13)	0.0193(3)
C1	0.6332(3)	0.4250(2)	0.9155(2)	0.0137(4)
N1	0.6794(3)	0.58515(19)	0.93919(18)	0.0135(4)
F2	0.8557(2)	0.11936(15)	0.72198(14)	0.0231(3)
C2	0.7682(3)	0.3460(2)	0.8362(2)	0.0154(5)
C3	0.7230(4)	0.1908(3)	0.8002(2)	0.0162(5)
F3	0.4924(2)	-0.03909(14)	0.80850(13)	0.0216(3)
F4	0.2272(2)	0.10625(14)	0.96435(13)	0.0184(3)
C4	0.5409(4)	0.1112(2)	0.8444(2)	0.0163(5)
C5	0.4073(3)	0.1871(2)	0.9254(2)	0.0149(5)
F5	1.07158(19)	0.75313(15)	0.87437(13)	0.0202(3)
C6	0.4532(3)	0.3433(2)	0.9666(2)	0.0141(5)
F6	1.0953(2)	0.86634(15)	0.62765(14)	0.0252(3)
C7	0.6965(3)	0.6456(2)	0.8065(2)	0.0141(5)
F7	0.7356(2)	0.82018(16)	0.42890(14)	0.0284(4)
C8	0.8925(3)	0.7283(2)	0.7784(2)	0.0149(5)
F8	0.3485(2)	0.65887(16)	0.47817(13)	0.0238(3)
C9	0.9057(4)	0.7860(3)	0.6517(2)	0.0184(5)
F9	0.3245(2)	0.54294(14)	0.72402(13)	0.0201(3)
C10	0.7228(4)	0.7626(3)	0.5503(2)	0.0192(5)
C11	0.5272(4)	0.6822(3)	0.5758(2)	0.0171(5)
C12	0.5152(3)	0.6234(2)	0.7027(2)	0.0142(5)

*Table S 7 Atomic coordinates and U_{eq} [Å^2] for **4** (CH_2Cl_2)*

Atom	***x***	***y***	***z***	U_{eq}
Al2	0.54004(5)	0.26344(2)	0.46540(4)	0.02049(17)
F4	-0.19575(13)	0.83901(5)	0.44135(8)	0.0359(4)
C4	-0.2369(2)	0.78157(10)	0.38320(14)	0.0289(6)
Al1	0.30480(6)	0.50210(3)	0.72613(4)	0.02083(17)

F6	0.04698(14)	0.77483(6)	0.73531(8)	0.0393(5)
C6	-0.13736(19)	0.77503(9)	0.47737(13)	0.0229(6)
C5	-0.1893(2)	0.79910(9)	0.43391(14)	0.0262(6)
F5	-0.02062(13)	0.82345(5)	0.64475(8)	0.0344(4)
F7	0.04968(12)	0.69371(6)	0.72024(8)	0.0343(4)
C7	-0.05354(18)	0.76716(9)	0.57741(13)	0.0230(6)
F8	-0.01693(13)	0.65978(5)	0.61370(8)	0.0361(4)
C8	-0.0194(2)	0.78347(9)	0.63427(13)	0.0266(6)
F9	0.06286(12)	0.71219(5)	0.44798(8)	0.0302(4)
C9	0.0154(2)	0.75882(10)	0.68167(13)	0.0281(6)
F00B	0.78123(12)	0.42960(5)	0.64625(8)	0.0316(4)
F10	0.13286(13)	0.64589(6)	0.39669(10)	0.0418(5)
C10	0.0164(2)	0.71697(10)	0.67374(14)	0.0281(6)
F12	-0.07561(14)	0.56262(6)	0.48442(11)	0.0451(5)
C12	-0.05230(18)	0.72457(9)	0.56933(13)	0.0233(6)
C11	-0.0175(2)	0.70020(9)	0.61882(14)	0.0268(6)
F11	0.06445(14)	0.57099(6)	0.41608(11)	0.0457(5)
C14	0.0290(2)	0.67536(9)	0.45690(13)	0.0258(6)
F14	0.08171(12)	0.79880(5)	0.48822(8)	0.0328(4)
C13	-0.0438(2)	0.67164(9)	0.49070(14)	0.0260(6)
F13	-0.15024(13)	0.62888(6)	0.53005(9)	0.0385(4)
F15	0.17309(12)	0.87040(6)	0.48789(9)	0.0406(5)
C15	0.0649(2)	0.64152(10)	0.43126(15)	0.0306(7)
F18	-0.16508(12)	0.86568(5)	0.55974(8)	0.0318(4)
C18	-0.0790(2)	0.63321(10)	0.49915(14)	0.0301(7)
C17	-0.0422(2)	0.59927(9)	0.47504(16)	0.0326(7)
F17	-0.07478(13)	0.93774(5)	0.55773(9)	0.0368(4)
C16	0.0300(2)	0.60386(10)	0.44039(15)	0.0329(7)
F16	0.09419(13)	0.93959(6)	0.52294(9)	0.0393(4)
C19	-0.04317(19)	0.83148(9)	0.52345(13)	0.0240(6)
C24	-0.0828(2)	0.86709(9)	0.54102(13)	0.0258(6)
C23	-0.0365(2)	0.90350(9)	0.54089(14)	0.0288(6)
C22	0.0497(2)	0.90440(10)	0.52325(14)	0.0302(7)
C21	0.0898(2)	0.86931(10)	0.50508(14)	0.0296(7)
C20	0.0433(2)	0.83294(9)	0.50489(13)	0.0262(6)
F3	-0.28638(13)	0.80457(6)	0.34246(9)	0.0393(5)
C3	-0.2356(2)	0.73976(10)	0.37523(14)	0.0287(6)
N2	-0.08514(16)	0.79209(7)	0.52802(11)	0.0226(5)
F2	-0.28355(13)	0.72331(6)	0.32664(8)	0.0384(4)
C2	-0.1879(2)	0.71541(9)	0.41814(14)	0.0278(6)
N1	-0.08306(16)	0.70839(7)	0.51209(11)	0.0245(5)
F1	-0.19348(13)	0.67536(5)	0.41072(9)	0.0369(4)
C1	-0.13626(19)	0.73237(9)	0.46938(13)	0.0232(6)
O1_3	0.3514(2)	0.53779(11)	0.77930(14)	0.0273(7)
C1_3	0.3660(4)	0.55162(17)	0.8372(3)	0.0283(13)
C2_3	0.3961(4)	0.59692(17)	0.8345(2)	0.0405(11)
F1_3	0.3235(2)	0.62095(9)	0.81975(14)	0.0495(8)
F2_3	0.4358(2)	0.61073(9)	0.88891(13)	0.0466(8)
F3_3	0.4515(2)	0.60338(10)	0.79361(14)	0.0456(8)
C3_3	0.4445(4)	0.52726(19)	0.8741(3)	0.0415(14)
F4_3	0.4377(2)	0.48821(8)	0.86221(13)	0.0449(8)
F5_3	0.5263(2)	0.53965(14)	0.86046(18)	0.0573(10)
F6_3	0.4448(3)	0.53164(13)	0.93521(16)	0.0527(10)
C4_3	0.2801(4)	0.5489(2)	0.8705(3)	0.0396(14)
F7_3	0.2688(4)	0.51028(13)	0.8895(2)	0.0554(12)

F8_3	0.2829(3)	0.57252(13)	0.91979(18)	0.0478(10)
F9_3	0.2065(2)	0.55817(14)	0.83323(15)	0.0544(9)
O1_4	0.1988(6)	0.5172(3)	0.6911(4)	0.0294(19)
C1_4	0.1528(4)	0.54393(19)	0.6513(3)	0.0292(13)
C2_4	0.1834(5)	0.5396(2)	0.5861(3)	0.0469(17)
F1_4	0.2599(2)	0.55963(14)	0.58248(19)	0.0532(10)
F2_4	0.1211(3)	0.5544(2)	0.54259(18)	0.0728(16)
F3_4	0.1985(3)	0.50064(16)	0.5735(2)	0.0580(13)
C3_4	0.0503(3)	0.53339(16)	0.6476(2)	0.0366(11)
F4_4	0.02699(19)	0.52552(13)	0.70343(15)	0.0488(9)
F5_4	0.0313(4)	0.50001(18)	0.6147(2)	0.0595(14)
F6_4	-0.0043(2)	0.56302(14)	0.62302(18)	0.0509(10)
C4_4	0.1671(4)	0.58834(17)	0.6737(3)	0.0437(12)
F7_4	0.1191(3)	0.59601(14)	0.7206(2)	0.0568(11)
F8_4	0.1407(2)	0.61537(11)	0.62845(19)	0.0628(11)
F9_4	0.2523(2)	0.59548(9)	0.69268(17)	0.0515(10)
O1_5	0.2932(5)	0.45816(15)	0.7651(2)	0.0287(12)
C1_5	0.2558(5)	0.4202(2)	0.7642(3)	0.0401(18)
C2_5	0.3356(6)	0.3894(3)	0.7835(5)	0.067(2)
F1_5	0.3973(5)	0.40330(18)	0.8254(4)	0.0754(17)
F2_5	0.3037(5)	0.35391(15)	0.8023(4)	0.095(2)
F3_5	0.3780(6)	0.3809(3)	0.7350(4)	0.095(3)
C3_5	0.1992(7)	0.4099(2)	0.7036(3)	0.084(2)
F4_5	0.1190(5)	0.4296(2)	0.6996(3)	0.106(2)
F5_5	0.2416(6)	0.42134(19)	0.6571(2)	0.127(3)
F6_5	0.1897(6)	0.36876(17)	0.6992(3)	0.098(2)
C4_5	0.1935(6)	0.4184(3)	0.8165(4)	0.0444(18)
F7_5	0.1446(6)	0.4512(2)	0.8194(3)	0.0610(19)
F8_5	0.1401(5)	0.3858(3)	0.8128(3)	0.058(2)
F9_5	0.2445(5)	0.41657(19)	0.8708(3)	0.0784(17)
O1_6	0.3732(7)	0.5005(4)	0.6681(5)	0.027(2)
C1_6	0.4589(5)	0.4999(2)	0.6534(3)	0.0275(14)
C2_6	0.5088(4)	0.54083(19)	0.6706(4)	0.0642(18)
F1_6	0.5401(3)	0.54008(19)	0.7305(2)	0.0902(18)
F2_6	0.5767(3)	0.54724(14)	0.6357(3)	0.0893(18)
F3_6	0.4513(3)	0.57158(13)	0.6596(3)	0.0756(15)
C3_6	0.4559(4)	0.4932(3)	0.5837(3)	0.073(2)
F4_6	0.3950(3)	0.4674(2)	0.5628(2)	0.0962(18)
F5_6	0.4295(6)	0.5287(4)	0.5553(5)	0.105(2)
F6_6	0.5359(2)	0.48085(19)	0.56728(15)	0.0717(17)
C4_6	0.5141(4)	0.4642(2)	0.6863(3)	0.0471(16)
F7_6	0.4866(4)	0.42919(13)	0.6611(3)	0.0945(19)
F8_6	0.6039(4)	0.4693(3)	0.6832(3)	0.060(2)
F9_6	0.5014(10)	0.4649(4)	0.7447(5)	0.057(2)
O1_7	0.5740(3)	0.28029(11)	0.53925(15)	0.0304(8)
C1_7	0.5805(3)	0.31200(12)	0.57863(18)	0.0327(9)
C2_7	0.6088(3)	0.35200(12)	0.54811(19)	0.0370(9)
F1_7	0.69558(19)	0.35081(8)	0.53957(14)	0.0559(7)
F2_7	0.5968(4)	0.38526(12)	0.58010(17)	0.0564(10)
F3_7	0.5635(2)	0.35656(7)	0.49328(11)	0.0535(8)
C3_7	0.4886(3)	0.31934(15)	0.6047(2)	0.0542(12)
F4_7	0.4511(3)	0.28417(12)	0.6169(2)	0.0851(13)
F5_7	0.4308(2)	0.33919(11)	0.56373(16)	0.0749(10)
F6_7	0.4989(3)	0.34099(13)	0.6564(2)	0.0768(13)
C4_7	0.6548(4)	0.30119(14)	0.6330(2)	0.0499(12)

F7_7	0.6232(3)	0.27520(9)	0.67068(13)	0.0720(10)
F8_7	0.6832(3)	0.33438(9)	0.66517(14)	0.0693(10)
F9_7	0.72713(19)	0.28495(9)	0.61214(13)	0.0594(8)
O1_8	0.43661(14)	0.28484(7)	0.44044(10)	0.0318(5)
C1_8	0.3773(2)	0.29671(9)	0.39224(14)	0.0296(6)
C2_8	0.3385(3)	0.25865(11)	0.35675(19)	0.0535(10)
F1_8	0.27837(19)	0.23940(8)	0.38791(14)	0.0752(8)
F2_8	0.29667(18)	0.26753(7)	0.30160(12)	0.0668(7)
F3_8	0.40543(19)	0.23267(7)	0.34891(12)	0.0687(8)
C3_8	0.4209(2)	0.32554(11)	0.34829(15)	0.0362(7)
F4_8	0.47860(13)	0.35051(6)	0.37856(9)	0.0438(5)
F5_8	0.46733(16)	0.30447(9)	0.31008(10)	0.0596(7)
F6_8	0.35844(14)	0.34792(7)	0.31410(9)	0.0471(5)
C4_8	0.3000(2)	0.31950(11)	0.41901(16)	0.0395(8)
F7_8	0.32581(15)	0.35684(6)	0.43613(10)	0.0472(5)
F8_8	0.22476(12)	0.32206(7)	0.37774(11)	0.0475(5)
F9_8	0.27595(15)	0.30019(8)	0.46740(11)	0.0580(6)
O1_9	0.6128(5)	0.2766(3)	0.4130(3)	0.0260(15)
C1_9	0.6910(4)	0.26892(15)	0.3895(2)	0.0261(11)
C2_9	0.6960(4)	0.22498(15)	0.3651(2)	0.0526(13)
F1_9	0.7170(6)	0.19877(16)	0.4099(4)	0.077(2)
F2_9	0.7574(4)	0.22127(15)	0.3253(3)	0.0805(16)
F3_9	0.6165(5)	0.21338(19)	0.3381(3)	0.0718(16)
C3_9	0.6977(3)	0.29927(14)	0.3361(2)	0.0380(11)
F4_9	0.6707(4)	0.33545(18)	0.3494(3)	0.0543(14)
F5_9	0.6455(7)	0.2878(3)	0.2868(3)	0.074(2)
F6_9	0.7823(3)	0.30234(16)	0.32080(18)	0.0458(10)
C4_9	0.7732(3)	0.27572(15)	0.43938(19)	0.0385(11)
F7_9	0.7880(5)	0.31446(18)	0.4501(3)	0.0654(15)
F8_9	0.8502(3)	0.26022(17)	0.4251(2)	0.0535(13)
F9_9	0.7561(6)	0.2591(2)	0.4917(2)	0.0469(14)
O1_10	0.5340(10)	0.21156(19)	0.4703(5)	0.033(3)
C1_10	0.5107(5)	0.1768(2)	0.4967(3)	0.0298(16)
C2_10	0.4625(3)	0.18519(15)	0.5548(2)	0.0375(12)
F1_10	0.5214(3)	0.19598(18)	0.6020(2)	0.0531(12)
F2_10	0.4171(8)	0.1527(3)	0.5710(4)	0.0473(17)
F3_10	0.4029(9)	0.2153(3)	0.5445(7)	0.0476(19)
C3_10	0.4473(4)	0.15155(16)	0.4502(3)	0.0472(14)
F4_10	0.4768(9)	0.1526(4)	0.3949(4)	0.069(2)
F5_10	0.3646(5)	0.1668(3)	0.4445(3)	0.0678(18)
F6_10	0.4447(4)	0.11228(14)	0.4681(3)	0.0640(15)
C4_10	0.6005(4)	0.15186(15)	0.5160(2)	0.0404(13)
F7_10	0.6289(4)	0.1340(2)	0.4678(2)	0.0497(14)
F8_10	0.5878(8)	0.12241(19)	0.5570(4)	0.069(2)
F9_10	0.6638(6)	0.1759(4)	0.5421(6)	0.059(2)
Cl1_11	0.04217(6)	0.29951(3)	0.68899(4)	0.0412(2)
Cl2_11	0.01068(6)	0.21385(3)	0.65660(4)	0.04001(19)
C1_11	-0.0319(3)	0.25760(11)	0.69005(18)	0.0442(9)
H1A_11	-0.091512	0.264783	0.667521	0.053
H1AB_11	-0.041283	0.251488	0.732995	0.053
Cl1_12	0.70345(6)	0.04643(3)	0.55305(4)	0.0410(2)
Cl2_12	0.70627(6)	-0.04233(3)	0.55830(4)	0.03761(19)
C1_12	0.7708(2)	0.00232(10)	0.55146(16)	0.0374(7)
H1A_12	0.820761	0.003411	0.585528	0.045
H1AB_12	0.798141	0.001465	0.512465	0.045

O1_19	0.5341(19)	0.2112(3)	0.4653(9)	0.020(4)
C1_19	0.5176(7)	0.1770(4)	0.4962(5)	0.027(3)
C2_19	0.4208(6)	0.1771(3)	0.5156(5)	0.039(2)
F1_19	0.3584(8)	0.1702(5)	0.4681(5)	0.057(3)
F2_19	0.4046(18)	0.1499(8)	0.5574(10)	0.059(4)
F3_19	0.4024(19)	0.2140(6)	0.5369(14)	0.047(3)
C3_19	0.5875(6)	0.1715(3)	0.5546(4)	0.031(2)
F4_19	0.6695(10)	0.1830(8)	0.5443(9)	0.043(3)
F5_19	0.5647(6)	0.1946(3)	0.6005(4)	0.0419(19)
F6_19	0.5911(13)	0.1328(3)	0.5728(7)	0.047(3)
C4_19	0.5286(7)	0.1399(3)	0.4537(4)	0.044(2)
F7_19	0.6121(9)	0.1337(5)	0.4454(5)	0.054(3)
F8_19	0.4948(8)	0.1058(3)	0.4744(6)	0.067(3)
F9_19	0.4841(15)	0.1481(5)	0.3979(6)	0.045(3)
O1_2	0.2020(10)	0.5239(6)	0.7036(8)	0.025(3)
C1_2	0.1396(8)	0.5375(3)	0.6591(5)	0.033(3)
C2_2	0.0864(6)	0.5724(3)	0.6864(4)	0.046(2)
F1_2	0.1312(6)	0.6069(2)	0.6893(5)	0.058(2)
F2_2	0.0059(5)	0.5780(3)	0.6522(5)	0.059(2)
F3_2	0.0687(5)	0.5637(2)	0.7414(3)	0.063(2)
C3_2	0.0734(7)	0.5020(3)	0.6411(5)	0.045(2)
F4_2	0.1191(5)	0.46832(19)	0.6309(3)	0.062(2)
F5_2	0.0221(4)	0.4937(2)	0.6848(4)	0.0546(18)
F6_2	0.0211(9)	0.5096(3)	0.5897(5)	0.059(3)
C4_2	0.1830(7)	0.5538(3)	0.6034(5)	0.042(3)
F7_2	0.2089(8)	0.5227(3)	0.5703(5)	0.060(2)
F8_2	0.1246(5)	0.5774(3)	0.5687(4)	0.067(2)
F9_2	0.2570(4)	0.5760(2)	0.6201(4)	0.0529(18)
O1_13	0.3789(13)	0.5076(7)	0.6728(10)	0.030(4)
C1_13	0.4478(8)	0.4952(3)	0.6426(5)	0.029(2)
C2_13	0.4719(5)	0.5309(3)	0.6013(4)	0.045(2)
F1_13	0.4758(6)	0.5649(2)	0.6300(4)	0.0582(18)
F2_13	0.5529(4)	0.5242(3)	0.5818(4)	0.068(3)
F3_13	0.4090(10)	0.5364(5)	0.5524(8)	0.082(3)
C3_13	0.4174(6)	0.4572(3)	0.6019(4)	0.056(2)
F4_13	0.3303(5)	0.4605(2)	0.5802(3)	0.069(2)
F5_13	0.4659(6)	0.4518(3)	0.5577(3)	0.077(3)
F6_13	0.4231(6)	0.4238(2)	0.6363(3)	0.0620(19)
C4_13	0.5305(6)	0.4837(3)	0.6899(5)	0.037(2)
F7_13	0.5057(17)	0.4612(6)	0.7351(8)	0.050(3)
F8_13	0.5899(8)	0.4603(4)	0.6631(5)	0.054(3)
F9_13	0.5759(5)	0.5158(2)	0.7100(3)	0.066(2)
O1_14	0.286(3)	0.4536(6)	0.7484(19)	0.042(6)
C1_14	0.2586(12)	0.4187(5)	0.7714(8)	0.043(4)
C2_14	0.3087(13)	0.3833(5)	0.7432(8)	0.045(4)
F1_14	0.3918(13)	0.3891(7)	0.7768(12)	0.059(3)
F2_14	0.2768(15)	0.3475(4)	0.7566(9)	0.050(4)
F3_14	0.3240(15)	0.3848(5)	0.6867(7)	0.049(3)
C3_14	0.1557(12)	0.4153(7)	0.7657(11)	0.067(4)
F4_14	0.1217(17)	0.4501(8)	0.7821(15)	0.071(4)
F5_14	0.125(2)	0.4102(10)	0.7069(12)	0.088(4)
F6_14	0.124(3)	0.3867(11)	0.7996(18)	0.063(4)
C4_14	0.3036(14)	0.4148(7)	0.8397(8)	0.066(5)
F7_14	0.253(2)	0.4315(10)	0.8778(13)	0.075(4)
F8_14	0.315(2)	0.3761(7)	0.8539(13)	0.083(5)

F9_14	0.3869(14)	0.4310(8)	0.8399(13)	0.074(4)
O1_15	0.6155(16)	0.2744(10)	0.4144(13)	0.037(6)
C1_15	0.6937(10)	0.2708(4)	0.3900(6)	0.034(3)
C2_15	0.6753(11)	0.2510(5)	0.3253(6)	0.066(4)
F1_15	0.644(2)	0.2789(7)	0.2842(11)	0.058(4)
F2_15	0.7512(14)	0.2363(6)	0.3083(9)	0.086(4)
F3_15	0.6126(18)	0.2228(8)	0.3243(12)	0.089(5)
C3_15	0.7598(9)	0.2421(5)	0.4300(6)	0.051(3)
F4_15	0.761(2)	0.2483(8)	0.4886(7)	0.059(4)
F5_15	0.7355(18)	0.2031(5)	0.4221(12)	0.066(4)
F6_15	0.8401(10)	0.2449(6)	0.4105(9)	0.060(4)
C4_15	0.7401(9)	0.3129(4)	0.3843(7)	0.052(3)
F7_15	0.7822(18)	0.3253(7)	0.4378(8)	0.069(4)
F8_15	0.8000(10)	0.3118(6)	0.3436(7)	0.058(3)
F9_15	0.6788(16)	0.3409(7)	0.3682(11)	0.067(4)
O1_16	0.3469(6)	0.5184(3)	0.7977(4)	0.0306(18)
C1_16	0.3730(8)	0.5499(4)	0.8349(5)	0.032(3)
C2_16	0.3981(8)	0.5874(3)	0.7968(5)	0.048(2)
F1_16	0.3366(6)	0.5924(2)	0.7481(3)	0.059(2)
F2_16	0.4039(7)	0.6213(3)	0.8309(4)	0.061(2)
F3_16	0.4786(6)	0.5818(3)	0.7768(4)	0.055(2)
C3_16	0.4584(9)	0.5365(4)	0.8787(6)	0.046(3)
F4_16	0.4345(8)	0.5125(3)	0.9226(5)	0.059(2)
F5_16	0.5155(6)	0.5158(3)	0.8475(4)	0.057(2)
F6_16	0.5025(6)	0.5686(3)	0.9043(4)	0.065(3)
C4_16	0.2955(9)	0.5614(4)	0.8733(6)	0.046(3)
F7_16	0.2551(10)	0.5281(3)	0.8917(7)	0.060(3)
F8_16	0.3263(8)	0.5810(3)	0.9252(5)	0.056(3)
F9_16	0.2361(7)	0.5854(4)	0.8411(5)	0.078(3)
O1_17	0.565(3)	0.2866(10)	0.5326(10)	0.059(7)
C1_17	0.5655(12)	0.3121(6)	0.5797(8)	0.047(4)
C2_17	0.6485(13)	0.3034(6)	0.6279(9)	0.069(5)
F1_17	0.7248(13)	0.3142(8)	0.6065(11)	0.079(4)
F2_17	0.6363(19)	0.3242(8)	0.6782(9)	0.079(5)
F3_17	0.6574(18)	0.2639(6)	0.6385(13)	0.088(7)
C3_17	0.4787(13)	0.3043(7)	0.6107(10)	0.074(4)
F4_17	0.4065(11)	0.3017(7)	0.5692(10)	0.070(5)
F5_17	0.488(2)	0.2683(8)	0.6396(14)	0.096(5)
F6_17	0.467(2)	0.3343(10)	0.6488(16)	0.083(5)
C4_17	0.5743(14)	0.3551(6)	0.5520(10)	0.059(5)
F7_17	0.4953(15)	0.3667(8)	0.5225(12)	0.103(8)
F8_17	0.601(3)	0.3817(10)	0.5954(13)	0.067(5)
F9_17	0.6372(14)	0.3527(6)	0.5131(10)	0.057(3)
O1_18	0.2899(11)	0.4496(3)	0.7359(7)	0.032(3)
C1_18	0.2670(9)	0.4158(4)	0.7664(5)	0.036(3)
C2_18	0.2173(8)	0.3861(4)	0.7202(5)	0.062(3)
F1_18	0.2609(7)	0.3842(3)	0.6711(4)	0.068(2)
F2_18	0.2186(8)	0.3481(2)	0.7426(5)	0.066(2)
F3_18	0.1293(7)	0.3914(4)	0.7016(6)	0.085(4)
C3_18	0.2057(10)	0.4263(5)	0.8167(7)	0.050(3)
F4_18	0.2551(9)	0.4421(4)	0.8654(5)	0.072(3)
F5_18	0.1481(13)	0.4556(6)	0.7987(8)	0.066(3)
F6_18	0.1601(10)	0.3945(4)	0.8343(6)	0.061(3)
C4_18	0.3559(9)	0.3945(4)	0.7979(6)	0.043(3)
F7_18	0.4114(8)	0.4213(4)	0.8282(6)	0.057(3)

F8_18	0.3386(10)	0.3657(4)	0.8383(6)	0.074(3)
F9_18	0.4010(9)	0.3767(5)	0.7571(5)	0.054(3)
N1_1	0.85813(16)	0.55408(7)	0.75407(11)	0.0227(5)
F1_1	0.79770(13)	0.59455(6)	0.64489(8)	0.0355(4)
C1_1	0.82386(18)	0.53365(9)	0.70118(12)	0.0215(6)
N2_1	0.85257(16)	0.47007(7)	0.75543(10)	0.0222(5)
F2_1	0.73016(13)	0.55339(6)	0.54455(8)	0.0399(5)
C3_1	0.7580(2)	0.53342(10)	0.59554(13)	0.0296(7)
F3_1	0.72279(13)	0.47117(7)	0.54597(8)	0.0391(5)
C4_1	0.7549(2)	0.49133(10)	0.59616(13)	0.0287(7)
F4_1	0.95940(14)	0.42949(6)	0.85224(9)	0.0418(5)
C5_1	0.78532(19)	0.47024(9)	0.64823(13)	0.0252(6)
F5_1	1.06096(15)	0.47096(7)	0.93860(9)	0.0510(6)
C6_1	0.82119(18)	0.49064(9)	0.70167(12)	0.0216(6)
F6_1	1.07429(14)	0.55246(7)	0.93243(9)	0.0464(5)
C7_1	0.90840(19)	0.49036(9)	0.80096(12)	0.0233(6)
F7_1	0.98355(13)	0.59369(6)	0.84021(9)	0.0401(5)
C8_1	0.9597(2)	0.46977(10)	0.84909(14)	0.0294(6)
F8_1	0.70398(11)	0.55606(5)	0.81046(8)	0.0286(4)
C9_1	1.0126(2)	0.49096(11)	0.89367(14)	0.0356(8)
F9_1	0.63565(13)	0.62636(6)	0.85210(9)	0.0401(5)
C10_1	1.0193(2)	0.53276(10)	0.89065(14)	0.0327(7)
F10_1	0.71635(14)	0.69843(6)	0.83098(10)	0.0458(5)
C11_1	0.9713(2)	0.55380(10)	0.84387(14)	0.0295(7)
F11_1	0.86280(14)	0.70061(6)	0.76736(11)	0.0451(5)
C12_1	0.91287(19)	0.53304(9)	0.79941(13)	0.0240(6)
F12_1	0.93106(13)	0.63060(6)	0.72790(10)	0.0397(5)
C13_1	0.81967(19)	0.59242(9)	0.77012(13)	0.0243(6)
F13_1	0.69124(12)	0.46716(5)	0.80321(7)	0.0274(4)
C14_1	0.74356(19)	0.59168(9)	0.80121(13)	0.0240(6)
F14_1	0.60596(13)	0.39634(6)	0.82356(9)	0.0367(4)
C15_1	0.7087(2)	0.62729(10)	0.82220(14)	0.0290(6)
F15_1	0.68790(14)	0.32431(6)	0.80261(10)	0.0424(5)
C16_1	0.7497(2)	0.66388(10)	0.81114(15)	0.0338(7)
F16_1	0.84867(15)	0.32336(6)	0.75604(10)	0.0445(5)
F17_1	0.93072(13)	0.39476(6)	0.73232(9)	0.0383(4)
C17_1	0.8244(2)	0.66508(10)	0.77887(16)	0.0331(7)
C18_1	0.8588(2)	0.62943(10)	0.75861(15)	0.0306(7)
C19_1	0.8124(2)	0.43152(9)	0.76835(13)	0.0251(6)
C20_1	0.7295(2)	0.43172(9)	0.79163(12)	0.0236(6)
C21_1	0.6866(2)	0.39572(9)	0.80278(13)	0.0280(6)
C22_1	0.7285(2)	0.35939(9)	0.79185(14)	0.0320(7)
C23_1	0.8107(2)	0.35889(9)	0.76840(15)	0.0323(7)
C24_1	0.8524(2)	0.39494(10)	0.75621(14)	0.0295(6)
C2_1	0.79213(19)	0.55419(9)	0.64738(14)	0.0263(6)

*Table S 8 Atomic coordinates and U_{eq} [Å^2] for **4 (oDFB)***

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.82071(4)	0.57512(2)	0.58284(4)	0.00903(17)
Al2	0.67562(4)	0.74192(2)	0.41338(4)	0.00846(17)
Al3	0.82060(4)	-0.09037(2)	0.57989(3)	0.00847(17)
Al4	0.82330(4)	0.24313(2)	0.58740(3)	0.00845(17)
Al5	0.68104(4)	0.07705(2)	0.41653(3)	0.00751(16)

Al6	0.32055(4)	0.59145(2)	0.58364(4)	0.00908(17)
O1_2	0.6672(6)	0.77096(10)	0.4229(4)	0.019(2)
C1_2	0.6396(3)	0.79076(12)	0.4019(3)	0.0210(14)
C2_2	0.5707(3)	0.79187(10)	0.4042(2)	0.0212(12)
F1_2	0.53406(15)	0.77907(6)	0.36597(14)	0.0294(8)
F2_2	0.5482(6)	0.81326(15)	0.3982(5)	0.0299(18)
F3_2	0.56485(19)	0.78376(8)	0.44925(17)	0.0395(11)
C3_2	0.6756(3)	0.81100(12)	0.4343(3)	0.0435(19)
F4_2	0.73700(19)	0.80761(7)	0.4439(3)	0.066(2)
F5_2	0.6626(3)	0.81309(8)	0.48000(19)	0.0616(15)
F6_2	0.6624(6)	0.83107(14)	0.4079(4)	0.055(2)
C4_2	0.6413(3)	0.79327(12)	0.3439(3)	0.0327(15)
F7_2	0.6976(2)	0.79912(9)	0.3410(2)	0.0573(15)
F8_2	0.6014(3)	0.80904(10)	0.3172(3)	0.0342(14)
F9_2	0.6266(2)	0.77339(7)	0.31835(15)	0.0410(11)
O1_3	0.6687(14)	0.7706(2)	0.4264(9)	0.012(4)
C1_3	0.6420(6)	0.7906(3)	0.4058(5)	0.019(3)
C2_3	0.6253(6)	0.7905(2)	0.3446(5)	0.025(3)
F1_3	0.5734(4)	0.77863(14)	0.3233(3)	0.035(2)
F2_3	0.6204(8)	0.8120(3)	0.3259(9)	0.041(4)
F3_3	0.6709(5)	0.78078(16)	0.3287(3)	0.032(2)
C3_3	0.6887(6)	0.8103(3)	0.4270(5)	0.028(3)
F4_3	0.7152(5)	0.80763(15)	0.4782(3)	0.036(2)
F5_3	0.7327(4)	0.81094(17)	0.4008(5)	0.045(3)
F6_3	0.6615(14)	0.8310(3)	0.4223(11)	0.052(4)
C4_3	0.5806(6)	0.7942(2)	0.4219(5)	0.025(3)
F7_3	0.5941(5)	0.79974(18)	0.4731(3)	0.040(3)
F8_3	0.5442(14)	0.8107(4)	0.3948(12)	0.028(3)
F9_3	0.5473(4)	0.77482(15)	0.4151(4)	0.031(2)
O1_4	0.70015(11)	0.72901(4)	0.47418(8)	0.0134(4)
C1_4	0.69558(14)	0.72875(6)	0.52388(12)	0.0143(6)
C2_4	0.73635(18)	0.70873(6)	0.55357(14)	0.0238(7)
F1_4	0.79699(11)	0.71444(5)	0.56427(10)	0.0318(6)
F2_4	0.72450(14)	0.70393(5)	0.59938(9)	0.0378(6)
F3_4	0.72727(13)	0.69009(4)	0.52438(9)	0.0329(6)
C3_4	0.62669(17)	0.72511(7)	0.52475(13)	0.0214(7)
F4_4	0.58853(10)	0.73735(4)	0.48722(9)	0.0257(5)
F5_4	0.60969(12)	0.70320(5)	0.51611(10)	0.0323(6)
F6_4	0.61665(12)	0.73131(5)	0.57073(9)	0.0360(6)
C4_4	0.71905(16)	0.75211(6)	0.55247(13)	0.0187(7)
F7_4	0.67594(11)	0.76850(4)	0.53887(9)	0.0251(5)
F8_4	0.73398(12)	0.75000(4)	0.60464(8)	0.0290(5)
F9_4	0.76965(11)	0.75936(4)	0.53999(9)	0.0271(5)
O1_5	0.7318(5)	0.7360(3)	0.3817(6)	0.020(3)
C1_5	0.7929(5)	0.73337(14)	0.3841(3)	0.0171(16)
C2_5	0.7960(5)	0.72482(16)	0.3295(3)	0.0293(19)
F1_5	0.7845(4)	0.70205(11)	0.3243(3)	0.0497(18)
F2_5	0.8527(5)	0.7279(2)	0.3222(5)	0.037(2)
F3_5	0.7553(4)	0.73548(15)	0.2908(3)	0.0383(17)
C3_5	0.8263(5)	0.75697(16)	0.3957(4)	0.0226(17)
F4_5	0.8110(4)	0.76761(12)	0.4355(3)	0.0310(15)
F5_5	0.8096(7)	0.7708(2)	0.3542(4)	0.035(2)
F6_5	0.8880(5)	0.75500(19)	0.4092(6)	0.034(2)
C4_5	0.8256(4)	0.71586(14)	0.4271(3)	0.0331(17)
F7_5	0.8398(2)	0.72577(12)	0.4747(2)	0.0380(14)

F8_5	0.8791(3)	0.70814(16)	0.4195(3)	0.054(2)
F9_5	0.7887(3)	0.69799(10)	0.4274(3)	0.0478(16)
O1_6	0.60376(11)	0.73212(4)	0.37528(9)	0.0152(5)
C1_6	0.57158(15)	0.71552(6)	0.34478(12)	0.0181(7)
C2_6	0.59044(19)	0.71333(9)	0.29264(16)	0.0352(10)
F1_6	0.64323(13)	0.70165(7)	0.29944(13)	0.0584(10)
F2_6	0.54684(13)	0.70238(6)	0.25477(11)	0.0493(8)
F3_6	0.59935(14)	0.73379(6)	0.27457(10)	0.0474(8)
C3_6	0.50083(16)	0.72182(7)	0.33215(14)	0.0221(7)
F4_6	0.48694(11)	0.72993(5)	0.37368(10)	0.0325(6)
F5_6	0.48644(11)	0.73786(4)	0.29461(9)	0.0292(5)
F6_6	0.46378(11)	0.70349(5)	0.31451(10)	0.0314(6)
C4_6	0.5828(2)	0.69191(7)	0.37334(18)	0.0400(11)
F7_6	0.55337(16)	0.69103(5)	0.41055(12)	0.0522(9)
F8_6	0.56290(15)	0.67402(5)	0.34098(13)	0.0548(9)
F9_6	0.64284(14)	0.68910(5)	0.39652(14)	0.0557(10)
O1_7	0.79399(11)	0.23289(4)	0.52438(9)	0.0134(4)
C1_7	0.80577(15)	0.22184(5)	0.48352(12)	0.0138(6)
C2_7	0.74205(18)	0.21864(7)	0.44151(14)	0.0240(8)
F1_7	0.70787(12)	0.20243(5)	0.45541(11)	0.0350(6)
F2_7	0.74756(13)	0.21323(5)	0.39424(9)	0.0372(7)
F3_7	0.70912(12)	0.23819(5)	0.43645(9)	0.0344(6)
C3_7	0.85043(19)	0.23585(7)	0.45981(15)	0.0261(8)
F4_7	0.89722(12)	0.24418(5)	0.49808(11)	0.0349(6)
F5_7	0.82087(15)	0.25345(5)	0.43145(11)	0.0427(7)
F6_7	0.87493(15)	0.22329(5)	0.42805(11)	0.0414(7)
C4_7	0.83462(17)	0.19768(6)	0.50004(13)	0.0182(7)
F7_7	0.89592(11)	0.19935(4)	0.52223(9)	0.0279(5)
F8_7	0.82623(12)	0.18361(4)	0.45883(8)	0.0265(5)
F9_7	0.80982(12)	0.18817(4)	0.53492(9)	0.0268(5)
O1_8	0.88487(10)	0.22611(4)	0.62113(9)	0.0136(4)
C1_8	0.93793(14)	0.22415(5)	0.66011(11)	0.0130(6)
C2_8	0.98937(16)	0.24071(7)	0.65134(13)	0.0216(7)
F1_8	0.98089(11)	0.26198(4)	0.66582(9)	0.0281(5)
F2_8	1.04676(10)	0.23419(5)	0.67872(10)	0.0371(6)
F3_8	0.98764(11)	0.24134(5)	0.60092(9)	0.0339(6)
C3_8	0.96065(19)	0.19885(7)	0.66076(15)	0.0273(8)
F4_8	0.91326(14)	0.18434(4)	0.65480(10)	0.0400(7)
F5_8	0.98646(13)	0.19534(5)	0.62186(10)	0.0439(8)
F6_8	1.00334(13)	0.19347(5)	0.70591(10)	0.0386(7)
C4_8	0.92720(15)	0.22993(6)	0.71455(12)	0.0142(6)
F7_8	0.89690(11)	0.21296(4)	0.73119(9)	0.0289(5)
F8_8	0.98076(10)	0.23322(4)	0.75182(8)	0.0202(4)
F9_8	0.89285(10)	0.24876(4)	0.71156(8)	0.0228(5)
O1_9	0.8516(3)	0.27078(6)	0.5865(2)	0.0146(10)
C1_9	0.83694(19)	0.29297(8)	0.57494(16)	0.0153(8)
C2_9	0.7761(2)	0.29547(8)	0.52872(19)	0.0306(11)
F1_9	0.78751(18)	0.29062(6)	0.48299(11)	0.0458(9)
F2_9	0.7517(2)	0.31653(7)	0.5253(2)	0.0443(13)
F3_9	0.73310(13)	0.28071(5)	0.53468(14)	0.0399(8)
C3_9	0.8274(2)	0.30543(8)	0.62439(18)	0.0248(10)
F4_9	0.87097(17)	0.29921(5)	0.66701(10)	0.0323(7)
F5_9	0.77252(16)	0.29958(6)	0.63205(15)	0.0426(9)
F6_9	0.8290(3)	0.32822(7)	0.6207(2)	0.0362(12)
C4_9	0.8917(2)	0.30473(8)	0.55888(19)	0.0260(10)

F7_9	0.94010(14)	0.30812(5)	0.60043(13)	0.0343(7)
F8_9	0.8754(2)	0.32515(6)	0.53585(15)	0.0427(10)
F9_9	0.91080(17)	0.29161(5)	0.52520(13)	0.0388(8)
O1_10	0.65042(11)	0.10414(4)	0.41825(9)	0.0153(5)
C1_10	0.66356(16)	0.12644(5)	0.43086(13)	0.0172(6)
C2_10	0.67169(19)	0.13957(6)	0.38200(15)	0.0242(8)
F1_10	0.72768(13)	0.13478(5)	0.37483(12)	0.0397(7)
F2_10	0.66866(13)	0.16233(4)	0.38635(10)	0.0331(6)
F3_10	0.62895(13)	0.13317(4)	0.33906(9)	0.0307(5)
C3_10	0.6080(2)	0.13693(6)	0.44756(15)	0.0258(8)
F4_10	0.58948(15)	0.12326(5)	0.48059(11)	0.0401(7)
F5_10	0.55936(12)	0.14056(5)	0.40615(10)	0.0351(6)
F6_10	0.62325(16)	0.15721(4)	0.47186(12)	0.0467(8)
C4_10	0.7235(2)	0.12905(6)	0.47729(15)	0.0281(8)
F7_10	0.71329(15)	0.12316(5)	0.52282(10)	0.0427(7)
F8_10	0.74574(15)	0.15042(4)	0.48213(12)	0.0476(8)
F9_10	0.76885(12)	0.11506(4)	0.47083(11)	0.0367(6)
O1_11	0.73959(11)	0.07837(4)	0.38544(10)	0.0169(5)
C1_11	0.79085(15)	0.06909(6)	0.37572(13)	0.0189(7)
C2_11	0.84010(17)	0.06135(8)	0.42675(15)	0.0279(8)
F1_11	0.82387(13)	0.04164(5)	0.44372(11)	0.0365(6)
F2_11	0.89688(11)	0.05911(6)	0.41979(11)	0.0442(7)
F3_11	0.84395(11)	0.07677(5)	0.46497(10)	0.0354(6)
C3_11	0.81976(19)	0.08802(8)	0.34819(17)	0.0320(9)
F4_11	0.77571(13)	0.09850(6)	0.31094(12)	0.0439(7)
F5_11	0.84838(13)	0.10393(5)	0.38263(13)	0.0453(7)
F6_11	0.86124(12)	0.07956(6)	0.32480(12)	0.0442(7)
C4_11	0.77260(17)	0.04796(7)	0.33895(15)	0.0265(8)
F7_11	0.74460(13)	0.05444(6)	0.28974(10)	0.0404(7)
F8_11	0.82178(12)	0.03519(5)	0.33681(11)	0.0404(7)
F9_11	0.73347(12)	0.03452(5)	0.35511(11)	0.0356(6)
O1_12	0.71292(11)	0.06679(4)	0.47924(9)	0.0145(5)
C1_12	0.70259(15)	0.05527(5)	0.52027(12)	0.0131(6)
C2_12	0.76376(18)	0.05571(6)	0.56482(14)	0.0229(7)
F1_12	0.80751(12)	0.04261(5)	0.55491(10)	0.0339(6)
F2_12	0.75663(13)	0.04901(5)	0.61153(9)	0.0373(6)
F3_12	0.78751(12)	0.07707(4)	0.57150(9)	0.0294(5)
C3_12	0.64964(18)	0.06639(7)	0.53924(14)	0.0247(8)
F4_12	0.60325(11)	0.07273(5)	0.49826(10)	0.0304(5)
F5_12	0.66979(14)	0.08530(5)	0.56792(10)	0.0367(6)
F6_12	0.62626(13)	0.05249(5)	0.56917(11)	0.0390(7)
C4_12	0.68413(19)	0.02983(6)	0.50381(14)	0.0247(8)
F7_12	0.62477(12)	0.02846(4)	0.47702(10)	0.0358(6)
F8_12	0.69360(13)	0.01598(4)	0.54557(9)	0.0321(6)
F9_12	0.71809(14)	0.02185(4)	0.47339(10)	0.0360(6)
O1_13	0.62124(11)	0.05930(4)	0.38328(9)	0.0144(5)
C1_13	0.56861(14)	0.05657(5)	0.34440(12)	0.0117(6)
C2_13	0.51542(16)	0.07261(7)	0.35215(14)	0.0220(7)
F1_13	0.52252(11)	0.09406(4)	0.33696(9)	0.0270(5)
F2_13	0.45883(11)	0.06553(5)	0.32461(10)	0.0364(6)
F3_13	0.51606(11)	0.07343(5)	0.40233(9)	0.0335(6)
C3_13	0.54748(18)	0.03122(6)	0.34500(15)	0.0265(8)
F4_13	0.59596(13)	0.01718(4)	0.35095(11)	0.0371(6)
F5_13	0.52284(13)	0.02751(5)	0.38430(11)	0.0434(7)
F6_13	0.50484(13)	0.02509(4)	0.30050(10)	0.0404(7)

C4_13	0.57911(16)	0.06197(6)	0.28989(13)	0.0168(6)
F7_13	0.61019(12)	0.04514(4)	0.27428(9)	0.0304(5)
F8_13	0.52485(10)	0.06448(4)	0.25220(8)	0.0220(4)
F9_13	0.61138(10)	0.08123(4)	0.29147(8)	0.0228(5)
O1_14	0.76378(11)	0.24308(5)	0.61756(10)	0.0184(5)
C1_14	0.71360(15)	0.23297(6)	0.62694(13)	0.0198(7)
C2_14	0.68082(19)	0.25157(8)	0.65234(17)	0.0334(9)
F1_14	0.65085(13)	0.26668(6)	0.61591(13)	0.0478(8)
F2_14	0.63938(12)	0.24277(6)	0.67505(11)	0.0431(7)
F3_14	0.72226(14)	0.26325(6)	0.68897(12)	0.0445(7)
C3_14	0.73390(17)	0.21266(7)	0.66584(15)	0.0262(8)
F4_14	0.77574(11)	0.19984(4)	0.65184(11)	0.0334(6)
F5_14	0.76006(12)	0.22016(6)	0.71467(9)	0.0397(7)
F6_14	0.68605(12)	0.19915(5)	0.66775(11)	0.0368(6)
C4_14	0.66678(18)	0.22397(8)	0.57573(15)	0.0295(9)
F7_14	0.68751(13)	0.20434(5)	0.56048(10)	0.0368(6)
F8_14	0.61039(12)	0.22014(6)	0.58194(11)	0.0448(8)
F9_14	0.66115(12)	0.23904(5)	0.53694(10)	0.0372(6)
O1_15	0.34455(13)	0.56332(4)	0.58709(11)	0.0221(5)
C1_15	0.33020(16)	0.54118(6)	0.57442(13)	0.0178(6)
C2_15	0.3838(2)	0.52955(8)	0.55706(18)	0.0407(11)
F1_15	0.43325(15)	0.52543(6)	0.59837(13)	0.0518(8)
F2_15	0.36549(19)	0.50922(6)	0.53413(14)	0.0639(10)
F3_15	0.4037(2)	0.54236(7)	0.52444(16)	0.0727(12)
C3_15	0.2695(2)	0.53923(7)	0.52921(19)	0.0419(12)
F4_15	0.22807(14)	0.55476(5)	0.53363(16)	0.0613(10)
F5_15	0.2803(2)	0.54435(6)	0.48242(12)	0.0658(11)
F6_15	0.24404(16)	0.51868(5)	0.52424(15)	0.0677(12)
C4_15	0.3228(2)	0.52857(8)	0.62393(18)	0.0368(10)
F7_15	0.26756(19)	0.53479(7)	0.63244(18)	0.0756(12)
F8_15	0.32206(15)	0.50569(5)	0.61856(13)	0.0538(9)
F9_15	0.36640(17)	0.53414(6)	0.66572(11)	0.0521(8)
O1_16	0.26164(15)	0.59319(6)	0.61437(14)	0.0178(7)
C1_16	0.2112(2)	0.60372(10)	0.6223(2)	0.0178(10)
C2_16	0.2314(3)	0.62412(11)	0.6612(2)	0.0258(13)
F1_16	0.2554(2)	0.61663(9)	0.71014(15)	0.0387(10)
F2_16	0.1842(3)	0.63843(11)	0.6620(3)	0.0352(14)
F3_16	0.2748(2)	0.63652(11)	0.6477(2)	0.0319(12)
C3_16	0.1665(3)	0.61288(10)	0.5708(2)	0.0288(12)
F4_16	0.15982(19)	0.59757(8)	0.53165(14)	0.0368(9)
F5_16	0.1878(2)	0.63212(7)	0.55489(14)	0.0387(9)
F6_16	0.1090(2)	0.61731(10)	0.57545(18)	0.0444(11)
C4_16	0.1759(3)	0.58561(11)	0.6471(3)	0.0317(13)
F7_16	0.1454(3)	0.57060(14)	0.6110(3)	0.0493(14)
F8_16	0.1352(2)	0.59515(9)	0.6693(2)	0.0436(12)
F9_16	0.21693(19)	0.57388(7)	0.68439(16)	0.0431(10)
O1_17	0.29309(18)	0.60108(6)	0.52095(12)	0.0131(7)
C1_17	0.3060(2)	0.61122(10)	0.4795(2)	0.0130(10)
C2_17	0.3379(4)	0.63509(13)	0.4939(3)	0.0255(16)
F1_17	0.3995(3)	0.63304(16)	0.5101(3)	0.062(2)
F2_17	0.3244(6)	0.64931(18)	0.4530(4)	0.0247(17)
F3_17	0.3187(4)	0.64454(13)	0.5321(3)	0.0440(19)
C3_17	0.2436(3)	0.61437(10)	0.4365(2)	0.0244(12)
F4_17	0.2096(2)	0.59516(8)	0.43201(16)	0.0343(11)
F5_17	0.20929(15)	0.63120(6)	0.44883(16)	0.0341(8)

F6_17	0.2508(2)	0.61906(7)	0.38913(12)	0.0374(10)
C4_17	0.3512(3)	0.59659(9)	0.4579(2)	0.0260(10)
F7_17	0.3216(2)	0.57856(7)	0.43019(18)	0.0427(11)
F8_17	0.37731(19)	0.60837(6)	0.42574(15)	0.0382(10)
F9_17	0.39721(16)	0.58864(6)	0.49746(15)	0.0359(9)
O1_18	0.89378(12)	0.56471(4)	0.61766(10)	0.0111(5)
C1_18	0.92736(16)	0.54762(6)	0.64656(14)	0.0137(7)
C2_18	0.99668(17)	0.55525(7)	0.66140(15)	0.0186(7)
F1_18	1.00885(11)	0.57034(5)	0.70096(10)	0.0251(6)
F2_18	1.03572(11)	0.53726(5)	0.67705(10)	0.0258(6)
F3_18	1.01094(11)	0.56521(5)	0.62149(10)	0.0230(5)
C3_18	0.9201(2)	0.52494(7)	0.61382(16)	0.0234(8)
F4_18	0.85951(14)	0.52128(5)	0.58897(13)	0.0319(7)
F5_18	0.95117(14)	0.52627(5)	0.57791(11)	0.0322(6)
F6_18	0.94025(14)	0.50652(4)	0.64431(12)	0.0342(7)
C4_18	0.90759(19)	0.54320(8)	0.69733(15)	0.0248(9)
F7_18	0.85513(12)	0.53060(5)	0.68698(12)	0.0358(7)
F8_18	0.95089(13)	0.53189(5)	0.73400(10)	0.0340(7)
F9_18	0.89585(14)	0.56271(6)	0.71865(10)	0.0334(7)
O1_19	0.82871(12)	0.60414(4)	0.57417(11)	0.0215(5)
C1_19	0.85606(17)	0.62399(6)	0.59443(15)	0.0223(7)
C2_19	0.92419(18)	0.62509(7)	0.58979(17)	0.0282(8)
F1_19	0.96251(11)	0.61247(4)	0.62786(11)	0.0346(6)
F2_19	0.94675(12)	0.64662(4)	0.59572(11)	0.0349(6)
F3_19	0.92743(13)	0.61739(5)	0.54451(11)	0.0381(6)
C3_19	0.8182(2)	0.64436(7)	0.56417(19)	0.0373(10)
F4_19	0.75709(13)	0.64061(5)	0.55505(16)	0.0567(10)
F5_19	0.82974(17)	0.64671(5)	0.51722(13)	0.0558(9)
F6_19	0.83157(14)	0.66427(4)	0.59047(14)	0.0548(10)
C4_19	0.8571(2)	0.62616(7)	0.65357(17)	0.0303(9)
F7_19	0.80104(13)	0.63135(6)	0.65825(13)	0.0465(8)
F8_19	0.89622(13)	0.64198(5)	0.67890(11)	0.0389(6)
F9_19	0.87290(15)	0.60603(5)	0.67815(10)	0.0393(6)
O1_20	0.7716(4)	0.5683(3)	0.6208(4)	0.0151(19)
C1_20	0.7116(3)	0.56477(11)	0.6209(3)	0.0152(13)
C2_20	0.6848(3)	0.54271(12)	0.5902(3)	0.0310(15)
F1_20	0.6661(3)	0.54661(11)	0.5384(2)	0.0441(14)
F2_20	0.6353(2)	0.53452(9)	0.6037(2)	0.0400(13)
F3_20	0.7276(2)	0.52622(9)	0.5983(3)	0.0453(15)
C3_20	0.7111(4)	0.56221(13)	0.6794(3)	0.0236(15)
F4_20	0.7484(4)	0.57755(10)	0.7094(3)	0.0334(14)
F5_20	0.7313(2)	0.54119(9)	0.6979(2)	0.0374(12)
F6_20	0.6535(4)	0.5650(2)	0.6854(4)	0.035(2)
C4_20	0.6703(4)	0.58557(13)	0.5968(3)	0.0224(14)
F7_20	0.6805(5)	0.60363(15)	0.6293(3)	0.0345(16)
F8_20	0.6093(4)	0.58081(13)	0.5847(4)	0.0310(17)
F9_20	0.6827(5)	0.59264(12)	0.5523(3)	0.0352(18)
O1_21	0.79349(18)	0.56340(6)	0.52114(11)	0.0146(7)
C1_21	0.79570(17)	0.56266(6)	0.47108(14)	0.0153(7)
C2_21	0.8601(2)	0.55641(9)	0.46625(18)	0.0318(11)
F1_21	0.8730(2)	0.53428(6)	0.47476(13)	0.0501(11)
F2_21	0.8686(2)	0.56240(11)	0.41949(16)	0.0507(11)
F3_21	0.90410(15)	0.56760(6)	0.50345(15)	0.0355(8)
C3_21	0.77604(18)	0.58649(7)	0.44403(15)	0.0184(7)
F4_21	0.72836(12)	0.59544(5)	0.45890(11)	0.0288(6)

F5_21	0.82251(12)	0.60141(4)	0.45618(10)	0.0259(6)
F6_21	0.75776(14)	0.58450(5)	0.39149(10)	0.0278(6)
C4_21	0.7468(2)	0.54468(8)	0.44259(16)	0.0338(11)
F7_21	0.68941(14)	0.55204(6)	0.43494(12)	0.0468(9)
F8_21	0.7541(3)	0.53918(9)	0.39475(13)	0.0622(14)
F9_21	0.7536(2)	0.52523(5)	0.47053(13)	0.0510(11)
O1_22	0.38173(13)	0.60804(4)	0.61874(10)	0.0244(6)
C1_22	0.43435(15)	0.61016(6)	0.65708(12)	0.0161(6)
C2_22	0.48586(19)	0.59371(8)	0.64747(16)	0.0301(9)
F1_22	0.47794(12)	0.57233(4)	0.66197(10)	0.0336(6)
F2_22	0.54333(13)	0.60030(7)	0.67415(13)	0.0548(9)
F3_22	0.48367(16)	0.59318(6)	0.59693(11)	0.0520(8)
C3_22	0.4571(2)	0.63530(7)	0.65741(16)	0.0348(10)
F4_22	0.40963(16)	0.64979(4)	0.65282(12)	0.0523(9)
F5_22	0.48204(18)	0.63908(6)	0.61792(12)	0.0616(10)
F6_22	0.50038(15)	0.64069(5)	0.70228(11)	0.0469(8)
C4_22	0.42443(17)	0.60425(7)	0.71143(14)	0.0217(7)
F7_22	0.39556(13)	0.62124(5)	0.72879(11)	0.0393(6)
F8_22	0.47895(11)	0.60072(4)	0.74832(9)	0.0284(5)
F9_22	0.39106(12)	0.58522(4)	0.70891(9)	0.0310(5)
O1_23	0.89188(11)	-0.09920(4)	0.61973(9)	0.0142(4)
C1_23	0.92414(15)	-0.11515(6)	0.65315(12)	0.0171(6)
C2_23	0.90695(18)	-0.11447(8)	0.70617(14)	0.0302(9)
F1_23	0.85307(11)	-0.12545(5)	0.70259(11)	0.0398(7)
F2_23	0.95004(12)	-0.12476(6)	0.74528(9)	0.0407(7)
F3_23	0.89996(13)	-0.09290(5)	0.72010(9)	0.0372(6)
C3_23	0.99480(16)	-0.10984(7)	0.66344(13)	0.0212(7)
F4_23	1.00755(10)	-0.10357(5)	0.61970(9)	0.0268(5)
F5_23	1.01172(11)	-0.09269(5)	0.69782(9)	0.0313(6)
F6_23	1.03065(11)	-0.12801(5)	0.68322(9)	0.0300(5)
C4_23	0.91030(17)	-0.13956(6)	0.62881(15)	0.0235(7)
F7_23	0.93734(12)	-0.14253(4)	0.59056(10)	0.0312(5)
F8_23	0.93034(13)	-0.15637(4)	0.66378(11)	0.0358(6)
F9_23	0.84908(11)	-0.14246(4)	0.60826(11)	0.0326(6)
O1_24	0.79711(10)	-0.10483(4)	0.52054(8)	0.0111(4)
C1_24	0.80317(14)	-0.10595(5)	0.47137(12)	0.0126(6)
C2_24	0.78007(16)	-0.08332(6)	0.44051(13)	0.0196(7)
F1_24	0.82352(11)	-0.06709(4)	0.45188(9)	0.0259(5)
F2_24	0.76543(12)	-0.08651(4)	0.38807(8)	0.0292(5)
F3_24	0.72940(10)	-0.07534(4)	0.45166(9)	0.0253(5)
C3_24	0.76201(17)	-0.12627(6)	0.44297(14)	0.0224(7)
F4_24	0.76999(12)	-0.14453(4)	0.47378(9)	0.0310(5)
F5_24	0.70142(10)	-0.12055(4)	0.43102(9)	0.0264(5)
F6_24	0.77452(13)	-0.13224(5)	0.39806(9)	0.0358(6)
C4_24	0.87187(16)	-0.11013(6)	0.47156(13)	0.0203(7)
F7_24	0.88823(11)	-0.13195(4)	0.48210(10)	0.0298(5)
F8_24	0.88302(12)	-0.10501(5)	0.42568(9)	0.0318(6)
F9_24	0.90949(10)	-0.09732(4)	0.50836(8)	0.0237(5)
O1_25	0.76556(11)	-0.09531(4)	0.61336(9)	0.0157(5)
C1_25	0.70500(15)	-0.09788(6)	0.61142(14)	0.0188(7)
C2_25	0.70098(19)	-0.10453(9)	0.66701(17)	0.0386(11)
F1_25	0.71485(18)	-0.12675(7)	0.67570(18)	0.0798(14)
F2_25	0.64396(12)	-0.10107(6)	0.67327(11)	0.0456(8)
F3_25	0.74068(13)	-0.09273(8)	0.70311(11)	0.0637(11)
C3_25	0.66985(18)	-0.07472(8)	0.59592(17)	0.0317(9)

F4_25	0.68484(13)	-0.06522(6)	0.55545(13)	0.0560(10)
F5_25	0.68463(15)	-0.05988(5)	0.63564(15)	0.0528(8)
F6_25	0.60756(12)	-0.07750(6)	0.58212(12)	0.0500(9)
C4_25	0.6722(2)	-0.11613(9)	0.5706(2)	0.0488(13)
F7_25	0.65790(15)	-0.10746(8)	0.52148(13)	0.0735(13)
F8_25	0.61940(16)	-0.12378(7)	0.57969(19)	0.0812(15)
F9_25	0.70887(18)	-0.13389(6)	0.5718(2)	0.0816(15)
O1_26	0.8282(3)	-0.06193(6)	0.5630(2)	0.0153(9)
C1_26	0.8544(2)	-0.04151(8)	0.58078(19)	0.0200(9)
C2_26	0.8259(3)	-0.02304(8)	0.5383(2)	0.0435(14)
F1_26	0.8500(3)	-0.02426(7)	0.49827(15)	0.0662(14)
F2_26	0.8365(4)	-0.00188(9)	0.5588(4)	0.0722(17)
F3_26	0.7638(2)	-0.02608(10)	0.5222(2)	0.0698(18)
C3_26	0.8418(3)	-0.03483(10)	0.6334(2)	0.0467(15)
F4_26	0.8518(3)	-0.05361(7)	0.66593(14)	0.0556(12)
F5_26	0.7842(2)	-0.02819(8)	0.6268(2)	0.0744(17)
F6_26	0.8819(3)	-0.01884(9)	0.6604(3)	0.0653(17)
C4_26	0.9265(2)	-0.04221(8)	0.5882(2)	0.0296(11)
F7_26	0.95570(16)	-0.05309(6)	0.63181(16)	0.0512(11)
F8_26	0.9513(3)	-0.02104(10)	0.5922(3)	0.0382(11)
F9_26	0.9386(2)	-0.05264(7)	0.5476(2)	0.0528(12)
C1_27	1.08995(18)	0.48832(7)	0.62419(15)	0.0249(8)
C2_27	1.07767(16)	0.47101(7)	0.65547(15)	0.0244(8)
C3_27	1.12051(18)	0.46403(7)	0.70072(16)	0.0269(8)
H3_27	1.111031	0.452079	0.721736	0.032
C4_27	1.17752(19)	0.47481(9)	0.71483(16)	0.0333(10)
H4_27	1.207990	0.470284	0.745997	0.040
C5_27	1.1908(2)	0.49217(10)	0.68398(19)	0.0467(13)
H5_27	1.230360	0.499500	0.694251	0.056
C6_27	1.1474(2)	0.49903(8)	0.63837(18)	0.0382(10)
H6_27	1.156841	0.510906	0.617170	0.046
F1_27	1.04638(13)	0.49377(5)	0.57953(11)	0.0431(7)
F2_27	1.02166(13)	0.46043(6)	0.63920(11)	0.0492(9)
C1_28	1.09235(17)	0.82518(7)	0.62918(15)	0.0238(8)
C2_28	1.07547(16)	0.80834(7)	0.65916(14)	0.0234(8)
C3_28	1.11805(17)	0.79902(7)	0.70205(14)	0.0225(7)
H3_28	1.105934	0.787408	0.722483	0.027
C4_28	1.17882(17)	0.80690(7)	0.71483(15)	0.0255(8)
H4_28	1.208927	0.800673	0.744316	0.031
C5_28	1.19594(19)	0.82382(8)	0.68483(16)	0.0317(9)
H5_28	1.237944	0.828998	0.693658	0.038
C6_28	1.15238(18)	0.83335(7)	0.64187(15)	0.0248(8)
H6_28	1.163909	0.845239	0.621778	0.030
F1_28	1.04916(13)	0.83323(6)	0.58675(11)	0.0471(8)
F2_28	1.01567(12)	0.80074(6)	0.64469(11)	0.0504(9)
C1_29	0.41783(18)	0.97471(7)	0.33865(15)	0.0270(8)
C2_29	0.3982(2)	0.99087(7)	0.36862(16)	0.0312(9)
C3_29	0.3375(2)	0.99835(8)	0.35366(19)	0.0381(10)
H3_29	0.323735	1.009723	0.373693	0.046
C4_29	0.2967(2)	0.98920(8)	0.30921(18)	0.0382(11)
H4_29	0.254459	0.994174	0.298998	0.046
C5_29	0.31644(19)	0.97291(8)	0.27947(16)	0.0317(9)
H5_29	0.287980	0.966652	0.249042	0.038
C6_29	0.37781(18)	0.96577(7)	0.29417(15)	0.0244(8)
H6_29	0.392120	0.954762	0.273636	0.029

F1_29	0.47777(13)	0.96752(7)	0.35396(12)	0.0599(11)
F2_29	0.43995(17)	0.99796(7)	0.41295(12)	0.0592(10)
C1_30	0.41942(17)	0.63973(7)	0.33908(15)	0.0239(8)
C2_30	0.40464(18)	0.65750(7)	0.36800(15)	0.0263(8)
C3_30	0.34663(19)	0.66747(7)	0.35302(15)	0.0268(8)
H3_30	0.336599	0.679995	0.372229	0.032
C4_30	0.30289(19)	0.65879(7)	0.30900(16)	0.0280(8)
H4_30	0.261976	0.665046	0.298913	0.034
C5_30	0.31831(17)	0.64114(7)	0.27973(15)	0.0246(8)
H5_30	0.288230	0.635538	0.249446	0.030
C6_30	0.37749(17)	0.63165(7)	0.29458(14)	0.0225(7)
H6_30	0.388786	0.619783	0.274322	0.027
F1_30	0.47692(12)	0.63019(6)	0.35556(12)	0.0511(9)
F2_30	0.44792(13)	0.66409(6)	0.41178(11)	0.0475(8)
C1_31	0.91723(16)	-0.13820(6)	0.34790(14)	0.0181(7)
C2_31	0.91906(16)	-0.15639(6)	0.38142(13)	0.0173(6)
C3_31	0.87203(18)	-0.17235(6)	0.37121(15)	0.0243(8)
H3_31	0.873745	-0.185030	0.394184	0.029
C4_31	0.82223(18)	-0.16977(7)	0.32717(15)	0.0264(8)
H4_31	0.789217	-0.180654	0.319788	0.032
C5_31	0.82030(17)	-0.15125(7)	0.29356(15)	0.0246(8)
H5_31	0.785914	-0.149564	0.263250	0.029
C6_31	0.86791(18)	-0.13530(7)	0.30386(14)	0.0250(8)
H6_31	0.866629	-0.122599	0.281036	0.030
F1_31	0.96457(11)	-0.12276(4)	0.35992(10)	0.0302(5)
F2_31	0.96792(11)	-0.15810(4)	0.42464(9)	0.0247(5)
N1_32	0.54816(11)	0.90159(4)	0.38724(10)	0.0087(5)
F1_32	0.50458(10)	0.91015(4)	0.47680(8)	0.0183(4)
C2_32	0.53371(15)	0.92650(6)	0.45770(12)	0.0128(6)
N2_32	0.61528(12)	0.93620(5)	0.35518(10)	0.0092(5)
F2_32	0.51637(10)	0.95171(4)	0.52099(8)	0.0202(4)
C3_32	0.54076(15)	0.94771(6)	0.48175(13)	0.0142(6)
F3_32	0.58392(12)	0.98453(4)	0.49149(9)	0.0241(5)
C4_32	0.57577(16)	0.96468(6)	0.46647(13)	0.0152(6)
F4_32	0.63671(10)	0.97742(3)	0.41357(8)	0.0176(4)
C5_32	0.60200(15)	0.96080(5)	0.42595(12)	0.0116(6)
F5_32	0.69152(10)	0.92456(4)	0.29093(8)	0.0177(4)
C6_32	0.59304(14)	0.93987(5)	0.39878(11)	0.0083(5)
F6_32	0.68797(11)	0.88268(4)	0.24930(9)	0.0219(5)
C7_32	0.61795(14)	0.91394(5)	0.33682(11)	0.0084(5)
F7_32	0.61718(11)	0.84951(3)	0.27444(8)	0.0204(4)
C8_32	0.65373(15)	0.90888(5)	0.30258(12)	0.0118(6)
F8_32	0.55013(10)	0.85708(3)	0.34125(9)	0.0185(4)
C9_32	0.65337(16)	0.88725(6)	0.28155(13)	0.0146(6)
F9_32	0.55522(9)	0.86179(4)	0.44818(8)	0.0181(4)
C10_32	0.61699(16)	0.87016(6)	0.29483(13)	0.0141(6)
F10_32	0.45135(10)	0.83641(4)	0.44590(9)	0.0225(5)
C11_32	0.58278(15)	0.87446(5)	0.32967(12)	0.0122(6)
F11_32	0.33926(10)	0.85025(4)	0.38680(9)	0.0234(5)
C12_32	0.58240(14)	0.89642(5)	0.35191(11)	0.0094(5)
F12_32	0.32786(9)	0.88920(4)	0.32749(9)	0.0238(5)
C13_32	0.49422(14)	0.88806(5)	0.38809(12)	0.0095(5)
F13_32	0.43082(9)	0.91448(4)	0.33037(8)	0.0169(4)
C14_32	0.43599(14)	0.89510(6)	0.35806(12)	0.0111(6)
F14_32	0.72296(9)	0.96294(4)	0.36503(8)	0.0194(4)

C15_32	0.38319(15)	0.88244(6)	0.35705(13)	0.0148(6)
F15_32	0.72936(12)	0.99527(4)	0.29321(10)	0.0303(6)
C16_32	0.38903(16)	0.86264(6)	0.38697(13)	0.0161(6)
F16_32	0.62829(15)	1.00425(4)	0.21262(10)	0.0382(7)
C17_32	0.44679(16)	0.85556(6)	0.41773(13)	0.0149(6)
F17_32	0.52071(14)	0.98062(5)	0.20192(10)	0.0400(7)
C18_32	0.49951(14)	0.86821(6)	0.41858(12)	0.0121(6)
F18_32	0.51578(10)	0.94691(4)	0.27221(8)	0.0213(4)
C19_32	0.61891(15)	0.95485(5)	0.32047(12)	0.0107(6)
C20_32	0.67359(16)	0.96749(6)	0.32564(13)	0.0150(6)
C21_32	0.67691(19)	0.98394(6)	0.28908(14)	0.0197(7)
C22_32	0.6250(2)	0.98829(6)	0.24783(15)	0.0246(8)
C23_32	0.57003(19)	0.97622(7)	0.24214(14)	0.0229(8)
C24_32	0.56735(16)	0.95939(6)	0.27834(13)	0.0153(6)
C1_32	0.55843(14)	0.92209(5)	0.41502(12)	0.0086(5)
N1_33	0.95577(12)	0.39950(4)	0.60603(10)	0.0094(5)
F1_33	0.96365(10)	0.35414(4)	0.64907(9)	0.0203(4)
C2_33	0.93114(15)	0.37040(6)	0.66467(12)	0.0133(6)
N2_33	0.88696(12)	0.43166(5)	0.64383(10)	0.0105(5)
F2_33	0.90783(10)	0.34371(4)	0.72226(8)	0.0203(4)
C3_33	0.90182(16)	0.36462(6)	0.70212(12)	0.0138(6)
F3_33	0.83335(11)	0.37399(4)	0.75207(9)	0.0227(5)
C4_33	0.86368(16)	0.38036(6)	0.71822(13)	0.0156(6)
F4_33	0.81795(10)	0.41661(4)	0.71161(9)	0.0214(4)
C5_33	0.85743(15)	0.40217(6)	0.69801(13)	0.0145(6)
F5_33	0.85493(10)	0.47308(4)	0.58642(8)	0.0187(4)
C6_33	0.88991(14)	0.40921(6)	0.66184(12)	0.0109(6)
F6_33	0.89808(10)	0.48246(4)	0.50441(8)	0.0207(4)
C7_33	0.90466(14)	0.43655(6)	0.59844(12)	0.0105(6)
F7_33	0.96433(11)	0.45115(4)	0.46797(8)	0.0224(5)
C8_33	0.89031(15)	0.45753(5)	0.57179(12)	0.0119(6)
F8_33	0.98939(10)	0.41004(4)	0.51329(8)	0.0216(5)
C9_33	0.91183(15)	0.46250(6)	0.52906(13)	0.0135(6)
F9_33	0.95476(9)	0.36345(4)	0.53556(9)	0.0218(5)
C10_33	0.94655(16)	0.44627(6)	0.51046(13)	0.0163(6)
F10_33	1.05999(11)	0.33934(4)	0.53753(9)	0.0278(5)
C11_33	0.95940(15)	0.42529(6)	0.53450(13)	0.0131(6)
F11_33	1.16839(10)	0.35037(4)	0.60755(10)	0.0270(5)
C12_33	0.93995(14)	0.42014(5)	0.57936(12)	0.0097(5)
F12_33	1.17472(10)	0.38624(4)	0.67475(9)	0.0255(5)
C13_33	1.01131(14)	0.38731(5)	0.60358(12)	0.0115(6)
F13_33	1.07002(10)	0.41091(4)	0.67107(8)	0.0186(4)
C14_33	1.06774(15)	0.39321(6)	0.63867(12)	0.0119(6)
F14_33	0.77507(9)	0.45459(4)	0.63472(8)	0.0214(4)
C15_33	1.12102(15)	0.38084(6)	0.64019(13)	0.0152(6)
F15_33	0.76453(11)	0.48896(4)	0.70177(10)	0.0265(5)
C16_33	1.11784(15)	0.36256(6)	0.60617(14)	0.0168(6)
F16_33	0.86540(12)	0.50131(4)	0.78027(8)	0.0253(5)
C17_33	1.06203(17)	0.35675(6)	0.57002(14)	0.0180(7)
F17_33	0.97595(12)	0.47982(4)	0.79234(9)	0.0282(5)
C18_33	1.00885(15)	0.36913(6)	0.56893(13)	0.0147(6)
F18_33	0.98542(9)	0.44493(4)	0.72613(8)	0.0200(4)
C19_33	0.88068(14)	0.44981(5)	0.67876(12)	0.0110(6)
C20_33	0.82394(15)	0.46088(6)	0.67329(13)	0.0143(6)
C21_33	0.81860(16)	0.47827(6)	0.70730(13)	0.0160(6)

C22_33	0.87033(18)	0.48462(6)	0.74746(13)	0.0176(7)
C23_33	0.92697(17)	0.47348(6)	0.75388(13)	0.0179(7)
C24_33	0.93158(15)	0.45607(6)	0.71973(12)	0.0137(6)
C1_33	0.92591(14)	0.39280(5)	0.64355(12)	0.0108(6)
N1_34	0.94783(12)	0.73533(5)	0.60755(10)	0.0100(5)
F1_34	0.94624(10)	0.69069(3)	0.65250(9)	0.0196(4)
C2_34	0.91448(15)	0.70802(5)	0.66553(12)	0.0122(6)
N2_34	0.88213(12)	0.76991(4)	0.64137(10)	0.0094(5)
F2_34	0.88045(11)	0.68272(4)	0.72034(9)	0.0213(4)
C3_34	0.88073(16)	0.70350(6)	0.70050(12)	0.0140(6)
F3_34	0.81060(11)	0.71586(4)	0.74683(9)	0.0232(5)
C4_34	0.84471(16)	0.72072(6)	0.71458(13)	0.0158(6)
F4_34	0.80670(10)	0.75793(4)	0.70628(8)	0.0183(4)
C5_34	0.84395(15)	0.74230(6)	0.69406(12)	0.0133(6)
F5_34	0.86080(11)	0.81140(4)	0.58364(8)	0.0212(4)
C6_34	0.87988(14)	0.74765(5)	0.65934(11)	0.0099(5)
F6_34	0.90937(11)	0.81833(4)	0.50376(8)	0.0220(5)
C7_34	0.90309(14)	0.77378(5)	0.59744(11)	0.0100(5)
F7_34	0.97361(11)	0.78511(4)	0.47136(8)	0.0214(4)
C8_34	0.89392(15)	0.79471(6)	0.57038(12)	0.0127(6)
F8_34	0.98684(10)	0.74359(4)	0.51615(8)	0.0188(4)
C9_34	0.91846(16)	0.79857(6)	0.52910(13)	0.0137(6)
F9_34	0.94235(9)	0.69587(4)	0.54560(8)	0.0206(4)
C10_34	0.95163(16)	0.78123(6)	0.51212(12)	0.0148(6)
F10_34	1.04667(11)	0.67109(4)	0.54725(9)	0.0241(5)
C11_34	0.95917(14)	0.76008(6)	0.53615(12)	0.0122(6)
F11_34	1.15865(10)	0.68500(4)	0.60808(9)	0.0227(5)
C12_34	0.93642(14)	0.75590(5)	0.57999(12)	0.0096(5)
F12_34	1.16800(9)	0.72344(4)	0.66865(8)	0.0204(4)
C13_34	1.00212(14)	0.72202(5)	0.60664(12)	0.0107(6)
F13_34	1.06445(9)	0.74835(4)	0.66544(8)	0.0157(4)
C14_34	1.05993(15)	0.72924(6)	0.63713(12)	0.0115(6)
F14_34	0.77534(10)	0.79728(4)	0.62926(9)	0.0218(4)
C15_34	1.11315(14)	0.71661(6)	0.63824(12)	0.0136(6)
F15_34	0.76815(12)	0.83002(4)	0.69982(11)	0.0329(6)
C16_34	1.10806(15)	0.69722(6)	0.60776(13)	0.0154(6)
F16_34	0.86642(14)	0.83720(4)	0.78518(9)	0.0350(6)
C17_34	1.05037(16)	0.69004(6)	0.57619(13)	0.0148(6)
F17_34	0.97298(13)	0.81249(4)	0.79839(9)	0.0350(6)
C18_34	0.99742(15)	0.70254(6)	0.57567(13)	0.0140(6)
F18_34	0.97945(10)	0.77966(4)	0.72720(8)	0.0216(4)
C19_34	0.87826(15)	0.78852(5)	0.67640(12)	0.0112(6)
C20_34	0.82399(16)	0.80120(6)	0.66985(13)	0.0151(6)
C21_34	0.81996(18)	0.81774(6)	0.70637(15)	0.0204(7)
C22_34	0.8706(2)	0.82141(6)	0.75002(14)	0.0215(8)
C23_34	0.92474(19)	0.80874(6)	0.75683(13)	0.0203(7)
C24_34	0.92813(16)	0.79228(6)	0.72005(12)	0.0151(6)
C1_34	0.91466(14)	0.73002(5)	0.64351(11)	0.0092(5)
N1_35	0.54673(12)	0.56744(5)	0.38915(10)	0.0103(5)
F1_35	0.54564(10)	0.52204(4)	0.34769(9)	0.0219(4)
C2_35	0.57659(15)	0.53903(6)	0.33208(13)	0.0134(6)
N2_35	0.61239(12)	0.60094(5)	0.35226(10)	0.0103(5)
F2_35	0.60595(10)	0.51259(4)	0.27686(8)	0.0222(5)
C3_35	0.60779(15)	0.53368(6)	0.29578(13)	0.0154(6)
F3_35	0.67420(11)	0.54492(4)	0.24487(9)	0.0267(5)

C4_35	0.64280(17)	0.55036(6)	0.27897(13)	0.0173(7)
F4_35	0.68303(11)	0.58745(4)	0.28440(9)	0.0232(5)
C5_35	0.64581(16)	0.57244(6)	0.29867(13)	0.0153(6)
F5_35	0.64152(11)	0.64215(4)	0.41001(8)	0.0212(4)
C6_35	0.61285(15)	0.57831(6)	0.33467(12)	0.0114(6)
F6_35	0.59660(12)	0.65058(4)	0.49153(8)	0.0249(5)
C7_35	0.59411(14)	0.60520(5)	0.39743(11)	0.0082(5)
F7_35	0.53118(11)	0.61852(4)	0.52675(8)	0.0244(5)
C8_35	0.60658(15)	0.62626(5)	0.42429(12)	0.0124(6)
F8_35	0.51174(10)	0.57697(4)	0.48230(8)	0.0204(4)
C9_35	0.58430(16)	0.63075(6)	0.46682(13)	0.0156(6)
F9_35	0.55208(10)	0.52972(4)	0.45598(9)	0.0226(5)
C10_35	0.55046(16)	0.61411(6)	0.48488(13)	0.0146(6)
F10_35	0.44860(11)	0.50506(4)	0.45618(10)	0.0272(5)
C11_35	0.53978(15)	0.59300(6)	0.46092(13)	0.0138(6)
F11_35	0.33656(10)	0.51768(4)	0.39312(9)	0.0242(5)
C12_35	0.56023(14)	0.58815(5)	0.41608(12)	0.0104(5)
F12_35	0.32668(9)	0.55479(4)	0.32834(8)	0.0200(4)
C13_35	0.49229(14)	0.55465(5)	0.39197(12)	0.0113(6)
F13_35	0.42967(9)	0.57970(4)	0.32979(8)	0.0156(4)
C14_35	0.43464(14)	0.56116(5)	0.36018(12)	0.0098(5)
F14_35	0.71995(10)	0.62771(4)	0.35870(10)	0.0295(5)
C15_35	0.38153(14)	0.54867(6)	0.35993(12)	0.0126(6)
F15_35	0.72269(14)	0.66032(5)	0.28672(13)	0.0421(7)
C16_35	0.38661(15)	0.52976(6)	0.39281(13)	0.0144(6)
F16_35	0.61996(17)	0.66800(4)	0.20598(10)	0.0452(8)
C17_35	0.44416(16)	0.52333(6)	0.42531(14)	0.0154(6)
F17_35	0.51367(15)	0.64417(5)	0.19839(10)	0.0431(7)
C18_35	0.49689(15)	0.53573(6)	0.42484(13)	0.0140(6)
F18_35	0.51126(10)	0.61122(4)	0.27074(9)	0.0218(4)
C19_35	0.61535(15)	0.61943(5)	0.31623(13)	0.0127(6)
C20_35	0.66936(17)	0.63180(6)	0.31997(15)	0.0198(7)
C21_35	0.6712(2)	0.64841(7)	0.28260(17)	0.0271(9)
C22_35	0.6185(2)	0.65224(7)	0.24192(16)	0.0299(10)
C23_35	0.5640(2)	0.63999(6)	0.23767(14)	0.0256(8)
C24_35	0.56293(16)	0.62332(6)	0.27507(13)	0.0156(6)
C1_35	0.57807(14)	0.56140(5)	0.35276(12)	0.0103(5)
N1_36	1.10875(12)	-0.10033(5)	0.34971(10)	0.0108(5)
F1_36	1.13698(10)	-0.14145(4)	0.40897(8)	0.0190(4)
C2_36	1.10394(14)	-0.12492(6)	0.42322(12)	0.0117(6)
N2_36	1.04300(12)	-0.06647(5)	0.38562(10)	0.0106(5)
F2_36	1.09719(10)	-0.14793(4)	0.49376(8)	0.0200(4)
C3_36	1.08377(15)	-0.12865(6)	0.46714(13)	0.0135(6)
F3_36	1.03435(10)	-0.11512(4)	0.52881(8)	0.0201(4)
C4_36	1.05106(15)	-0.11152(6)	0.48538(12)	0.0130(6)
F4_36	1.01004(10)	-0.07483(4)	0.47982(8)	0.0172(4)
C5_36	1.03868(14)	-0.09096(6)	0.45929(12)	0.0113(6)
F5_36	1.03956(11)	-0.02165(3)	0.34083(9)	0.0217(4)
C6_36	1.05757(14)	-0.08682(5)	0.41373(12)	0.0103(5)
F6_36	1.09826(12)	-0.01285(4)	0.26843(8)	0.0242(5)
C7_36	1.07362(14)	-0.06076(5)	0.34818(12)	0.0104(5)
F7_36	1.17018(11)	-0.04465(4)	0.24054(9)	0.0262(5)
C8_36	1.07103(16)	-0.03866(6)	0.32650(12)	0.0140(6)
F8_36	1.18062(11)	-0.08690(4)	0.28199(9)	0.0240(5)
C9_36	1.10202(17)	-0.03367(6)	0.28950(13)	0.0164(6)

F9_36	1.22250(9)	-0.12228(4)	0.36097(8)	0.0196(4)
C10_36	1.13825(17)	-0.05021(6)	0.27431(13)	0.0181(7)
F10_36	1.23638(10)	-0.15683(4)	0.29585(9)	0.0227(5)
C11_36	1.14228(16)	-0.07191(6)	0.29511(13)	0.0151(6)
F11_36	1.13612(11)	-0.17194(4)	0.22003(9)	0.0228(5)
C12_36	1.10833(15)	-0.07788(6)	0.33088(12)	0.0119(6)
F12_36	1.02363(11)	-0.15187(4)	0.20658(9)	0.0274(5)
C13_36	1.11641(15)	-0.11922(6)	0.31676(12)	0.0118(6)
F13_36	1.01086(10)	-0.11625(4)	0.26959(8)	0.0218(4)
C14_36	1.06607(15)	-0.12635(6)	0.27687(12)	0.0133(6)
F14_36	1.05125(10)	-0.02923(4)	0.45390(9)	0.0222(5)
C15_36	1.07201(16)	-0.14442(6)	0.24432(13)	0.0170(7)
F15_36	0.94972(11)	-0.00296(4)	0.45346(9)	0.0258(5)
C16_36	1.12968(17)	-0.15470(6)	0.25110(13)	0.0151(6)
F16_36	0.83772(10)	-0.01349(4)	0.38765(9)	0.0231(5)
C17_36	1.18098(15)	-0.14719(6)	0.29042(13)	0.0142(6)
F17_36	0.82456(10)	-0.05054(4)	0.32276(9)	0.0238(5)
C18_36	1.17402(14)	-0.12962(6)	0.32322(12)	0.0126(6)
F18_36	0.92574(9)	-0.07672(4)	0.32395(8)	0.0184(4)
C19_36	0.98968(14)	-0.05307(6)	0.38851(12)	0.0117(6)
C20_36	0.99562(15)	-0.03451(6)	0.42230(13)	0.0143(6)
C21_36	0.94447(16)	-0.02109(6)	0.42208(14)	0.0174(7)
C22_36	0.88658(15)	-0.02663(6)	0.38823(13)	0.0153(6)
C23_36	0.88009(15)	-0.04535(6)	0.35528(13)	0.0159(6)
C24_36	0.93153(15)	-0.05868(6)	0.35574(12)	0.0123(6)
C1_36	1.09111(14)	-0.10422(5)	0.39518(12)	0.0098(5)
N1_37	0.45421(12)	0.76732(5)	0.60550(10)	0.0107(5)
F1_37	0.45892(10)	0.81276(3)	0.64740(9)	0.0193(4)
C2_37	0.42747(15)	0.79611(5)	0.66345(12)	0.0115(6)
N2_37	0.38769(12)	0.73440(4)	0.64350(10)	0.0088(5)
F2_37	0.40126(10)	0.82288(3)	0.71960(8)	0.0179(4)
C3_37	0.39688(15)	0.80192(6)	0.70037(12)	0.0130(6)
F3_37	0.32965(10)	0.79174(4)	0.75048(8)	0.0191(4)
C4_37	0.36061(15)	0.78559(6)	0.71675(12)	0.0127(6)
F4_37	0.31816(10)	0.74902(4)	0.71209(9)	0.0205(4)
C5_37	0.35637(15)	0.76352(6)	0.69745(12)	0.0129(6)
F5_37	0.35833(10)	0.69255(4)	0.58664(8)	0.0187(4)
C6_37	0.38906(14)	0.75692(5)	0.66163(11)	0.0096(5)
F6_37	0.39812(10)	0.68490(4)	0.50218(8)	0.0202(4)
C7_37	0.40483(14)	0.72992(5)	0.59783(11)	0.0090(5)
F7_37	0.46141(10)	0.71691(4)	0.46494(8)	0.0199(4)
C8_37	0.39159(15)	0.70890(6)	0.57104(12)	0.0126(6)
F8_37	0.48539(10)	0.75785(4)	0.51112(8)	0.0178(4)
C9_37	0.41152(15)	0.70452(6)	0.52737(12)	0.0130(6)
F9_37	0.44868(10)	0.80329(4)	0.53457(9)	0.0224(5)
C10_37	0.44452(15)	0.72115(6)	0.50813(12)	0.0129(6)
F10_37	0.55100(11)	0.82920(4)	0.53518(10)	0.0304(6)
C11_37	0.45729(14)	0.74205(6)	0.53273(12)	0.0118(6)
F11_37	0.66172(10)	0.81883(4)	0.60293(10)	0.0266(5)
C12_37	0.43885(13)	0.74678(5)	0.57836(12)	0.0093(5)
F12_37	0.67293(9)	0.78266(4)	0.67022(9)	0.0243(5)
C13_37	0.50861(14)	0.78010(5)	0.60219(12)	0.0111(6)
F13_37	0.57055(9)	0.75699(4)	0.66888(8)	0.0180(4)
C14_37	0.56602(14)	0.77459(6)	0.63620(12)	0.0121(6)
F14_37	0.27375(9)	0.71322(4)	0.63493(8)	0.0184(4)

C15_37	0.61830(15)	0.78757(6)	0.63652(13)	0.0154(6)
F15_37	0.26041(10)	0.67910(4)	0.70146(9)	0.0219(4)
C16_37	0.61276(15)	0.80602(6)	0.60252(14)	0.0165(6)
F16_37	0.36200(11)	0.66363(4)	0.77579(9)	0.0236(5)
C17_37	0.55552(16)	0.81120(6)	0.56741(14)	0.0164(6)
F17_37	0.47485(11)	0.68278(5)	0.78621(9)	0.0308(6)
C18_37	0.50351(14)	0.79825(6)	0.56712(13)	0.0144(6)
F18_37	0.48686(10)	0.71846(4)	0.72240(8)	0.0224(5)
C19_37	0.38023(14)	0.71591(5)	0.67761(12)	0.0103(5)
C20_37	0.32240(14)	0.70581(6)	0.67244(12)	0.0123(6)
C21_37	0.31581(16)	0.68846(6)	0.70573(13)	0.0146(6)
C22_37	0.36774(17)	0.68072(6)	0.74410(13)	0.0172(7)
C23_37	0.42543(16)	0.69062(6)	0.74948(13)	0.0168(6)
C24_37	0.43187(15)	0.70844(6)	0.71664(13)	0.0140(6)
C1_37	0.42419(14)	0.77363(5)	0.64288(12)	0.0098(5)
C1_38	0.57879(16)	0.67703(6)	0.61186(13)	0.0188(7)
C2_38	0.57937(16)	0.69536(6)	0.64472(14)	0.0196(7)
C3_38	0.62703(18)	0.69866(7)	0.68967(14)	0.0243(8)
H3_38	0.626831	0.711314	0.712302	0.029
C4_38	0.67543(18)	0.68289(7)	0.70086(15)	0.0261(8)
H4_38	0.709548	0.684835	0.731279	0.031
C5_38	0.67431(19)	0.66411(7)	0.66762(16)	0.0286(9)
H5_38	0.707486	0.653295	0.675894	0.034
C6_38	0.6256(2)	0.66113(7)	0.62302(15)	0.0267(8)
H6_38	0.624625	0.648320	0.600547	0.032
F1_38	0.53035(11)	0.67501(4)	0.56816(9)	0.0278(5)
F2_38	0.53133(12)	0.71067(5)	0.63166(10)	0.0350(6)
O1_1	0.8022(17)	0.5581(5)	0.5280(8)	0.018(6)
C1_1	0.8055(10)	0.5580(3)	0.4779(9)	0.024(4)
C2_1	0.7724(12)	0.5356(4)	0.4516(9)	0.050(4)
F1_1	0.8154(13)	0.5194(3)	0.4525(9)	0.036(5)
F2_1	0.740(2)	0.5395(8)	0.4017(11)	0.063(5)
F3_1	0.7297(16)	0.5316(6)	0.4774(15)	0.051(5)
C3_1	0.7655(10)	0.5789(3)	0.4520(10)	0.034(5)
F4_1	0.7745(19)	0.5966(5)	0.4858(14)	0.090(12)
F5_1	0.7053(10)	0.5722(4)	0.4443(11)	0.032(6)
F6_1	0.7806(14)	0.5857(5)	0.4092(11)	0.032(4)
C4_1	0.8733(11)	0.5584(5)	0.4749(12)	0.032(5)
F7_1	0.9023(15)	0.5767(5)	0.5011(19)	0.037(5)
F8_1	0.878(2)	0.5598(11)	0.4258(14)	0.047(5)
F9_1	0.9024(16)	0.5391(5)	0.4961(14)	0.047(5)
O1_39	0.7259(8)	0.7349(5)	0.3762(9)	0.011(3)
C1_39	0.7861(6)	0.73180(19)	0.3766(4)	0.014(2)
C2_39	0.8126(5)	0.70973(19)	0.4079(5)	0.030(2)
F1_39	0.7696(5)	0.69326(14)	0.3963(5)	0.048(2)
F2_39	0.8630(5)	0.7023(2)	0.3949(5)	0.047(3)
F3_39	0.8289(4)	0.7138(2)	0.4596(4)	0.043(2)
C3_39	0.8262(8)	0.7527(2)	0.4013(6)	0.026(3)
F4_39	0.8169(12)	0.7706(3)	0.3686(7)	0.040(3)
F5_39	0.8126(7)	0.7593(2)	0.4451(5)	0.036(3)
F6_39	0.8871(7)	0.7482(3)	0.4138(10)	0.037(3)
C4_39	0.7881(7)	0.7294(2)	0.3185(5)	0.026(2)
F7_39	0.7501(7)	0.7448(2)	0.2888(5)	0.033(2)
F8_39	0.8451(7)	0.7328(4)	0.3125(8)	0.033(3)
F9_39	0.7689(5)	0.70845(19)	0.3001(4)	0.044(2)

O1_40	0.8493(18)	0.2709(3)	0.5887(18)	0.016(7)
C1_40	0.8358(8)	0.2931(4)	0.5794(7)	0.016(4)
C2_40	0.8839(9)	0.3037(4)	0.5532(7)	0.026(4)
F1_40	0.8700(12)	0.2977(4)	0.5027(7)	0.034(4)
F2_40	0.8849(16)	0.3265(3)	0.5562(11)	0.037(4)
F3_40	0.9409(8)	0.2962(4)	0.5771(9)	0.031(4)
C3_40	0.8413(10)	0.3056(4)	0.6324(7)	0.023(4)
F4_40	0.8107(10)	0.2940(3)	0.6606(7)	0.028(4)
F5_40	0.9006(9)	0.3063(3)	0.6609(7)	0.027(4)
F6_40	0.820(2)	0.3270(4)	0.6260(17)	0.029(5)
C4_40	0.7693(9)	0.2967(4)	0.5420(7)	0.022(4)
F7_40	0.7262(8)	0.2940(4)	0.5679(8)	0.034(5)
F8_40	0.7642(19)	0.3174(4)	0.5193(16)	0.038(5)
F9_40	0.7552(9)	0.2808(3)	0.5042(6)	0.021(4)
O1_41	0.7658(9)	0.5685(6)	0.6147(11)	0.012(4)
C1_41	0.7057(8)	0.5659(2)	0.6144(5)	0.018(3)
C2_41	0.7040(8)	0.5573(3)	0.6696(6)	0.028(3)
F1_41	0.7453(8)	0.5686(2)	0.7073(6)	0.030(3)
F2_41	0.6475(9)	0.5604(5)	0.6771(10)	0.033(4)
F3_41	0.7180(7)	0.5348(2)	0.6745(5)	0.040(2)
C3_41	0.6723(6)	0.5483(2)	0.5720(6)	0.034(3)
F4_41	0.6582(7)	0.5579(3)	0.5244(5)	0.043(3)
F5_41	0.7083(6)	0.5305(2)	0.5691(6)	0.050(3)
F6_41	0.6191(6)	0.5406(3)	0.5794(6)	0.044(3)
C4_41	0.6715(10)	0.5893(3)	0.6033(7)	0.026(3)
F7_41	0.6852(13)	0.5997(3)	0.5629(7)	0.036(4)
F8_41	0.6098(9)	0.5870(4)	0.5911(11)	0.032(3)
F9_41	0.6891(12)	0.6031(4)	0.6450(6)	0.033(3)
O1_42	0.8282(19)	-0.0618(3)	0.5689(14)	0.026(7)
C1_42	0.8523(9)	-0.0411(3)	0.5818(7)	0.030(4)
C2_42	0.9140(9)	-0.0379(4)	0.5673(8)	0.040(4)
F1_42	0.9031(14)	-0.0341(5)	0.5158(8)	0.070(7)
F2_42	0.948(2)	-0.0202(6)	0.5923(18)	0.041(5)
F3_42	0.9481(9)	-0.0568(3)	0.5781(10)	0.038(4)
C3_42	0.8638(10)	-0.0373(4)	0.6425(8)	0.056(5)
F4_42	0.8144(12)	-0.0458(5)	0.6553(9)	0.057(4)
F5_42	0.9148(11)	-0.0489(4)	0.6667(10)	0.091(8)
F6_42	0.8611(16)	-0.0146(4)	0.6494(15)	0.065(5)
C4_42	0.8037(10)	-0.0226(3)	0.5556(10)	0.059(5)
F7_42	0.7597(13)	-0.0229(4)	0.5816(14)	0.083(8)
F8_42	0.827(2)	-0.0014(4)	0.559(2)	0.071(5)
F9_42	0.7801(13)	-0.0277(5)	0.5049(10)	0.057(5)
O1_43	0.8637(10)	0.5631(4)	0.6237(9)	0.024(5)
C1_43	0.9201(8)	0.5561(3)	0.6549(6)	0.016(4)
C2_43	0.9705(8)	0.5712(3)	0.6400(7)	0.031(5)
F1_43	0.9583(11)	0.5725(5)	0.5879(6)	0.039(6)
F2_43	1.0276(8)	0.5626(4)	0.6575(10)	0.034(3)
F3_43	0.9696(12)	0.5926(3)	0.6593(9)	0.040(5)
C3_43	0.9233(9)	0.5620(3)	0.7122(6)	0.026(4)
F4_43	0.8975(11)	0.5463(4)	0.7360(8)	0.034(5)
F5_43	0.8914(8)	0.5817(3)	0.7131(6)	0.016(3)
F6_43	0.9801(7)	0.5677(4)	0.7418(7)	0.026(5)
C4_43	0.9181(10)	0.5313(3)	0.6344(9)	0.039(5)
F7_43	0.8696(14)	0.5289(5)	0.5895(10)	0.047(5)
F8_43	0.8994(13)	0.5150(4)	0.6611(8)	0.046(7)

F9_43	0.9689(12)	0.5264(5)	0.6198(13)	0.061(8)
O1_44	0.7374(10)	0.5677(4)	0.5811(9)	0.012(4)
C1_44	0.6975(8)	0.5614(3)	0.6089(7)	0.023(4)
C2_44	0.7260(10)	0.5418(3)	0.6481(8)	0.032(4)
F1_44	0.7570(14)	0.5268(4)	0.6268(13)	0.045(4)
F2_44	0.6832(12)	0.5299(5)	0.6636(11)	0.033(4)
F3_44	0.7660(11)	0.5504(5)	0.6911(9)	0.037(4)
C3_44	0.6818(10)	0.5824(3)	0.6387(8)	0.030(4)
F4_44	0.6456(13)	0.5973(5)	0.6055(10)	0.032(3)
F5_44	0.7339(11)	0.5938(5)	0.6624(11)	0.046(7)
F6_44	0.6537(14)	0.5775(6)	0.6755(11)	0.039(5)
C4_44	0.6365(9)	0.5523(4)	0.5695(8)	0.041(4)
F7_44	0.6216(14)	0.5654(5)	0.5264(9)	0.046(5)
F8_44	0.5881(10)	0.5524(5)	0.5897(12)	0.042(7)
F9_44	0.6455(14)	0.5309(4)	0.5554(13)	0.053(8)
O1_45	0.2452(5)	0.5994(2)	0.5840(5)	0.018(2)
C1_45	0.2032(6)	0.6044(2)	0.6102(5)	0.020(3)
C2_45	0.1436(7)	0.6142(2)	0.5709(5)	0.031(3)
F1_45	0.1295(6)	0.6023(2)	0.5262(4)	0.035(3)
F2_45	0.0946(6)	0.6136(3)	0.5907(6)	0.044(3)
F3_45	0.1528(6)	0.63610(18)	0.5598(4)	0.036(2)
C3_45	0.2303(8)	0.6224(3)	0.6536(6)	0.029(4)
F4_45	0.2694(7)	0.6127(3)	0.6955(5)	0.048(3)
F5_45	0.2586(9)	0.6390(4)	0.6337(8)	0.040(4)
F6_45	0.1850(11)	0.6325(4)	0.6699(10)	0.039(4)
C4_45	0.1848(7)	0.5821(3)	0.6349(6)	0.034(3)
F7_45	0.2358(6)	0.5706(2)	0.6598(5)	0.044(3)
F8_45	0.1520(7)	0.5866(3)	0.6690(6)	0.042(3)
F9_45	0.1512(10)	0.5684(4)	0.5973(8)	0.045(4)
O1_46	0.3186(6)	0.59640(17)	0.5157(4)	0.012(2)
C1_46	0.3077(6)	0.6110(2)	0.4744(5)	0.013(3)
C2_46	0.3307(6)	0.5994(2)	0.4301(5)	0.026(3)
F1_46	0.3872(5)	0.58994(18)	0.4494(5)	0.038(2)
F2_46	0.3355(7)	0.61371(18)	0.3924(4)	0.045(3)
F3_46	0.2913(7)	0.5826(2)	0.4076(5)	0.040(3)
C3_46	0.2362(6)	0.6157(2)	0.4526(5)	0.019(3)
F4_46	0.2178(4)	0.63108(16)	0.4828(4)	0.026(2)
F5_46	0.2043(7)	0.5964(2)	0.4525(5)	0.033(3)
F6_46	0.2214(6)	0.6240(2)	0.4034(4)	0.031(2)
C4_46	0.3366(8)	0.6349(3)	0.4937(8)	0.013(3)
F7_46	0.3052(9)	0.6455(4)	0.5245(9)	0.018(3)
F8_46	0.333(2)	0.6492(6)	0.4537(12)	0.023(4)
F9_46	0.3960(7)	0.6335(4)	0.5213(5)	0.014(2)

*Table S 9 Atomic coordinates and U_{eq} [Å^2] for **5***

Atom	***x***	***y***	***z***	U_{eq}
Sn1	0.35366(2)	0.87302(2)	0.71801(2)	0.02176(5)
Al2	0.35956(5)	0.50274(3)	0.58309(3)	0.01385(17)
Al1	0.37895(6)	0.84219(3)	0.36260(4)	0.01548(18)
O1_1	0.3647(8)	0.8872(5)	0.4273(5)	0.020(2)
C1_1	0.4006(4)	0.9200(3)	0.4743(3)	0.0203(14)
C2_1	0.4435(4)	0.8812(2)	0.5270(2)	0.0308(12)
F1_1	0.51739(18)	0.85998(11)	0.50680(12)	0.0405(9)

F2_1	0.4591(7)	0.9091(5)	0.5820(4)	0.0372(14)
F3_1	0.3914(3)	0.8380(2)	0.5397(2)	0.0528(14)
C3_1	0.3295(4)	0.9564(3)	0.5046(2)	0.0431(14)
F4_1	0.2776(3)	0.9791(2)	0.4588(3)	0.0544(15)
F5_1	0.2805(2)	0.92480(19)	0.54306(15)	0.0630(11)
F6_1	0.3604(10)	0.9983(5)	0.5414(4)	0.057(2)
C4_1	0.4706(3)	0.9601(2)	0.4477(2)	0.0305(12)
F7_1	0.4344(3)	1.00294(12)	0.41469(13)	0.0486(9)
F8_1	0.5202(9)	0.9838(5)	0.4929(7)	0.039(2)
F9_1	0.5210(3)	0.9321(2)	0.4069(2)	0.0410(11)
O1_2	0.4148(8)	0.8740(6)	0.2934(5)	0.019(2)
C1_2	0.3927(4)	0.9043(3)	0.2395(3)	0.0210(16)
C2_2	0.3387(4)	0.9565(2)	0.2573(3)	0.0272(12)
F1_2	0.3877(2)	0.99634(10)	0.28549(12)	0.0366(8)
F2_2	0.3003(9)	0.9800(4)	0.2049(5)	0.037(2)
F3_2	0.2774(3)	0.9433(2)	0.2985(2)	0.0318(10)
C3_2	0.3419(4)	0.8669(2)	0.1908(2)	0.0299(11)
F4_2	0.3773(5)	0.8151(3)	0.1873(5)	0.0460(17)
F5_2	0.26035(17)	0.86137(12)	0.20796(12)	0.0357(8)
F6_2	0.3414(7)	0.8880(5)	0.1313(5)	0.0368(19)
C4_2	0.4786(4)	0.9240(3)	0.2090(2)	0.0381(14)
F7_2	0.5163(2)	0.88202(17)	0.17813(14)	0.0499(9)
F8_2	0.4639(9)	0.9669(5)	0.1671(4)	0.050(2)
F9_2	0.5341(3)	0.9428(2)	0.2541(3)	0.0446(13)
O1_3	0.2795(8)	0.8137(10)	0.3424(11)	0.021(3)
C1_3	0.2061(7)	0.7931(4)	0.3670(5)	0.019(2)
C2_3	0.1856(4)	0.7378(2)	0.3297(2)	0.0301(15)
F1_3	0.2357(5)	0.6952(3)	0.3509(3)	0.0358(14)
F2_3	0.1035(4)	0.7204(3)	0.3349(4)	0.0375(14)
F3_3	0.2014(13)	0.7439(7)	0.2681(7)	0.033(2)
C3_3	0.1307(4)	0.8356(2)	0.3553(3)	0.0318(15)
F4_3	0.1537(18)	0.8876(5)	0.3724(11)	0.048(3)
F5_3	0.1073(8)	0.8382(3)	0.2943(4)	0.0431(19)
F6_3	0.0604(5)	0.8210(5)	0.3882(3)	0.0445(18)
C4_3	0.2122(4)	0.7797(3)	0.4405(3)	0.0334(15)
F7_3	0.2012(6)	0.8256(3)	0.4765(3)	0.0438(17)
F8_3	0.1527(12)	0.7417(7)	0.4586(9)	0.038(3)
F9_3	0.2884(11)	0.7577(10)	0.4560(12)	0.045(3)
O1_4	0.45613(13)	0.79285(8)	0.38619(9)	0.0211(4)
C1_4	0.51450(19)	0.75404(13)	0.36667(13)	0.0243(7)
C2_4	0.4698(2)	0.70558(14)	0.32912(17)	0.0352(8)
F1_4	0.41263(13)	0.72634(8)	0.28681(9)	0.0408(5)
F2_4	0.52557(14)	0.67346(8)	0.29604(10)	0.0470(5)
F3_4	0.42742(14)	0.67140(9)	0.36888(11)	0.0516(6)
C3_4	0.5611(2)	0.72993(16)	0.42750(16)	0.0410(9)
F4_4	0.61897(14)	0.76726(10)	0.45065(10)	0.0550(6)
F5_4	0.50527(15)	0.71869(10)	0.47278(9)	0.0560(6)
F6_4	0.60311(15)	0.68119(9)	0.41496(10)	0.0559(6)
C4_4	0.5832(2)	0.78176(15)	0.32295(16)	0.0352(8)
F7_4	0.60596(13)	0.83258(9)	0.34439(10)	0.0469(5)
F8_4	0.65489(13)	0.74993(10)	0.31966(11)	0.0496(6)
F9_4	0.55282(13)	0.78803(9)	0.26288(8)	0.0430(5)
O1_5	0.33387(14)	0.48178(9)	0.50567(8)	0.0222(5)
C1_5	0.35518(19)	0.47761(12)	0.44346(12)	0.0188(6)
C2_5	0.4341(2)	0.43779(13)	0.43499(13)	0.0255(7)

F1_5	0.50768(11)	0.46424(8)	0.45030(8)	0.0328(4)
F2_5	0.44057(12)	0.41884(8)	0.37463(8)	0.0332(4)
F3_5	0.42841(12)	0.39256(8)	0.47327(8)	0.0357(5)
C3_5	0.2757(2)	0.45160(13)	0.40721(13)	0.0251(7)
F4_5	0.20316(12)	0.47621(8)	0.42555(8)	0.0330(4)
F5_5	0.26858(12)	0.39635(8)	0.41935(8)	0.0329(4)
F6_5	0.27979(13)	0.45755(8)	0.34367(7)	0.0381(5)
C4_5	0.3754(2)	0.53656(13)	0.41441(13)	0.0226(7)
F7_5	0.30449(12)	0.56690(7)	0.40435(8)	0.0310(4)
F8_5	0.41616(12)	0.53277(8)	0.35843(7)	0.0317(4)
F9_5	0.42672(12)	0.56593(7)	0.45495(8)	0.0326(4)
O1_6	0.2956(4)	0.46541(18)	0.6354(2)	0.0171(9)
C1_6	0.2599(3)	0.41439(18)	0.64988(19)	0.0194(10)
C2_6	0.2052(2)	0.39016(15)	0.59257(17)	0.0304(10)
F1_6	0.2565(3)	0.36671(16)	0.54955(16)	0.0454(9)
F2_6	0.14947(18)	0.35054(11)	0.61208(14)	0.0482(8)
F3_6	0.16188(18)	0.43069(12)	0.56356(14)	0.0456(8)
C3_6	0.2002(3)	0.42427(17)	0.70779(19)	0.0391(11)
F4_6	0.2376(3)	0.45708(12)	0.75155(14)	0.0545(10)
F5_6	0.1263(4)	0.4499(3)	0.6877(2)	0.0590(15)
F6_6	0.1784(2)	0.37563(9)	0.73675(12)	0.0504(8)
C4_6	0.3310(2)	0.37135(14)	0.66926(17)	0.0267(8)
F7_6	0.3662(2)	0.38381(17)	0.7259(3)	0.0482(10)
F8_6	0.3022(2)	0.31795(13)	0.67234(14)	0.0324(7)
F9_6	0.39438(19)	0.37186(15)	0.62699(16)	0.0393(8)
O1_7	0.46811(13)	0.49134(8)	0.59591(9)	0.0218(5)
C1_7	0.54213(19)	0.50478(12)	0.62833(13)	0.0211(6)
C2_7	0.5242(2)	0.53308(14)	0.69425(13)	0.0302(8)
F1_7	0.50480(13)	0.58810(8)	0.68748(8)	0.0363(5)
F2_7	0.59321(13)	0.53000(8)	0.73426(8)	0.0421(5)
F3_7	0.45821(13)	0.50836(9)	0.72224(8)	0.0426(5)
C3_7	0.5928(2)	0.44875(13)	0.63980(15)	0.0311(8)
F4_7	0.58973(13)	0.41586(8)	0.58773(9)	0.0364(5)
F5_7	0.55906(13)	0.41921(8)	0.68786(9)	0.0406(5)
F6_7	0.67620(12)	0.45747(8)	0.65453(9)	0.0392(5)
C4_7	0.5957(2)	0.54588(13)	0.58690(14)	0.0268(7)
F7_7	0.62951(12)	0.51873(8)	0.53701(8)	0.0378(5)
F8_7	0.66016(12)	0.57028(8)	0.61988(8)	0.0369(5)
F9_7	0.54598(12)	0.58754(8)	0.56282(8)	0.0332(4)
O1_8	0.3423(9)	0.5750(4)	0.5964(5)	0.0169(18)
C1_8	0.2808(6)	0.6141(4)	0.6080(4)	0.0212(7)
C2_8	0.2488(4)	0.6086(3)	0.6786(3)	0.0329(14)
F1_8	0.1912(2)	0.56729(13)	0.68257(19)	0.0525(12)
F2_8	0.2083(8)	0.6560(6)	0.6970(9)	0.040(2)
F3_8	0.3135(4)	0.5985(4)	0.7187(4)	0.058(2)
C3_8	0.3252(4)	0.6724(2)	0.5995(3)	0.0329(13)
F4_8	0.3744(6)	0.6731(6)	0.5494(4)	0.057(2)
F5_8	0.3757(2)	0.68425(15)	0.6510(2)	0.0541(11)
F6_8	0.2689(10)	0.7154(5)	0.5932(6)	0.044(2)
C4_8	0.2037(4)	0.6098(3)	0.5600(3)	0.0360(16)
F7_8	0.2260(3)	0.62667(19)	0.50193(14)	0.0576(13)
F8_8	0.1355(11)	0.6409(7)	0.5798(8)	0.044(3)
F9_8	0.1769(5)	0.5570(3)	0.5554(3)	0.060(2)
C1_10	0.8090(2)	0.65356(16)	0.48530(15)	0.0358(8)
C2_10	0.7983(3)	0.7002(2)	0.52323(17)	0.0508(11)

C3_10	0.8619(3)	0.74204(19)	0.52607(19)	0.0608(12)
H3_10	0.855336	0.774478	0.552708	0.073
C4_10	0.9336(3)	0.7356(2)	0.48995(18)	0.0537(12)
H4_10	0.977070	0.764037	0.491129	0.064
C5_10	0.9437(3)	0.68984(18)	0.45293(18)	0.0517(11)
H5_10	0.994414	0.685906	0.428337	0.062
C6_10	0.8803(3)	0.64776(17)	0.45011(18)	0.0486(10)
H6_10	0.887518	0.615315	0.423567	0.058
F1_10	0.74758(16)	0.61360(11)	0.48384(11)	0.0643(7)
F2_10	0.72754(19)	0.70423(15)	0.55860(13)	0.0913(10)
N1_11	0.4626(2)	0.80211(13)	0.68055(13)	0.0409(8)
C1_11	0.5101(2)	0.77021(14)	0.66055(14)	0.0309(8)
C2_11	0.5702(2)	0.72944(15)	0.63436(17)	0.0393(9)
H2A_11	0.567550	0.731124	0.587267	0.059
H2B_11	0.554839	0.691133	0.648600	0.059
H2C_11	0.628928	0.738512	0.649526	0.059
N1_12	0.46803(18)	0.88818(11)	0.79896(12)	0.0295(6)
C1_12	0.5254(2)	0.90357(13)	0.82862(14)	0.0287(7)
C2_12	0.5987(2)	0.92356(17)	0.86765(18)	0.0446(10)
H2A_12	0.647828	0.897920	0.862083	0.067
H2B_12	0.582878	0.924222	0.913046	0.067
H2C_12	0.614605	0.961941	0.854000	0.067
N1_13	0.25519(18)	0.90307(11)	0.80259(12)	0.0294(6)
C1_13	0.2030(2)	0.92493(13)	0.83095(14)	0.0254(7)
C2_13	0.1359(2)	0.95253(14)	0.86691(15)	0.0342(8)
H2A_13	0.139743	0.993752	0.861027	0.051
H2B_13	0.143070	0.943358	0.912680	0.051
H2C_13	0.079276	0.939175	0.851373	0.051
N1_14	0.2217(2)	0.81941(12)	0.68085(12)	0.0361(7)
C1_14	0.1608(2)	0.80159(13)	0.65750(14)	0.0295(7)
C2_14	0.0829(2)	0.77852(15)	0.62725(17)	0.0403(9)
H2A_14	0.084467	0.784926	0.580711	0.060
H2B_14	0.032242	0.797445	0.644821	0.060
H2C_14	0.079659	0.737655	0.635842	0.060
N1_15	0.34555(16)	0.79579(11)	0.78254(11)	0.0242(6)
C1_15	0.3450(2)	0.75470(14)	0.80995(14)	0.0309(8)
C2_15	0.3438(3)	0.70114(16)	0.8446(2)	0.0560(12)
H2A_15	0.308517	0.673576	0.820530	0.084
H2B_15	0.319212	0.707085	0.887185	0.084
H2C_15	0.402849	0.686643	0.849615	0.084
O1_16	0.2761(11)	0.8152(13)	0.3478(15)	0.017(4)
C1_16	0.2004(10)	0.7937(6)	0.3686(7)	0.024(4)
C2_16	0.1531(5)	0.8397(3)	0.4072(4)	0.034(2)
F1_16	0.1860(9)	0.8460(4)	0.4652(5)	0.044(2)
F2_16	0.0686(8)	0.8270(7)	0.4134(5)	0.046(3)
F3_16	0.156(2)	0.8900(8)	0.3788(14)	0.043(4)
C3_16	0.1437(5)	0.7746(3)	0.3109(4)	0.033(2)
F4_16	0.1869(19)	0.7474(12)	0.2668(10)	0.039(4)
F5_16	0.1073(11)	0.8187(4)	0.2813(6)	0.041(2)
F6_16	0.0791(6)	0.7402(4)	0.3295(6)	0.048(2)
C4_16	0.2207(5)	0.7415(4)	0.4130(4)	0.034(2)
F7_16	0.2407(7)	0.6966(4)	0.3790(4)	0.0397(19)
F8_16	0.1537(17)	0.7284(10)	0.4497(13)	0.039(4)
F9_16	0.2891(16)	0.7545(14)	0.4498(17)	0.043(4)
O1_17	0.3341(19)	0.5710(9)	0.5988(13)	0.030(5)

C1_17	0.2780(12)	0.6146(8)	0.6055(7)	0.0212(7)
C2_17	0.3057(7)	0.6655(5)	0.5640(5)	0.033(2)
F1_17	0.2891(6)	0.6556(3)	0.5021(2)	0.042(2)
F2_17	0.263(2)	0.7129(11)	0.5790(12)	0.036(3)
F3_17	0.3892(11)	0.6756(11)	0.5679(9)	0.043(4)
C3_17	0.2770(9)	0.6327(5)	0.6772(5)	0.033(3)
F4_17	0.2793(10)	0.5883(6)	0.7149(7)	0.048(4)
F5_17	0.3481(5)	0.6639(3)	0.6917(4)	0.050(2)
F6_17	0.2120(18)	0.6666(12)	0.6930(19)	0.043(5)
C4_17	0.1870(8)	0.5949(6)	0.5832(5)	0.029(3)
F7_17	0.1524(4)	0.5617(3)	0.6267(4)	0.050(2)
F8_17	0.134(2)	0.6386(14)	0.5703(16)	0.034(4)
F9_17	0.1907(11)	0.5633(7)	0.5298(5)	0.044(3)
O1_18	0.364(3)	0.8925(16)	0.4202(16)	0.016(5)
C1_18	0.4024(12)	0.9201(9)	0.4694(11)	0.025(5)
C2_18	0.4968(10)	0.9362(7)	0.4542(7)	0.034(4)
F1_18	0.5493(5)	0.8919(4)	0.4640(5)	0.044(3)
F2_18	0.529(3)	0.9781(16)	0.490(2)	0.030(4)
F3_18	0.5012(13)	0.9510(8)	0.3939(7)	0.049(5)
C3_18	0.3468(10)	0.9746(7)	0.4757(8)	0.045(4)
F4_18	0.2648(10)	0.9598(8)	0.4780(9)	0.045(4)
F5_18	0.3648(10)	1.0100(4)	0.4280(5)	0.056(3)
F6_18	0.365(3)	1.0032(16)	0.5302(14)	0.044(5)
C4_18	0.4013(11)	0.8847(7)	0.5320(8)	0.038(4)
F7_18	0.3207(7)	0.8835(5)	0.5566(4)	0.048(3)
F8_18	0.454(3)	0.908(2)	0.5759(17)	0.049(6)
F9_18	0.4271(11)	0.8324(6)	0.5225(7)	0.045(4)
O1_19	0.421(3)	0.8723(18)	0.2942(13)	0.019(7)
C1_19	0.4022(11)	0.9035(8)	0.2412(10)	0.018(4)
C2_19	0.3930(10)	0.8632(6)	0.1812(6)	0.033(3)
F1_19	0.4707(8)	0.8477(5)	0.1615(4)	0.051(3)
F2_19	0.360(2)	0.8925(16)	0.1320(14)	0.039(5)
F3_19	0.3498(14)	0.8169(8)	0.1951(12)	0.039(4)
C3_19	0.3159(10)	0.9361(7)	0.2485(7)	0.034(4)
F4_19	0.3091(10)	0.9561(8)	0.3074(7)	0.044(4)
F5_19	0.2484(5)	0.9032(5)	0.2376(5)	0.051(3)
F6_19	0.309(3)	0.9814(13)	0.2099(15)	0.031(4)
C4_19	0.4755(11)	0.9470(6)	0.2310(8)	0.040(4)
F7_19	0.4668(8)	0.9900(4)	0.2716(4)	0.055(3)
F8_19	0.478(3)	0.9680(13)	0.1714(11)	0.032(4)
F9_19	0.5515(12)	0.9226(9)	0.2418(10)	0.056(5)
O1_20	0.296(3)	0.4580(14)	0.6235(17)	0.039(9)
C1_20	0.2686(13)	0.4110(9)	0.6533(9)	0.027(5)
C2_20	0.1688(12)	0.4145(8)	0.6520(9)	0.044(5)
F1_20	0.144(3)	0.4459(17)	0.7024(14)	0.051(6)
F2_20	0.1376(13)	0.3616(7)	0.6598(14)	0.074(7)
F3_20	0.1368(13)	0.4335(10)	0.5968(9)	0.056(5)
C3_20	0.2974(14)	0.3579(9)	0.6157(10)	0.049(5)
F4_20	0.3789(14)	0.3650(13)	0.6008(11)	0.053(5)
F5_20	0.251(2)	0.3503(13)	0.5617(12)	0.056(6)
F6_20	0.2883(19)	0.3112(9)	0.6501(9)	0.039(5)
C4_20	0.3023(15)	0.4076(9)	0.7242(9)	0.051(5)
F7_20	0.3860(16)	0.3979(14)	0.724(2)	0.060(6)
F8_20	0.2555(14)	0.3702(7)	0.7572(6)	0.057(5)
F9_20	0.2924(16)	0.4593(8)	0.7496(10)	0.062(5)

*Table S 10 Atomic coordinates and U_{eq} [Å^2] for **6***

Atom	*x*	*y*	*z*	U_{eq}
Sn1	0.83077(2)	0.47786(2)	0.24364(2)	0.02791(6)
N1	0.73727(17)	0.65634(16)	0.28577(9)	0.0247(4)
C1	0.8434(2)	0.73050(18)	0.27964(11)	0.0249(5)
H1	0.840826	0.797144	0.287171	0.030
Al1	0.36941(5)	0.72087(5)	0.13125(3)	0.01629(13)
C2	0.6498(2)	0.6734(2)	0.29861(11)	0.0309(5)
H2	0.646505	0.735943	0.304109	0.037
N2	0.71412(17)	0.55816(16)	0.28117(10)	0.0278(4)
Al2	0.12559(5)	0.25584(5)	0.37722(3)	0.01819(13)
C3	0.5675(2)	0.5842(2)	0.30216(12)	0.0358(6)
H3	0.495806	0.571737	0.310319	0.043
N3	0.86638(16)	0.69983(16)	0.21869(9)	0.0244(4)
N2A	0.7191(2)	0.37118(17)	0.29898(10)	0.0329(5)
C2A	0.5923(3)	0.2344(3)	0.31876(14)	0.0386(6)
H2A	0.534667	0.167056	0.313011	0.046
N3A	0.58578(16)	0.26971(16)	0.17683(9)	0.0253(4)
C3A	0.6449(3)	0.3106(3)	0.37252(14)	0.0451(7)
H3A	0.630981	0.307636	0.411617	0.054
N4A	0.65748(18)	0.36695(16)	0.17836(10)	0.0276(4)
C4A	0.7232(3)	0.3937(3)	0.35864(13)	0.0402(7)
H4A	0.773068	0.458134	0.387744	0.048
N5A	0.70561(17)	0.20017(15)	0.18913(10)	0.0252(4)
C5A	0.4888(2)	0.2333(2)	0.14160(11)	0.0302(5)
H5A	0.426793	0.167512	0.133515	0.036
N6A	0.80492(17)	0.28295(16)	0.19484(10)	0.0286(4)
C6A	0.4970(2)	0.3089(2)	0.11991(12)	0.0334(6)
H6A	0.442090	0.306687	0.094149	0.040
C7A	0.6025(2)	0.3901(2)	0.14342(12)	0.0321(5)
H7A	0.631625	0.453522	0.135649	0.039
C8A	0.7080(2)	0.10946(18)	0.16269(11)	0.0271(5)
H8A	0.648519	0.041949	0.153905	0.033
C9A	0.8123(2)	0.1338(2)	0.15114(11)	0.0292(5)
H9A	0.840486	0.087376	0.132965	0.035
C10A	0.8689(2)	0.24213(19)	0.17185(11)	0.0270(5)
H10A	0.944110	0.281410	0.169631	0.032
C1A	0.6150(2)	0.21679(19)	0.20997(11)	0.0265(5)
H1A	0.550224	0.147370	0.202088	0.032
C10	1.0331(2)	0.7157(2)	0.36971(13)	0.0349(6)
H10	1.065375	0.679470	0.381895	0.042
C9	1.0694(2)	0.8214(2)	0.39576(13)	0.0356(6)
H9	1.128704	0.869401	0.427686	0.043
C8	1.0013(2)	0.8412(2)	0.36551(12)	0.0303(5)
H8	1.004069	0.906566	0.372179	0.036
C7	0.8845(2)	0.6033(2)	0.13691(12)	0.0324(6)
H7	0.880467	0.544633	0.105899	0.039
C6	0.9330(2)	0.7022(2)	0.13469(13)	0.0361(6)
H6	0.967498	0.723837	0.102996	0.043
N6	0.94815(19)	0.67124(17)	0.32577(10)	0.0322(5)
N5	0.92895(17)	0.74981(16)	0.32416(9)	0.0260(4)
C5	0.9213(2)	0.7625(2)	0.18733(12)	0.0307(5)

H5	0.946948	0.835073	0.199705	0.037
N4	0.84399(18)	0.60044(17)	0.18808(10)	0.0289(4)
C4	0.6106(2)	0.5150(2)	0.29129(12)	0.0336(6)
H4	0.571462	0.445970	0.291103	0.040
N1A	0.63718(18)	0.27230(17)	0.27464(10)	0.0293(4)
O1_1	0.50560(14)	0.74785(14)	0.13699(8)	0.0290(4)
C1_1	0.58245(18)	0.72701(17)	0.10950(10)	0.0215(4)
C2_1	0.6968(2)	0.81566(19)	0.14488(12)	0.0295(5)
F1_1	0.71743(12)	0.80482(12)	0.19749(7)	0.0334(3)
F2_1	0.77874(12)	0.81813(13)	0.11413(8)	0.0389(4)
F3_1	0.69888(14)	0.90655(12)	0.15776(9)	0.0451(4)
C3_1	0.5738(2)	0.7224(2)	0.04280(12)	0.0314(5)
F4_1	0.46990(13)	0.66500(14)	0.01538(7)	0.0372(4)
F5_1	0.60788(16)	0.81678(15)	0.04014(9)	0.0494(4)
F6_1	0.63295(14)	0.68229(15)	0.01098(7)	0.0417(4)
C4_1	0.5716(2)	0.62255(18)	0.11121(11)	0.0265(5)
F7_1	0.49162(13)	0.54273(11)	0.06857(7)	0.0352(3)
F8_1	0.66454(13)	0.61524(12)	0.10305(8)	0.0358(3)
F9_1	0.54765(14)	0.61126(12)	0.16385(7)	0.0383(4)
O1_2	0.3466(3)	0.7737(3)	0.08226(11)	0.0727(10)
C1_2	0.3041(2)	0.81611(19)	0.05507(10)	0.0257(5)
C2_2	0.2136(3)	0.7323(2)	0.00187(13)	0.0463(7)
F1_2	0.12283(18)	0.68012(16)	0.02248(10)	0.0664(6)
F2_2	0.18863(19)	0.7710(2)	-0.03561(9)	0.0697(7)
F3_2	0.2450(2)	0.66476(15)	-0.03007(11)	0.0866(9)
C3_2	0.3959(2)	0.8927(2)	0.03077(13)	0.0408(6)
F4_2	0.48549(16)	0.9510(3)	0.07120(10)	0.0940(10)
F5_2	0.42240(16)	0.84258(16)	-0.01836(8)	0.0473(4)
F6_2	0.36562(19)	0.95628(15)	0.01628(11)	0.0621(6)
C4_2	0.2539(2)	0.8760(2)	0.10064(12)	0.0331(5)
F7_2	0.33323(19)	0.96519(17)	0.13764(10)	0.0718(7)
F8_2	0.18717(18)	0.89699(18)	0.07352(10)	0.0565(5)
F9_2	0.19728(13)	0.82197(13)	0.13435(7)	0.0371(4)
O1_3	0.2918(2)	0.59090(15)	0.10675(13)	0.0679(9)
C1_3	0.2030(2)	0.50215(18)	0.10216(11)	0.0284(5)
C2_3	0.1595(3)	0.4393(2)	0.03420(12)	0.0372(6)
F1_3	0.10519(19)	0.47757(16)	0.01077(8)	0.0541(5)
F2_3	0.09007(16)	0.33988(12)	0.02426(8)	0.0497(5)
F3_3	0.24096(19)	0.44344(16)	0.00360(8)	0.0547(5)
C3_3	0.2349(2)	0.4391(2)	0.13178(13)	0.0393(6)
F4_3	0.29937(18)	0.4994(2)	0.18405(9)	0.0777(8)
F5_3	0.28922(14)	0.39597(15)	0.09697(8)	0.0447(4)
F6_3	0.14718(16)	0.36332(17)	0.14101(10)	0.0539(5)
C4_3	0.1124(2)	0.5228(2)	0.13367(12)	0.0319(5)
F7_3	0.13314(14)	0.54827(15)	0.19306(7)	0.0461(4)
F8_3	0.01269(12)	0.44094(12)	0.11437(8)	0.0398(4)
F9_3	0.10773(16)	0.60132(13)	0.12334(9)	0.0470(4)
O1_4	0.3371(10)	0.7637(7)	0.2040(4)	0.0179(16)
C1_4	0.3745(7)	0.8293(7)	0.2615(5)	0.0226(19)
C2_4	0.2735(5)	0.8206(4)	0.2924(2)	0.0293(12)
F1_4	0.2289(4)	0.7341(3)	0.30553(19)	0.0450(11)
F2_4	0.2998(14)	0.9012(8)	0.3442(4)	0.0375(19)
F3_4	0.1972(10)	0.8202(11)	0.2576(8)	0.0392(18)
C3_4	0.4461(4)	0.9428(4)	0.2649(2)	0.0292(12)
F4_4	0.5138(10)	0.9476(8)	0.2240(5)	0.0332(17)

F5_4	0.3835(4)	0.9833(3)	0.2527(2)	0.0393(9)
F6_4	0.5071(8)	1.0038(8)	0.3189(4)	0.0405(18)
C4_4	0.4453(5)	0.7971(5)	0.2939(3)	0.0330(13)
F7_4	0.5452(3)	0.8289(4)	0.27779(16)	0.0376(9)
F8_4	0.4587(11)	0.8380(10)	0.3541(4)	0.043(2)
F9_4	0.4001(6)	0.6959(5)	0.2797(3)	0.0424(12)
O1_5	0.1291(4)	0.3752(2)	0.3972(2)	0.0238(9)
C1_5	0.1720(3)	0.4691(3)	0.39096(15)	0.0231(8)
C2_5	0.1272(3)	0.5347(2)	0.43609(14)	0.0316(6)
F1_5	0.02336(16)	0.50614(15)	0.41583(11)	0.0481(5)
F2_5	0.1856(3)	0.6357(2)	0.44464(17)	0.0402(7)
F3_5	0.12886(19)	0.52214(14)	0.48904(9)	0.0401(5)
C3_5	0.2996(2)	0.5254(2)	0.40614(14)	0.0311(6)
F4_5	0.33962(19)	0.46048(19)	0.38133(13)	0.0425(6)
F5_5	0.33188(15)	0.56025(15)	0.46547(9)	0.0413(5)
F6_5	0.3466(4)	0.6057(2)	0.3867(2)	0.0405(8)
C4_5	0.1365(3)	0.4597(3)	0.32584(14)	0.0421(8)
F7_5	0.1994(2)	0.43247(17)	0.28837(9)	0.0599(7)
F8_5	0.1452(4)	0.5475(3)	0.3218(2)	0.0526(7)
F9_5	0.0333(2)	0.3880(2)	0.30502(12)	0.0653(8)
O1_6	0.1577(12)	0.2281(10)	0.3033(6)	0.0194(16)
C1_6	0.1951(5)	0.1718(5)	0.2621(3)	0.0238(13)
C2_6	0.3127(3)	0.1962(3)	0.28599(19)	0.0291(9)
F1_6	0.3109(3)	0.1480(3)	0.32467(11)	0.0350(7)
F2_6	0.3637(12)	0.1647(10)	0.2417(5)	0.0367(15)
F3_6	0.3746(9)	0.2977(6)	0.3139(4)	0.0416(16)
C3_6	0.1963(4)	0.2008(3)	0.20415(18)	0.0345(10)
F4_6	0.1039(10)	0.2029(9)	0.1904(8)	0.0439(16)
F5_6	0.2804(3)	0.2930(3)	0.21208(16)	0.0445(8)
F6_6	0.2070(4)	0.1329(4)	0.1563(2)	0.0470(11)
C4_6	0.1174(3)	0.0544(3)	0.24656(19)	0.0321(9)
F7_6	0.0238(4)	0.0251(4)	0.2115(2)	0.0450(10)
F8_6	0.1614(10)	-0.0048(7)	0.2169(3)	0.0424(17)
F9_6	0.0908(8)	0.0323(11)	0.2967(6)	0.0403(14)
O1_7	-0.0037(17)	0.173(3)	0.3801(18)	0.023(5)
C1_7	-0.1130(17)	0.1344(12)	0.3744(6)	0.024(3)
C2_7	-0.1468(14)	0.2011(10)	0.4266(6)	0.029(3)
F1_7	-0.0818(8)	0.3001(7)	0.4379(5)	0.041(3)
F2_7	-0.2510(15)	0.175(2)	0.4097(12)	0.043(4)
F3_7	-0.1332(8)	0.1872(8)	0.4790(4)	0.038(2)
C3_7	-0.1687(15)	0.0229(11)	0.3767(6)	0.031(4)
F4_7	-0.1690(8)	-0.0426(7)	0.3239(5)	0.050(3)
F5_7	-0.1153(7)	0.0158(7)	0.4202(5)	0.039(3)
F6_7	-0.2720(17)	-0.007(3)	0.3861(16)	0.041(4)
C4_7	-0.1618(13)	0.1301(11)	0.3133(6)	0.031(3)
F7_7	-0.1091(8)	0.1027(9)	0.2702(4)	0.035(2)
F8_7	-0.2665(12)	0.0579(11)	0.2961(9)	0.050(3)
F9_7	-0.1428(9)	0.2272(8)	0.3183(5)	0.053(3)
O1_8	0.2232(6)	0.2550(6)	0.4230(2)	0.0250(13)
C1_8	0.2554(3)	0.2591(3)	0.47829(19)	0.0225(8)
C2_8	0.1969(3)	0.1501(3)	0.48398(16)	0.0372(8)
F1_8	0.09358(18)	0.1256(2)	0.49297(13)	0.0526(7)
F2_8	0.2455(4)	0.1429(4)	0.52995(18)	0.0536(9)
F3_8	0.1955(3)	0.0788(3)	0.4338(2)	0.0585(9)
C3_8	0.3815(3)	0.2978(3)	0.48565(16)	0.0346(7)

F4_8	0.4320(3)	0.3793(2)	0.46778(17)	0.0453(7)
F5_8	0.40393(19)	0.2233(2)	0.45201(11)	0.0469(6)
F6_8	0.4250(5)	0.3242(5)	0.5426(2)	0.0497(10)
C4_8	0.2295(3)	0.3339(3)	0.52912(14)	0.0363(8)
F7_8	0.3022(3)	0.43208(17)	0.53762(11)	0.0585(7)
F8_8	0.2326(4)	0.3212(3)	0.58239(16)	0.0458(10)
F9_8	0.1291(3)	0.3216(3)	0.5142(2)	0.0503(10)
C1_9	0.0884(8)	0.0967(7)	0.0181(4)	0.048(2)
C2_9	0.1051(7)	0.0117(7)	-0.0034(4)	0.047(2)
C3_9	0.0203(12)	-0.0891(11)	-0.0206(8)	0.123(7)
H3_9	0.031734	-0.147435	-0.038934	0.148
C4_9	-0.0815(13)	-0.0985(11)	-0.0093(10)	0.127(7)
H4_9	-0.140454	-0.165220	-0.014904	0.152
C5_9	-0.0996(13)	-0.0164(10)	0.0093(10)	0.137(7)
H5_9	-0.172246	-0.027166	0.013648	0.165
C6_9	-0.0168(8)	0.0832(6)	0.0225(4)	0.046(2)
H6_9	-0.031670	0.140444	0.034262	0.055
F1_9	0.1696(5)	0.1836(5)	0.0363(4)	0.108(2)
F2_9	0.2002(5)	0.0252(5)	-0.0037(3)	0.0993(19)
C1_10	0.4646(8)	-0.0997(7)	0.4993(4)	0.042(2)
C2_10	0.3894(6)	-0.0753(6)	0.4791(3)	0.0310(15)
C3_10	0.4219(6)	0.0230(6)	0.4793(3)	0.0343(15)
H3_10	0.370037	0.039505	0.464848	0.041
C4_10	0.5255(11)	0.0957(12)	0.4996(10)	0.114(7)
H4_10	0.546611	0.164869	0.501953	0.137
C5_10	0.5996(13)	0.0708(14)	0.5166(9)	0.118(6)
H5_10	0.673852	0.122594	0.530194	0.142
C6_10	0.5709(12)	-0.0268(13)	0.5148(10)	0.134(7)
H6_10	0.625650	-0.044028	0.524392	0.161
F1_10	0.4326(4)	-0.1863(4)	0.5025(3)	0.0851(16)
F2_10	0.2907(4)	-0.1422(4)	0.4607(2)	0.0732(13)
O1_11	0.3531(9)	0.7872(6)	0.1985(4)	0.0195(15)
C1_11	0.3870(6)	0.8353(6)	0.2585(4)	0.0197(16)
C2_11	0.5063(4)	0.9246(4)	0.2709(2)	0.0275(10)
F1_11	0.5188(10)	0.9747(7)	0.2315(5)	0.042(2)
F2_11	0.5321(7)	0.9951(7)	0.3259(3)	0.0343(14)
F3_11	0.5791(3)	0.8887(3)	0.26504(15)	0.0408(9)
C3_11	0.3870(6)	0.7613(5)	0.2918(3)	0.0416(14)
F4_11	0.2863(4)	0.7022(3)	0.2985(2)	0.0709(16)
F5_11	0.4253(6)	0.6995(5)	0.2583(3)	0.0574(15)
F6_11	0.4471(11)	0.8108(9)	0.3460(4)	0.051(2)
C4_11	0.3102(4)	0.8818(5)	0.2850(2)	0.0347(12)
F7_11	0.2059(8)	0.8121(11)	0.2628(7)	0.048(2)
F8_11	0.3224(13)	0.9091(10)	0.3451(4)	0.053(3)
F9_11	0.3324(4)	0.9642(3)	0.2694(2)	0.0512(11)
O1_12	0.146(2)	0.2137(18)	0.3062(11)	0.023(4)
C1_12	0.1832(8)	0.1579(8)	0.2647(5)	0.021(2)
C2_12	0.1172(6)	0.1229(6)	0.2013(3)	0.0365(17)
F1_12	0.1042(19)	0.1999(16)	0.1940(14)	0.045(3)
F2_12	0.1667(8)	0.0915(6)	0.1568(4)	0.0494(19)
F3_12	0.0176(7)	0.0449(7)	0.1951(4)	0.0488(19)
C3_12	0.1692(6)	0.0608(5)	0.2793(3)	0.0292(15)
F4_12	0.2483(5)	0.0849(5)	0.3220(2)	0.0412(13)
F5_12	0.0729(13)	0.018(2)	0.2978(10)	0.040(3)
F6_12	0.1692(18)	-0.0117(13)	0.2307(5)	0.036(2)

C4_12	0.3067(6)	0.2255(6)	0.2641(4)	0.0369(17)
F7_12	0.3638(15)	0.2765(10)	0.3197(6)	0.040(3)
F8_12	0.353(2)	0.1672(18)	0.2341(10)	0.040(3)
F9_12	0.3228(6)	0.2937(4)	0.2372(3)	0.0522(15)
O1_13	0.222(3)	0.256(3)	0.4234(12)	0.029(8)
C1_13	0.2553(12)	0.2552(11)	0.4772(9)	0.032(4)
C2_13	0.1777(11)	0.2710(12)	0.5223(7)	0.047(3)
F1_13	0.0842(11)	0.1867(14)	0.5102(7)	0.077(4)
F2_13	0.223(2)	0.2886(18)	0.5776(8)	0.045(4)
F3_13	0.1616(19)	0.3494(16)	0.5208(14)	0.054(4)
C3_13	0.3736(12)	0.3446(11)	0.5028(7)	0.047(4)
F4_13	0.4323(16)	0.3423(15)	0.4581(9)	0.056(5)
F5_13	0.3735(15)	0.4343(9)	0.5233(7)	0.074(5)
F6_13	0.420(3)	0.338(3)	0.5495(12)	0.062(5)
C4_13	0.2532(14)	0.1497(12)	0.4688(8)	0.061(4)
F7_13	0.3338(17)	0.1445(16)	0.4409(8)	0.092(5)
F8_13	0.269(2)	0.138(3)	0.5209(10)	0.071(5)
F9_13	0.1571(16)	0.0763(17)	0.4355(12)	0.076(5)
O1_14	-0.0017(4)	0.1658(7)	0.3857(4)	0.0205(11)
C1_14	-0.1110(4)	0.1350(3)	0.37678(17)	0.0236(9)
C2_14	-0.1525(4)	0.1076(4)	0.3092(2)	0.0427(11)
F1_14	-0.15832(19)	0.0181(2)	0.27631(10)	0.0605(8)
F2_14	-0.2530(3)	0.1022(3)	0.30089(18)	0.0501(9)
F3_14	-0.08425(19)	0.1791(3)	0.28797(12)	0.0555(8)
C3_14	-0.1389(4)	0.2200(3)	0.4163(2)	0.0367(10)
F4_14	-0.07897(19)	0.26558(19)	0.47057(11)	0.0506(7)
F5_14	-0.11796(19)	0.29255(18)	0.39180(16)	0.0567(8)
F6_14	-0.2446(3)	0.1827(5)	0.4239(2)	0.0416(10)
C4_14	-0.1683(4)	0.0379(3)	0.39586(18)	0.0291(8)
F7_14	-0.15066(17)	0.06383(18)	0.45526(10)	0.0422(6)
F8_14	-0.2765(4)	-0.0151(7)	0.3771(3)	0.0405(12)
F9_14	-0.12774(19)	-0.02809(16)	0.37276(14)	0.0495(7)
O1_15	0.130(3)	0.371(2)	0.390(2)	0.026(9)
C1_15	0.1687(14)	0.4645(18)	0.3842(7)	0.028(9)
C2_15	0.2870(14)	0.5000(15)	0.3686(8)	0.034(5)
F1_15	0.2853(14)	0.4522(13)	0.3109(6)	0.039(4)
F2_15	0.338(4)	0.6013(16)	0.379(2)	0.045(5)
F3_15	0.344(2)	0.479(2)	0.4031(10)	0.047(5)
C3_15	0.1728(14)	0.5457(16)	0.4440(7)	0.036(7)
F4_15	0.0797(14)	0.5075(15)	0.4657(9)	0.041(4)
F5_15	0.2562(13)	0.5729(13)	0.4856(7)	0.044(5)
F6_15	0.185(3)	0.631(2)	0.4336(17)	0.043(5)
C4_15	0.0933(14)	0.4600(17)	0.3330(8)	0.044(8)
F7_15	0.0010(12)	0.4569(13)	0.3516(7)	0.040(4)
F8_15	0.142(3)	0.545(2)	0.318(2)	0.059(5)
F9_15	0.0724(17)	0.3779(15)	0.2851(8)	0.043(4)

*Table S 11 Atomic coordinates and U_{eq} [Å^2] for **7 vap dif.***

Atom	***x***	***y***	***z***	U_{eq}
Fe1	0.23422(2)	0.04901(2)	0.83362(2)	0.0537(2)
O1	0.1702(3)	0.0847(3)	0.8301(3)	0.064(2)
C1	0.1930(3)	0.0719(3)	0.8303(3)	0.048(2)
C2	0.2695(8)	0.0536(9)	0.8843(6)	0.094(7)

O2	0.2890(7)	0.0557(8)	0.9128(6)	0.124(7)
C3	0.227(4)	0.075(4)	0.885(2)	0.49(7)
O3	0.232(4)	0.095(3)	0.914(3)	0.70(7)
Al1	0.667(2)	0.3322(15)	0.59583(8)	0.0285(15)
Fe2	0.666667	0.333333	0.833333	0.0546(4)
Al2	0.42170(3)	0.28068(3)	0.75419(3)	0.0264(2)
Al3	0.18312(3)	0.23685(3)	0.91850(3)	0.0259(2)
C4	0.6917(16)	0.3991(7)	0.8348(15)	0.112(15)
O4	0.7065(16)	0.4357(9)	0.8302(15)	0.165(17)
O1_2	0.6782(2)	0.38249(17)	0.6100(2)	0.066(2)
C1_2	0.66759(15)	0.40978(15)	0.62393(15)	0.0448(11)
C2_2	0.69640(19)	0.45244(17)	0.60434(19)	0.0640(14)
F1_2	0.68512(19)	0.45195(17)	0.56752(13)	0.1070(17)
F2_2	0.69625(16)	0.48440(13)	0.62071(17)	0.0838(15)
F3_2	0.73682(12)	0.46102(14)	0.60629(18)	0.0880(15)
C3_2	0.6747(2)	0.4145(2)	0.66848(18)	0.0772(18)
F4_2	0.6579(3)	0.3762(2)	0.6843(2)	0.123(2)
F5_2	0.71494(17)	0.43629(17)	0.67745(15)	0.0981(16)
F6_2	0.6571(3)	0.4346(2)	0.68418(18)	0.119(2)
C4_2	0.62151(19)	0.3959(2)	0.6153(2)	0.0750(18)
F7_2	0.59607(13)	0.36575(13)	0.6392(2)	0.1007(18)
F8_2	0.6132(3)	0.4267(2)	0.6162(2)	0.106(2)
F9_2	0.61272(17)	0.3795(2)	0.57908(18)	0.106(2)
O1_3	0.6715(10)	0.3450(8)	0.5481(4)	0.036(6)
C1_3	0.6651(7)	0.3356(6)	0.5100(4)	0.044(3)
C2_3	0.6698(7)	0.3752(7)	0.4892(6)	0.060(5)
F1_3	0.6362(10)	0.3783(13)	0.4962(13)	0.079(6)
F2_3	0.6757(10)	0.3743(11)	0.4515(5)	0.100(8)
F3_3	0.7028(10)	0.4092(7)	0.5041(10)	0.084(7)
C3_3	0.6967(7)	0.3241(8)	0.4932(8)	0.067(5)
F4_3	0.7000(12)	0.2968(13)	0.5165(12)	0.075(9)
F5_3	0.7347(8)	0.3575(11)	0.4911(12)	0.090(8)
F6_3	0.6866(11)	0.3061(12)	0.4582(9)	0.081(8)
C4_3	0.6198(6)	0.2997(6)	0.5026(6)	0.056(4)
F7_3	0.6168(8)	0.2637(5)	0.5126(6)	0.086(6)
F8_3	0.6089(9)	0.2977(9)	0.4653(6)	0.085(7)
F9_3	0.5931(9)	0.3055(11)	0.5238(10)	0.070(6)
O1_4	0.45710(13)	0.31661(12)	0.72139(13)	0.0439(9)
C1_4	0.48644(18)	0.35664(16)	0.71239(16)	0.0444(13)
C2_4	0.4886(2)	0.35955(19)	0.66767(17)	0.0660(16)
F1_4	0.5046(2)	0.33668(19)	0.65349(15)	0.106(2)
F2_4	0.5122(2)	0.39775(15)	0.65468(14)	0.112(2)
F3_4	0.45130(18)	0.3444(2)	0.65197(14)	0.120(2)
C3_4	0.4757(2)	0.38941(18)	0.72850(19)	0.0669(16)
F4_4	0.4629(3)	0.38054(18)	0.76439(15)	0.113(2)
F5_4	0.44230(19)	0.3869(2)	0.7078(2)	0.1034(19)
F6_4	0.5058(2)	0.42806(14)	0.72528(18)	0.0926(18)
C4_4	0.52954(18)	0.36623(19)	0.72881(18)	0.0645(16)
F7_4	0.5302(2)	0.3726(2)	0.76772(19)	0.111(2)
F8_4	0.56122(16)	0.40052(16)	0.7140(2)	0.0972(18)
F9_4	0.53759(18)	0.33677(18)	0.7206(2)	0.111(2)
O1_5	0.4088(2)	0.23289(18)	0.73511(16)	0.0507(11)
C1_5	0.42058(14)	0.20555(14)	0.72312(13)	0.0353(9)
C2_5	0.42866(16)	0.20979(16)	0.67898(14)	0.0531(12)
F1_5	0.46519(13)	0.24411(12)	0.67160(13)	0.0841(12)

F2_5	0.42982(13)	0.17765(14)	0.66303(14)	0.0704(12)
F3_5	0.39879(15)	0.21300(17)	0.66006(12)	0.0816(13)
C3_5	0.38330(16)	0.16173(16)	0.73241(16)	0.0570(13)
F4_5	0.36931(17)	0.1597(2)	0.76861(14)	0.0972(17)
F5_5	0.35172(11)	0.15251(11)	0.70802(14)	0.0809(12)
F6_5	0.3920(3)	0.13140(19)	0.7283(2)	0.0889(17)
C4_5	0.46012(17)	0.21109(17)	0.74426(16)	0.0546(13)
F7_5	0.45151(15)	0.19780(15)	0.78084(10)	0.0833(13)
F8_5	0.4772(2)	0.19090(18)	0.7274(2)	0.0747(14)
F9_5	0.48908(13)	0.25176(12)	0.74574(15)	0.0781(13)
O1_6	0.4419(2)	0.2852(2)	0.79990(13)	0.0610(18)
C1_6	0.43894(15)	0.28407(16)	0.83899(14)	0.0420(11)
C2_6	0.48210(16)	0.29394(17)	0.85518(14)	0.0506(12)
F1_6	0.51057(12)	0.33366(13)	0.84997(15)	0.0853(13)
F2_6	0.48171(16)	0.28736(19)	0.89324(11)	0.0900(15)
F3_6	0.49624(15)	0.27154(17)	0.83822(13)	0.0885(15)
C3_6	0.40502(18)	0.24038(19)	0.85253(16)	0.0642(14)
F4_6	0.37187(14)	0.22527(18)	0.83041(15)	0.116(2)
F5_6	0.41907(19)	0.21212(13)	0.84822(16)	0.1021(16)
F6_6	0.39546(17)	0.23760(17)	0.88902(12)	0.0896(15)
C4_6	0.42821(17)	0.31676(19)	0.85455(15)	0.0562(13)
F7_6	0.38721(16)	0.3029(2)	0.84779(15)	0.1013(19)
F8_6	0.43393(16)	0.32365(17)	0.89177(13)	0.0795(14)
F9_6	0.4506(2)	0.35264(16)	0.83794(17)	0.117(2)
O1_7	0.3737(5)	0.2781(5)	0.7585(6)	0.055(4)
C1_7	0.3374(4)	0.2719(3)	0.7429(3)	0.049(3)
C2_7	0.3348(4)	0.2644(4)	0.6990(3)	0.067(3)
F1_7	0.3313(3)	0.2281(4)	0.6903(3)	0.112(4)
F2_7	0.3036(5)	0.2660(8)	0.6814(7)	0.097(3)
F3_7	0.3703(3)	0.2940(5)	0.6819(2)	0.113(5)
C3_7	0.3297(4)	0.3090(4)	0.7510(4)	0.072(3)
F4_7	0.3379(4)	0.3198(4)	0.7889(3)	0.097(3)
F5_7	0.3527(3)	0.3414(3)	0.7289(4)	0.108(3)
F6_7	0.2890(4)	0.2971(7)	0.7479(5)	0.086(4)
C4_7	0.3026(4)	0.2316(4)	0.7631(4)	0.077(3)
F7_7	0.2983(3)	0.2413(4)	0.7990(2)	0.114(4)
F8_7	0.2667(5)	0.2158(8)	0.7425(6)	0.103(4)
F9_7	0.3150(2)	0.2032(2)	0.7628(4)	0.101(3)
O1_8	0.1662(2)	0.24128(18)	0.87312(15)	0.0378(11)
C1_8	0.17002(16)	0.24066(16)	0.83405(17)	0.0390(11)
C2_8	0.21112(18)	0.28004(19)	0.82043(16)	0.0608(15)
F1_8	0.24344(11)	0.27560(18)	0.82694(12)	0.0771(13)
F2_8	0.2109(3)	0.2875(3)	0.78259(17)	0.091(2)
F3_8	0.21604(19)	0.31414(14)	0.83973(19)	0.0873(16)
C3_8	0.13226(19)	0.2420(2)	0.81691(18)	0.0670(16)
F4_8	0.0970(2)	0.2153(3)	0.8350(3)	0.0865(16)
F5_8	0.13695(19)	0.28021(17)	0.81983(16)	0.1012(17)
F6_8	0.1265(3)	0.2321(2)	0.77913(19)	0.094(2)
C4_8	0.1702(2)	0.20116(18)	0.81996(16)	0.0599(14)
F7_8	0.13177(16)	0.16775(13)	0.82180(16)	0.0822(15)
F8_8	0.1835(2)	0.20318(18)	0.78425(13)	0.0816(15)
F9_8	0.19540(16)	0.19405(15)	0.84360(12)	0.0747(13)
O1_9	0.23763(14)	0.2635(2)	0.91840(18)	0.0333(11)
C1_9	0.27365(14)	0.26945(14)	0.93440(13)	0.0316(10)
C2_9	0.28340(15)	0.23612(16)	0.91800(15)	0.0509(12)

F1_9	0.2849(2)	0.2367(2)	0.88009(13)	0.112(2)
F2_9	0.31967(13)	0.24111(18)	0.92946(16)	0.0853(14)
F3_9	0.2548(2)	0.19795(18)	0.9314(3)	0.121(3)
C3_9	0.27113(16)	0.26579(17)	0.97924(14)	0.0537(13)
F4_9	0.2665(3)	0.2974(3)	0.99393(19)	0.124(2)
F5_9	0.23927(19)	0.23126(19)	0.99016(12)	0.132(3)
F6_9	0.30449(17)	0.26957(18)	0.99576(17)	0.0905(17)
C4_9	0.30877(15)	0.31341(15)	0.92251(16)	0.0529(13)
F7_9	0.30048(15)	0.34227(11)	0.9323(2)	0.125(3)
F8_9	0.34566(14)	0.32453(15)	0.93717(19)	0.094(2)
F9_9	0.31337(17)	0.31434(19)	0.88298(14)	0.112(2)
O1_10	0.1644(2)	0.18553(17)	0.9330(2)	0.0421(8)
C1_10	0.13211(14)	0.14852(15)	0.94464(13)	0.0330(9)
C2_10	0.08926(13)	0.14183(13)	0.93049(14)	0.0416(10)
F1_10	0.08191(14)	0.17007(16)	0.9447(2)	0.127(3)
F2_10	0.05723(16)	0.10603(18)	0.9395(2)	0.094(2)
F3_10	0.08861(19)	0.1450(3)	0.89263(14)	0.112(2)
C3_10	0.13901(15)	0.11346(14)	0.92821(15)	0.0496(12)
F4_10	0.17523(16)	0.11835(18)	0.9394(2)	0.122(2)
F5_10	0.1385(3)	0.11341(17)	0.89032(13)	0.131(3)
F6_10	0.11051(16)	0.07570(12)	0.93795(15)	0.0751(15)
C4_10	0.13136(16)	0.14650(15)	0.98982(14)	0.0505(12)
F7_10	0.16648(14)	0.1507(2)	1.00333(14)	0.121(2)
F8_10	0.10195(19)	0.11109(18)	1.00409(19)	0.0800(15)
F9_10	0.1273(3)	0.1769(2)	1.00447(19)	0.124(3)
O1_11	0.1630(5)	0.2590(4)	0.9479(4)	0.067(3)
C1_11	0.1540(3)	0.2889(3)	0.9578(3)	0.050(2)
C2_11	0.1924(3)	0.3327(3)	0.9502(3)	0.067(2)
F1_11	0.2212(3)	0.3415(2)	0.9768(3)	0.106(3)
F2_11	0.1819(5)	0.3626(4)	0.9480(3)	0.084(3)
F3_11	0.20884(19)	0.33288(16)	0.9153(2)	0.0749(17)
C3_11	0.1171(3)	0.2852(3)	0.9339(3)	0.082(2)
F4_11	0.0866(2)	0.2436(2)	0.9315(3)	0.117(3)
F5_11	0.1279(2)	0.2975(2)	0.89833(19)	0.097(2)
F6_11	0.0984(5)	0.3045(4)	0.9498(6)	0.113(3)
C4_11	0.1420(4)	0.2822(3)	1.0011(3)	0.091(3)
F7_11	0.1050(3)	0.2497(2)	1.0066(3)	0.130(3)
F8_11	0.1426(6)	0.3154(5)	1.0171(6)	0.143(4)
F9_11	0.1717(4)	0.2788(3)	1.0212(2)	0.124(3)
C1_12	0.2115(2)	0.0079(2)	0.88023(17)	0.0375(15)
C2_12	0.2258(3)	-0.0093(4)	0.8512(2)	0.039(2)
C3_12	0.2020(4)	-0.0155(6)	0.8168(2)	0.0377(17)
C4_12	0.1722(3)	-0.0027(4)	0.8252(2)	0.0394(15)
C5_12	0.1779(2)	0.0111(3)	0.86477(18)	0.0341(13)
C6_12	0.1503(3)	0.0230(4)	0.8867(3)	0.090(3)
H6A_12	0.123412	-0.002265	0.892202	0.135
H6B_12	0.145422	0.042319	0.870952	0.135
H6C_12	0.163833	0.036547	0.911147	0.135
C7_12	0.1385(3)	-0.0076(4)	0.7979(3)	0.085(3)
H7A_12	0.147927	-0.006406	0.770996	0.127
H7B_12	0.132412	0.015090	0.802208	0.127
H7C_12	0.113211	-0.034598	0.802484	0.127
C8_12	0.2055(3)	-0.0360(3)	0.7807(2)	0.059(2)
H8A_12	0.191547	-0.030466	0.759140	0.088
H8B_12	0.192172	-0.066319	0.784860	0.088

H8C_12	0.235133	-0.024801	0.774253	0.088
C9_12	0.2572(3)	-0.0230(3)	0.8581(3)	0.067(2)
H9A_12	0.268259	-0.025998	0.833165	0.100
H9B_12	0.243734	-0.049947	0.871767	0.100
H9C_12	0.280219	-0.002027	0.874035	0.100
C10_12	0.2270(3)	0.0180(2)	0.92132(17)	0.072(2)
H10A_12	0.256198	0.024581	0.922415	0.108
H10B_12	0.209798	-0.006232	0.937987	0.108
H10C_12	0.225002	0.042117	0.930419	0.108
C1_13	0.2691(3)	0.1168(2)	0.8324(2)	0.0362(17)
C2_13	0.2944(2)	0.0995(2)	0.8433(2)	0.0394(17)
C3_13	0.2955(2)	0.0757(2)	0.8114(2)	0.0379(17)
C4_13	0.2695(5)	0.0759(5)	0.7815(3)	0.035(2)
C5_13	0.2539(4)	0.1022(4)	0.7940(3)	0.040(2)
C6_13	0.2302(5)	0.1157(5)	0.7680(3)	0.096(4)
H6A_13	0.249985	0.139660	0.752275	0.144
H6B_13	0.213380	0.123907	0.783943	0.144
H6C_13	0.211699	0.092543	0.750896	0.144
C7_13	0.2659(4)	0.0591(3)	0.7412(2)	0.060(3)
H7A_13	0.237788	0.049882	0.730995	0.089
H7B_13	0.270757	0.035284	0.741835	0.089
H7C_13	0.286791	0.081063	0.724388	0.089
C8_13	0.3241(3)	0.0581(3)	0.8082(4)	0.075(3)
H8A_13	0.308791	0.029843	0.797100	0.113
H8B_13	0.334543	0.056790	0.834064	0.113
H8C_13	0.347766	0.076066	0.791277	0.113
C9_13	0.3189(3)	0.1092(3)	0.8802(3)	0.084(3)
H9A_13	0.326259	0.087492	0.885160	0.125
H9B_13	0.301922	0.109951	0.901779	0.125
H9C_13	0.344504	0.136463	0.877889	0.125
C10_13	0.2650(4)	0.1496(3)	0.8538(3)	0.079(3)
H10A_13	0.252298	0.138820	0.879320	0.119
H10B_13	0.247172	0.157338	0.838920	0.119
H10C_13	0.292733	0.174388	0.857300	0.119
C1_14	0.6313(8)	0.3040(9)	0.784(2)	0.029(7)
C2_14	0.6398(9)	0.3460(10)	0.785(2)	0.031(6)
C3_14	0.6839(10)	0.3731(9)	0.786(4)	0.034(6)
C4_14	0.7026(8)	0.3475(10)	0.783(3)	0.037(7)
C5_14	0.6701(9)	0.3053(9)	0.778(2)	0.033(6)
C6_14	0.6753(15)	0.2712(12)	0.7599(16)	0.063(8)
H6A_14	0.670215	0.249868	0.779409	0.094
H6B_14	0.703805	0.283091	0.749702	0.094
H6C_14	0.655157	0.258472	0.738531	0.094
C7_14	0.7485(9)	0.3634(18)	0.779(2)	0.074(11)
H7A_14	0.754228	0.340550	0.783330	0.111
H7B_14	0.764219	0.386045	0.797249	0.111
H7C_14	0.757102	0.374050	0.752078	0.111
C8_14	0.7063(16)	0.4199(9)	0.7860(19)	0.047(9)
H8A_14	0.712174	0.429873	0.759059	0.070
H8B_14	0.732682	0.430877	0.800348	0.070
H8C_14	0.688708	0.429617	0.798296	0.070
C9_14	0.6074(13)	0.3590(16)	0.7848(14)	0.045(7)
H9A_14	0.600805	0.362384	0.757886	0.068
H9B_14	0.618152	0.385686	0.798633	0.068
H9C_14	0.582041	0.337550	0.797732	0.068

C10_14	0.5884(9)	0.2664(12)	0.7819(13)	0.042(8)
H10A_14	0.567465	0.275371	0.782024	0.063
H10B_14	0.583674	0.248053	0.804306	0.063
H10C_14	0.585843	0.251059	0.757857	0.063
C1_15	0.3013(3)	0.0914(4)	0.8223(4)	0.043(3)
C2_15	0.2788(7)	0.0797(9)	0.7868(5)	0.043(3)
C3_15	0.2473(5)	0.0909(6)	0.7890(4)	0.042(4)
C4_15	0.2506(4)	0.1098(4)	0.8256(3)	0.042(3)
C5_15	0.2840(4)	0.1108(4)	0.8461(3)	0.042(3)
C6_15	0.3006(7)	0.1316(8)	0.8845(4)	0.153(13)
H6A_15	0.311141	0.115965	0.899140	0.230
H6B_15	0.278099	0.132075	0.899231	0.230
H6C_15	0.323406	0.160321	0.880268	0.230
C7_15	0.2249(6)	0.1286(5)	0.8397(6)	0.103(8)
H7A_15	0.240725	0.159015	0.836095	0.155
H7B_15	0.218374	0.122110	0.867301	0.155
H7C_15	0.198767	0.116796	0.824743	0.155
C8_15	0.2183(7)	0.0877(8)	0.7569(5)	0.104(5)
H8A_15	0.230658	0.114239	0.742659	0.156
H8B_15	0.191384	0.081677	0.768028	0.156
H8C_15	0.213968	0.065102	0.739165	0.156
C9_15	0.2859(6)	0.0606(6)	0.7514(5)	0.076(5)
H9A_15	0.297984	0.081660	0.730772	0.114
H9B_15	0.259109	0.037127	0.742536	0.114
H9C_15	0.305136	0.050360	0.757662	0.114
C10_15	0.3391(5)	0.0887(9)	0.8308(7)	0.131(10)
H10A_15	0.350786	0.085086	0.806515	0.196
H10B_15	0.331714	0.064718	0.847955	0.196
H10C_15	0.359942	0.114476	0.843739	0.196
O1_16	0.2322(8)	0.2598(13)	0.9229(11)	0.055(7)
C1_16	0.2695(6)	0.2680(5)	0.9354(5)	0.048(4)
C2_16	0.3054(5)	0.2923(6)	0.9062(5)	0.069(4)
F1_16	0.2998(5)	0.3233(7)	0.8926(7)	0.071(4)
F2_16	0.3432(6)	0.3096(8)	0.9224(8)	0.092(6)
F3_16	0.3018(10)	0.2633(9)	0.8814(7)	0.120(6)
C3_16	0.2696(6)	0.2272(5)	0.9474(6)	0.078(5)
F4_16	0.2514(6)	0.2181(6)	0.9823(5)	0.068(4)
F5_16	0.2529(8)	0.2018(8)	0.9169(8)	0.087(5)
F6_16	0.3093(6)	0.2355(9)	0.9494(8)	0.095(5)
C4_16	0.2816(7)	0.2945(7)	0.9732(6)	0.103(5)
F7_16	0.2462(8)	0.2762(10)	0.9937(7)	0.101(5)
F8_16	0.3095(8)	0.2882(9)	0.9922(8)	0.097(5)
F9_16	0.2955(10)	0.3332(6)	0.9610(9)	0.144(10)
O1_17	0.1674(9)	0.2298(8)	0.8716(5)	0.057(7)
C1_17	0.1686(5)	0.2351(5)	0.8329(6)	0.053(4)
C2_17	0.1963(6)	0.2191(6)	0.8147(6)	0.083(5)
F1_17	0.1847(8)	0.1810(6)	0.8271(7)	0.103(5)
F2_17	0.1893(11)	0.2153(10)	0.7763(5)	0.099(6)
F3_17	0.2361(5)	0.2454(8)	0.8222(7)	0.100(6)
C3_17	0.1899(6)	0.2822(5)	0.8220(6)	0.083(5)
F4_17	0.1634(8)	0.2959(8)	0.8273(8)	0.122(5)
F5_17	0.2248(7)	0.3023(6)	0.8436(8)	0.087(6)
F6_17	0.2018(12)	0.2890(12)	0.7849(7)	0.093(5)
C4_17	0.1242(5)	0.2105(6)	0.8157(6)	0.066(5)
F7_17	0.0992(10)	0.2178(14)	0.8381(14)	0.093(6)

F8_17	0.1217(14)	0.2190(11)	0.7789(8)	0.101(6)
F9_17	0.1110(7)	0.1696(5)	0.8172(7)	0.092(5)
C1_18	0.1957(6)	-0.0008(6)	0.8784(4)	0.040(4)
C2_18	0.1727(8)	0.0087(10)	0.8513(5)	0.047(4)
C3_18	0.1791(8)	-0.0031(10)	0.8139(5)	0.039(4)
C4_18	0.2092(15)	-0.0159(18)	0.8170(6)	0.036(4)
C5_18	0.2186(10)	-0.0158(12)	0.8573(5)	0.039(5)
C6_18	0.2439(8)	-0.0345(9)	0.8720(9)	0.072(5)
H6A_18	0.246644	-0.031397	0.900309	0.108
H6B_18	0.271722	-0.020075	0.860037	0.108
H6C_18	0.229795	-0.064315	0.865220	0.108
C7_18	0.2221(9)	-0.0359(10)	0.7863(8)	0.066(6)
H7A_18	0.252312	-0.025068	0.788000	0.100
H7B_18	0.215271	-0.029355	0.760620	0.100
H7C_18	0.207099	-0.066292	0.790071	0.100
C8_18	0.1542(11)	-0.0059(12)	0.7785(8)	0.093(6)
H8A_18	0.141921	0.012149	0.781853	0.139
H8B_18	0.131762	-0.034916	0.774798	0.139
H8C_18	0.172536	0.003300	0.755652	0.139
C9_18	0.1405(9)	0.0206(12)	0.8617(10)	0.097(5)
H9A_18	0.112484	-0.003994	0.859482	0.145
H9B_18	0.142930	0.042502	0.843929	0.145
H9C_18	0.145144	0.031135	0.888457	0.145
C10_18	0.1910(8)	-0.0027(7)	0.9218(4)	0.090(9)
H10A_18	0.163712	-0.026486	0.928948	0.136
H10B_18	0.192912	0.023322	0.931225	0.136
H10C_18	0.213317	-0.006053	0.933618	0.136
O1_19	0.4544(6)	0.3252(5)	0.7363(5)	0.086(6)
C1_19	0.4851(5)	0.3575(5)	0.7172(4)	0.060(4)
C2_19	0.5053(5)	0.3474(6)	0.6832(5)	0.087(5)
F1_19	0.4738(7)	0.3193(7)	0.6615(6)	0.123(7)
F2_19	0.5291(8)	0.3817(7)	0.6614(7)	0.162(11)
F3_19	0.5288(7)	0.3327(7)	0.6974(8)	0.124(5)
C3_19	0.5183(5)	0.3817(6)	0.7493(5)	0.102(5)
F4_19	0.5025(6)	0.4002(6)	0.7710(6)	0.129(7)
F5_19	0.5243(7)	0.3520(6)	0.7654(7)	0.108(5)
F6_19	0.5546(5)	0.4086(6)	0.7337(7)	0.105(5)
C4_19	0.4694(6)	0.3869(5)	0.7029(5)	0.096(5)
F7_19	0.4426(7)	0.3822(7)	0.7312(7)	0.112(5)
F8_19	0.5013(6)	0.4262(5)	0.7030(7)	0.101(5)
F9_19	0.4522(8)	0.3739(6)	0.6684(6)	0.133(8)
O1_20	0.1645(12)	0.1872(9)	0.9295(14)	0.0421(8)
C1_20	0.1342(7)	0.1496(7)	0.9417(6)	0.044(4)
C2_20	0.1152(8)	0.1530(8)	0.9806(6)	0.073(5)
F1_20	0.0889(9)	0.1666(10)	0.9722(11)	0.128(5)
F2_20	0.0949(13)	0.1170(10)	0.9995(11)	0.087(6)
F3_20	0.1452(12)	0.1808(12)	1.0034(9)	0.110(7)
C3_20	0.1512(7)	0.1193(7)	0.9472(8)	0.101(4)
F4_20	0.1734(11)	0.1216(11)	0.9162(10)	0.119(6)
F5_20	0.1744(8)	0.1316(7)	0.9792(9)	0.126(9)
F6_20	0.1209(9)	0.0801(7)	0.9523(10)	0.081(5)
C4_20	0.0979(6)	0.1304(7)	0.9115(6)	0.068(5)
F7_20	0.1111(8)	0.1181(8)	0.8812(7)	0.127(11)
F8_20	0.0638(9)	0.1002(10)	0.9281(11)	0.087(7)
F9_20	0.0892(10)	0.1604(10)	0.9035(10)	0.089(5)

O1_21	0.6753(9)	0.3747(8)	0.6219(8)	0.044(5)
C1_21	0.6668(5)	0.4045(6)	0.6328(6)	0.059(4)
C2_21	0.7065(6)	0.4480(5)	0.6315(7)	0.078(5)
F1_21	0.7229(8)	0.4549(9)	0.5955(7)	0.091(5)
F2_21	0.6966(9)	0.4772(6)	0.6400(9)	0.089(5)
F3_21	0.7349(8)	0.4498(8)	0.6561(8)	0.102(5)
C3_21	0.6491(8)	0.3931(8)	0.6750(6)	0.097(5)
F4_21	0.6098(8)	0.3624(9)	0.6712(10)	0.133(9)
F5_21	0.6716(13)	0.3793(14)	0.6932(10)	0.114(5)
F6_21	0.6507(15)	0.4242(11)	0.6950(10)	0.112(6)
C4_21	0.6320(7)	0.4053(7)	0.6087(7)	0.080(5)
F7_21	0.6008(7)	0.3664(7)	0.6029(10)	0.092(5)
F8_21	0.6154(13)	0.4245(13)	0.6289(12)	0.105(6)
F9_21	0.6477(11)	0.4251(11)	0.5754(8)	0.139(10)
O1_22	0.4125(14)	0.2330(12)	0.7419(12)	0.0507(11)
C1_22	0.4177(6)	0.2024(8)	0.7264(6)	0.045(4)
C2_22	0.4015(7)	0.1921(8)	0.6842(6)	0.076(5)
F1_22	0.4157(11)	0.2289(9)	0.6664(8)	0.090(6)
F2_22	0.4146(10)	0.1685(11)	0.6670(11)	0.087(6)
F3_22	0.3599(7)	0.1715(10)	0.6832(10)	0.107(9)
C3_22	0.3942(8)	0.1621(8)	0.7509(7)	0.075(6)
F4_22	0.4137(11)	0.1686(11)	0.7846(7)	0.117(10)
F5_22	0.3552(8)	0.1533(12)	0.7568(11)	0.086(6)
F6_22	0.3930(19)	0.1293(12)	0.7339(15)	0.086(5)
C4_22	0.4650(6)	0.2165(7)	0.7269(7)	0.064(5)
F7_22	0.4798(8)	0.2352(9)	0.7610(8)	0.074(5)
F8_22	0.4709(15)	0.1840(11)	0.7236(15)	0.078(5)
F9_22	0.4845(9)	0.2433(9)	0.6985(9)	0.108(9)
C1_23	0.6902(8)	0.3743(8)	0.788(3)	0.032(5)
C2_23	0.6457(8)	0.3532(9)	0.788(2)	0.033(6)
C3_23	0.6298(8)	0.3103(9)	0.779(2)	0.031(7)
C4_23	0.6647(9)	0.3043(8)	0.775(2)	0.035(6)
C5_23	0.7018(8)	0.3439(10)	0.7786(19)	0.035(6)
C6_23	0.7455(9)	0.3520(18)	0.773(2)	0.076(10)
H6A_23	0.754321	0.361000	0.746082	0.114
H6B_23	0.746229	0.326272	0.778128	0.114
H6C_23	0.764409	0.374024	0.790858	0.114
C7_23	0.6632(15)	0.2635(9)	0.7692(15)	0.065(8)
H7A_23	0.668539	0.260584	0.741762	0.097
H7B_23	0.635411	0.240540	0.776481	0.097
H7C_23	0.684507	0.262501	0.785393	0.097
C8_23	0.5844(8)	0.2776(11)	0.7754(13)	0.043(7)
H8A_23	0.567066	0.288034	0.786926	0.064
H8B_23	0.579244	0.252066	0.788935	0.064
H8C_23	0.577405	0.271432	0.747828	0.064
C9_23	0.6196(12)	0.3738(14)	0.7916(12)	0.043(7)
H9A_23	0.631056	0.395282	0.811939	0.065
H9B_23	0.590732	0.352769	0.798187	0.065
H9C_23	0.619906	0.386881	0.766668	0.065
C10_23	0.7195(13)	0.4206(8)	0.7895(16)	0.049(9)
H10A_23	0.704150	0.434578	0.797983	0.074
H10B_23	0.731431	0.430847	0.763676	0.074
H10C_23	0.742045	0.426711	0.808018	0.074
O1_24	0.4436(8)	0.2921(7)	0.7977(6)	0.047(7)
C1_24	0.4415(5)	0.2880(5)	0.8366(6)	0.056(4)

C2_24	0.4302(6)	0.2446(5)	0.8531(6)	0.077(5)
F1_24	0.3983(6)	0.2152(5)	0.8326(6)	0.072(4)
F2_24	0.4174(8)	0.2412(9)	0.8901(6)	0.099(6)
F3_24	0.4649(8)	0.2416(10)	0.8517(7)	0.115(9)
C3_24	0.4874(5)	0.3194(6)	0.8484(6)	0.081(5)
F4_24	0.4945(10)	0.3570(6)	0.8382(10)	0.147(11)
F5_24	0.5121(6)	0.3117(9)	0.8258(7)	0.109(8)
F6_24	0.4949(9)	0.3134(9)	0.8845(6)	0.103(6)
C4_24	0.4085(6)	0.2979(6)	0.8531(6)	0.089(4)
F7_24	0.4089(7)	0.3280(6)	0.8312(5)	0.067(5)
F8_24	0.4167(9)	0.3120(10)	0.8895(6)	0.086(5)
F9_24	0.3719(5)	0.2607(7)	0.8501(6)	0.096(6)
O1_25	0.6785(15)	0.3450(16)	0.5455(7)	0.043(9)
C1_25	0.6711(8)	0.3389(8)	0.5071(7)	0.042(4)
C2_25	0.6775(8)	0.3028(7)	0.4925(8)	0.063(6)
F1_25	0.7192(8)	0.3179(11)	0.4944(11)	0.073(6)
F2_25	0.6655(13)	0.2936(14)	0.4556(9)	0.091(10)
F3_25	0.6573(13)	0.2688(9)	0.5141(12)	0.114(11)
C3_25	0.6280(8)	0.3331(9)	0.4966(9)	0.049(5)
F4_25	0.6290(15)	0.3695(12)	0.5011(19)	0.076(7)
F5_25	0.5992(12)	0.3060(17)	0.5213(16)	0.072(7)
F6_25	0.6149(17)	0.3194(19)	0.4607(11)	0.076(9)
C4_25	0.7053(9)	0.3780(8)	0.4849(9)	0.059(6)
F7_25	0.7089(16)	0.4123(10)	0.5006(16)	0.080(7)
F8_25	0.6959(16)	0.3758(16)	0.4475(8)	0.090(9)
F9_25	0.7409(10)	0.3777(15)	0.4890(16)	0.087(7)
O1_26	0.1653(6)	0.2593(5)	0.9530(4)	0.030(3)
C1_26	0.1583(4)	0.2905(4)	0.9630(4)	0.050(3)
C2_26	0.1133(4)	0.2784(4)	0.9511(4)	0.083(3)
F1_26	0.1049(4)	0.2618(5)	0.9155(3)	0.091(3)
F2_26	0.1081(9)	0.3114(7)	0.9528(10)	0.114(5)
F3_26	0.0864(3)	0.2484(3)	0.9759(4)	0.096(3)
C3_26	0.1622(4)	0.2976(4)	1.0078(4)	0.064(3)
F4_26	0.2032(3)	0.3160(4)	1.0172(3)	0.113(4)
F5_26	0.1431(4)	0.2608(3)	1.0257(3)	0.081(3)
F6_26	0.1474(9)	0.3217(7)	1.0196(9)	0.122(4)
C4_26	0.1890(4)	0.3329(5)	0.9441(4)	0.077(4)
F7_26	0.2280(3)	0.3401(3)	0.9473(5)	0.106(5)
F8_26	0.1894(8)	0.3648(6)	0.9630(5)	0.098(5)
F9_26	0.1785(6)	0.3324(4)	0.9068(3)	0.141(6)
O1_27	0.3797(4)	0.2877(5)	0.7537(6)	0.041(3)
C1_27	0.3408(4)	0.2758(3)	0.7409(3)	0.052(3)
C2_27	0.3416(5)	0.2798(4)	0.6963(4)	0.078(3)
F1_27	0.3622(4)	0.3211(3)	0.6875(3)	0.117(3)
F2_27	0.3034(6)	0.2606(8)	0.6815(8)	0.101(3)
F3_27	0.3621(3)	0.2623(4)	0.6809(2)	0.079(3)
C3_27	0.3076(4)	0.2309(4)	0.7514(4)	0.081(3)
F4_27	0.3120(4)	0.2235(3)	0.7885(3)	0.129(5)
F5_27	0.3111(3)	0.2035(3)	0.7278(4)	0.111(4)
F6_27	0.2680(5)	0.2236(8)	0.7502(7)	0.117(4)
C4_27	0.3300(4)	0.3078(4)	0.7594(4)	0.080(3)
F7_27	0.3197(4)	0.2964(4)	0.7970(3)	0.112(4)
F8_27	0.2995(4)	0.3094(6)	0.7401(5)	0.092(4)
F9_27	0.3625(3)	0.3466(3)	0.7575(4)	0.096(3)

*Table S 12 Table S 13 Atomic coordinates and U_{eq} [Å^2] for **7 layer.***

Atom	*x*	*y*	*z*	U_{eq}
Fe1	1.22085(7)	0.34162(6)	0.53791(4)	0.0332(3)
Fe2	0.29226(8)	0.83149(7)	0.71120(6)	0.0507(5)
Fe3	0.78346(6)	0.64672(5)	0.37684(4)	0.0259(3)
O1	1.3326(4)	0.2809(4)	0.5434(2)	0.050(2)
C1	1.2873(5)	0.3034(5)	0.5409(3)	0.047(3)
O2	0.2255(8)	0.7716(6)	0.7633(5)	0.113(6)
C2	0.2505(10)	0.7962(6)	0.7423(5)	0.084(6)
O3	0.6860(5)	0.7036(4)	0.3461(3)	0.068(3)
C3	0.7242(5)	0.6816(4)	0.3586(4)	0.045(3)
Al1	0.47182(12)	0.66205(10)	0.51762(7)	0.0215(5)
Al2	1.15297(12)	0.55398(10)	0.37171(8)	0.0266(6)
Al3	1.02291(13)	0.16169(10)	0.38797(7)	0.0236(6)
Al4	0.84771(12)	0.44424(11)	0.54212(7)	0.0252(6)
Al5	0.16403(11)	0.53711(10)	0.70696(8)	0.0271(5)
Al6	1.42978(13)	0.64450(10)	0.20403(8)	0.0301(6)
O1_1	1.0110(3)	0.1362(3)	0.42815(18)	0.0323(15)
C1_1	0.9843(4)	0.1393(3)	0.4600(2)	0.033(2)
C2_1	0.9727(4)	0.1946(4)	0.4707(2)	0.036(2)
F1_1	0.9251(3)	0.2133(2)	0.45465(18)	0.0425(15)
F2_1	0.9637(4)	0.1986(3)	0.50456(17)	0.0505(17)
F3_1	1.0188(3)	0.2232(3)	0.46198(19)	0.0464(16)
C3_1	1.0253(4)	0.1134(4)	0.4863(2)	0.038(2)
F4_1	1.0475(3)	0.0710(3)	0.47447(19)	0.0506(17)
F5_1	1.0698(3)	0.1436(3)	0.49452(19)	0.0535(18)
F6_1	0.9969(4)	0.1034(3)	0.51619(18)	0.057(2)
C4_1	0.9242(4)	0.1106(3)	0.4581(3)	0.035(2)
F7_1	0.9323(3)	0.0611(2)	0.4580(2)	0.0491(17)
F8_1	0.8897(3)	0.1208(3)	0.48555(18)	0.0481(17)
F9_1	0.8940(3)	0.1237(3)	0.43023(17)	0.0434(15)
O1_2	1.0472(3)	0.1143(2)	0.36079(19)	0.0302(14)
C1_2	1.0399(4)	0.0669(3)	0.3503(2)	0.033(2)
C2_2	1.0874(4)	0.0559(4)	0.3219(3)	0.041(2)
F1_2	1.1398(3)	0.0476(3)	0.3368(2)	0.0523(18)
F2_2	1.0739(4)	0.0155(3)	0.3024(2)	0.059(2)
F3_2	1.0934(3)	0.0947(3)	0.30064(18)	0.0466(16)
C3_2	0.9773(4)	0.0596(4)	0.3343(3)	0.043(2)
F4_2	0.9359(3)	0.0819(3)	0.3539(2)	0.0552(19)
F5_2	0.9751(4)	0.0809(4)	0.3030(2)	0.066(2)
F6_2	0.9622(4)	0.0117(3)	0.3301(3)	0.066(2)
C4_2	1.0477(5)	0.0288(3)	0.3802(3)	0.040(2)
F7_2	0.9985(3)	0.0264(3)	0.39971(19)	0.0519(18)
F8_2	1.0581(4)	-0.0181(2)	0.3681(2)	0.061(2)
F9_2	1.0935(3)	0.0426(3)	0.3998(2)	0.0546(18)
O1_3	0.9591(3)	0.1909(3)	0.3748(2)	0.0380(16)
C1_3	0.9341(4)	0.2292(4)	0.3567(2)	0.041(2)
C2_3	0.9566(5)	0.2811(4)	0.3683(2)	0.049(3)
F1_3	1.0091(4)	0.2924(3)	0.3544(2)	0.064(2)
F2_3	0.9198(5)	0.3189(3)	0.3600(2)	0.078(3)
F3_3	0.9623(5)	0.2816(3)	0.40244(18)	0.065(2)
C3_3	0.8661(5)	0.2260(5)	0.3620(3)	0.061(3)
F4_3	0.8474(4)	0.1783(4)	0.3601(3)	0.078(3)
F5_3	0.8503(4)	0.2426(4)	0.3931(2)	0.076(3)
F6_3	0.8370(4)	0.2522(4)	0.3382(2)	0.082(3)

C4_3	0.9480(5)	0.2237(5)	0.3174(3)	0.051(3)
F7_3	0.9175(4)	0.1855(4)	0.3031(2)	0.072(2)
F8_3	0.9353(4)	0.2642(4)	0.2993(2)	0.078(3)
F9_3	1.0050(3)	0.2110(3)	0.31297(18)	0.0549(19)
O1_4	1.0788(3)	0.2061(2)	0.38806(18)	0.0289(14)
C1_4	1.1384(4)	0.2142(3)	0.3886(2)	0.037(2)
C2_4	1.1675(5)	0.1900(4)	0.4204(3)	0.041(2)
F1_4	1.1472(3)	0.1445(3)	0.4261(2)	0.0514(17)
F2_4	1.2264(3)	0.1875(3)	0.4183(2)	0.059(2)
F3_4	1.1543(3)	0.2167(3)	0.44950(18)	0.0522(17)
C3_4	1.1497(5)	0.2714(4)	0.3889(3)	0.045(2)
F4_4	1.1372(4)	0.2916(3)	0.3574(2)	0.0556(19)
F5_4	1.1135(4)	0.2931(3)	0.4121(2)	0.060(2)
F6_4	1.2064(4)	0.2841(3)	0.3968(2)	0.063(2)
C4_4	1.1680(5)	0.1907(4)	0.3560(3)	0.045(2)
F7_4	1.1335(3)	0.1980(3)	0.32823(17)	0.0532(19)
F8_4	1.2194(4)	0.2128(4)	0.3481(3)	0.074(3)
F9_4	1.1767(3)	0.1420(3)	0.3595(2)	0.0542(18)
C1_5	1.2056(4)	0.3468(4)	0.4831(3)	0.033(2)
C2_5	1.1494(4)	0.3486(4)	0.4996(3)	0.041(3)
C3_5	1.1413(4)	0.3042(4)	0.5195(2)	0.031(2)
C4_5	1.1911(4)	0.2735(4)	0.5145(3)	0.035(2)
C5_5	1.2307(4)	0.2995(3)	0.4905(2)	0.0261(18)
C6_5	1.2839(6)	0.2784(5)	0.4729(4)	0.058(4)
H6A_5	1.274915	0.272740	0.448468	0.087
H6B_5	1.294723	0.246504	0.483725	0.087
H6C_5	1.316897	0.301952	0.474912	0.087
C7_5	1.1984(6)	0.2206(4)	0.5270(3)	0.048(3)
H7A_5	1.177586	0.197712	0.511408	0.073
H7B_5	1.181850	0.217511	0.550275	0.073
H7C_5	1.240545	0.211979	0.527519	0.073
C8_5	1.0854(5)	0.2887(6)	0.5376(3)	0.050(3)
H8A_5	1.065316	0.318507	0.546594	0.074
H8B_5	1.095086	0.266151	0.556678	0.074
H8C_5	1.059346	0.271493	0.521248	0.074
C9_5	1.1018(6)	0.3874(7)	0.4912(4)	0.068(5)
H9A_5	1.120480	0.419860	0.486847	0.103
H9B_5	1.074553	0.390354	0.510790	0.103
H9C_5	1.079820	0.376759	0.470719	0.103
C10_5	1.2297(5)	0.3844(5)	0.4580(3)	0.044(3)
H10A_5	1.216657	0.375822	0.434670	0.065
H10B_5	1.273007	0.384091	0.458992	0.065
H10C_5	1.215155	0.417827	0.464085	0.065
C1_6	1.2378(4)	0.4164(4)	0.5536(3)	0.042(2)
C2_6	1.1801(5)	0.4031(4)	0.5671(3)	0.043(2)
C3_6	1.1899(5)	0.3613(5)	0.5893(3)	0.048(3)
C4_6	1.2515(5)	0.3509(4)	0.5911(3)	0.044(2)
C5_6	1.2803(4)	0.3858(4)	0.5687(3)	0.039(2)
C6_6	1.3468(5)	0.3948(5)	0.5670(3)	0.045(3)
H6A_6	1.367808	0.363442	0.571685	0.068
H6B_6	1.358013	0.419873	0.584334	0.068
H6C_6	1.357457	0.407041	0.544028	0.068
C7_6	1.2789(8)	0.3145(5)	0.6165(3)	0.063(4)
H7A_6	1.256175	0.283216	0.616481	0.095
H7B_6	1.278289	0.329130	0.639653	0.095

H7C_6	1.319841	0.307525	0.609739	0.095
C8_6	1.1410(9)	0.3357(7)	0.6102(4)	0.084(6)
H8A_6	1.102592	0.350018	0.603967	0.125
H8B_6	1.148243	0.340949	0.634883	0.125
H8C_6	1.140988	0.299709	0.605246	0.125
C9_6	1.1279(6)	0.4370(6)	0.5642(5)	0.076(5)
H9A_6	1.128615	0.453894	0.541759	0.114
H9B_6	1.129265	0.462036	0.582639	0.114
H9C_6	1.091478	0.417307	0.566241	0.114
C10_6	1.2504(7)	0.4623(5)	0.5307(4)	0.062(4)
H10A_6	1.281655	0.454095	0.514123	0.093
H10B_6	1.263319	0.490331	0.545202	0.093
H10C_6	1.214370	0.471723	0.518284	0.093
O1_7	0.8879(4)	0.4933(3)	0.5572(2)	0.050(2)
C1_7	0.9285(4)	0.5302(3)	0.5518(2)	0.035(2)
C2_7	0.9197(5)	0.5551(4)	0.5159(3)	0.051(3)
F1_7	0.8626(4)	0.5576(5)	0.5088(3)	0.105(5)
F2_7	0.9444(5)	0.5998(3)	0.5134(2)	0.073(3)
F3_7	0.9429(6)	0.5263(4)	0.4912(2)	0.084(3)
C3_7	0.9924(5)	0.5111(5)	0.5537(3)	0.051(3)
F4_7	1.0080(5)	0.4994(4)	0.5860(2)	0.083(3)
F5_7	1.0000(5)	0.4703(4)	0.5335(3)	0.087(3)
F6_7	1.0324(3)	0.5448(4)	0.5440(3)	0.089(3)
C4_7	0.9183(5)	0.5695(4)	0.5807(3)	0.043(2)
F7_7	0.9197(5)	0.5479(3)	0.6109(2)	0.075(3)
F8_7	0.9602(4)	0.6050(3)	0.5822(2)	0.061(2)
F9_7	0.8674(4)	0.5933(4)	0.5750(3)	0.085(3)
C1_8	0.7330(4)	0.5939(4)	0.3457(2)	0.035(2)
C2_8	0.7551(4)	0.5689(3)	0.3747(2)	0.0331(19)
C3_8	0.8177(4)	0.5697(4)	0.3733(3)	0.039(2)
C4_8	0.8351(4)	0.5982(4)	0.3440(3)	0.040(2)
C5_8	0.7828(4)	0.6142(4)	0.3264(2)	0.035(2)
C6_8	0.7803(7)	0.6397(4)	0.2926(3)	0.048(3)
H6A_8	0.784351	0.614954	0.274128	0.071
H6B_8	0.812678	0.664076	0.291035	0.071
H6C_8	0.742372	0.657127	0.290273	0.071
C7_8	0.8982(5)	0.6042(5)	0.3312(3)	0.043(3)
H7A_8	0.914755	0.571259	0.325784	0.065
H7B_8	0.922091	0.620233	0.349172	0.065
H7C_8	0.898384	0.625128	0.310437	0.065
C8_8	0.8571(6)	0.5359(5)	0.3948(4)	0.052(3)
H8A_8	0.856244	0.501901	0.385238	0.079
H8B_8	0.842804	0.535282	0.418600	0.079
H8C_8	0.897779	0.548617	0.394275	0.079
C9_8	0.7175(7)	0.5396(5)	0.4002(3)	0.053(3)
H9A_8	0.689717	0.518210	0.387571	0.080
H9B_8	0.695357	0.563019	0.414769	0.080
H9C_8	0.743132	0.518799	0.414651	0.080
C10_8	0.6710(5)	0.5909(5)	0.3329(4)	0.048(3)
H10A_8	0.664275	0.617253	0.315778	0.072
H10B_8	0.643558	0.595373	0.352246	0.072
H10C_8	0.664270	0.558083	0.322286	0.072
C1_9	0.7980(4)	0.7227(3)	0.3938(2)	0.0292(19)
C2_9	0.7605(4)	0.6965(4)	0.4184(3)	0.032(2)
C3_9	0.7950(4)	0.6559(4)	0.4317(2)	0.0303(19)

C4_9	0.8523(4)	0.6579(4)	0.4158(3)	0.039(2)
C5_9	0.8530(4)	0.6975(4)	0.3913(3)	0.036(2)
C6_9	0.9046(5)	0.7166(5)	0.3699(3)	0.047(3)
H6A_9	0.891306	0.722483	0.346133	0.071
H6B_9	0.936371	0.691707	0.369875	0.071
H6C_9	0.919220	0.748059	0.379717	0.071
C7_9	0.9070(5)	0.6321(5)	0.4297(3)	0.050(3)
H7A_9	0.930103	0.618474	0.410438	0.075
H7B_9	0.895197	0.604740	0.445070	0.075
H7C_9	0.931084	0.656253	0.442463	0.075
C8_9	0.7736(7)	0.6216(5)	0.4604(3)	0.050(3)
H8A_9	0.730869	0.616497	0.458217	0.075
H8B_9	0.782385	0.636881	0.482795	0.075
H8C_9	0.793906	0.589231	0.458694	0.075
C9_9	0.7035(5)	0.7150(4)	0.4331(3)	0.042(3)
H9A_9	0.681676	0.733541	0.415401	0.062
H9B_9	0.711592	0.737132	0.452719	0.062
H9C_9	0.679723	0.686454	0.440896	0.062
C10_9	0.7865(6)	0.7736(4)	0.3780(4)	0.045(3)
H10A_9	0.804481	0.775094	0.355018	0.068
H10B_9	0.803870	0.799635	0.392662	0.068
H10C_9	0.743776	0.779061	0.376074	0.068
O1_11	1.4697(6)	0.6543(6)	0.2419(4)	0.042(4)
C1_11	1.5187(6)	0.6457(5)	0.2608(3)	0.057(3)
C2_11	1.5437(6)	0.5919(6)	0.2544(4)	0.061(4)
F1_11	1.5097(6)	0.5589(6)	0.2706(5)	0.105(5)
F2_11	1.5988(4)	0.5853(5)	0.2636(3)	0.064(3)
F3_11	1.5382(6)	0.5802(6)	0.2211(3)	0.077(4)
C3_11	1.5661(7)	0.6842(6)	0.2506(5)	0.080(5)
F4_11	1.5423(6)	0.7302(5)	0.2481(6)	0.118(6)
F5_11	1.5881(6)	0.6749(7)	0.2202(4)	0.097(5)
F6_11	1.6125(6)	0.6840(5)	0.2714(4)	0.091(4)
C4_11	1.5049(8)	0.6544(8)	0.2994(4)	0.095(6)
F7_11	1.5025(9)	0.7029(8)	0.3066(5)	0.148(8)
F8_11	1.5472(6)	0.6327(9)	0.3186(3)	0.128(8)
F9_11	1.4534(6)	0.6319(9)	0.3080(3)	0.130(7)
O1_12	1.3647(3)	0.6787(3)	0.2077(2)	0.0380(15)
C1_12	1.3394(5)	0.7202(4)	0.2221(3)	0.046(2)
C2_12	1.2770(5)	0.7258(5)	0.2066(4)	0.061(3)
F1_12	1.2801(4)	0.7214(4)	0.1726(2)	0.079(3)
F2_12	1.2546(5)	0.7727(4)	0.2127(3)	0.091(3)
F3_12	1.2397(4)	0.6917(4)	0.2187(4)	0.095(4)
C3_12	1.3345(5)	0.7150(4)	0.2624(3)	0.054(3)
F4_12	1.3848(5)	0.7293(4)	0.2781(2)	0.086(3)
F5_12	1.3224(5)	0.6691(3)	0.2712(2)	0.080(3)
F6_12	1.2930(5)	0.7441(3)	0.2763(3)	0.081(3)
C4_12	1.3760(6)	0.7686(4)	0.2151(3)	0.064(3)
F7_12	1.4356(4)	0.7605(4)	0.2186(3)	0.081(3)
F8_12	1.3586(6)	0.8075(4)	0.2341(3)	0.089(3)
F9_12	1.3717(6)	0.7822(4)	0.1818(2)	0.091(3)
O1_14	0.4462(3)	0.6131(2)	0.54308(18)	0.0264(14)
C1_14	0.4481(4)	0.5632(3)	0.5495(3)	0.041(2)
C2_14	0.5117(6)	0.5482(5)	0.5593(5)	0.095(5)
F1_14	0.5515(4)	0.5706(4)	0.5392(4)	0.112(5)
F2_14	0.5218(6)	0.4988(4)	0.5574(5)	0.146(7)

F3_14	0.5254(5)	0.5638(5)	0.5908(4)	0.123(5)
C3_14	0.4069(5)	0.5509(4)	0.5799(3)	0.045(2)
F4_14	0.3501(3)	0.5496(3)	0.5699(2)	0.0527(18)
F5_14	0.4085(5)	0.5865(3)	0.60452(18)	0.065(2)
F6_14	0.4169(4)	0.5067(3)	0.5936(2)	0.064(2)
C4_14	0.4279(6)	0.5335(4)	0.5170(3)	0.062(3)
F7_14	0.3814(5)	0.5548(4)	0.5017(2)	0.075(3)
F8_14	0.4124(5)	0.4860(3)	0.5255(3)	0.086(4)
F9_14	0.4726(6)	0.5295(3)	0.4951(3)	0.104(5)
O1_15	0.8706(11)	0.4242(8)	0.5033(4)	0.042(5)
C1_15	0.8873(5)	0.3900(5)	0.4793(3)	0.028(3)
C2_15	0.9276(8)	0.4130(7)	0.4512(5)	0.035(3)
F1_15	0.9044(6)	0.4566(5)	0.4396(5)	0.040(3)
F2_15	0.9337(10)	0.3829(10)	0.4243(6)	0.047(4)
F3_15	0.9812(8)	0.4224(11)	0.4632(5)	0.041(4)
C3_15	0.9202(6)	0.3461(5)	0.4971(4)	0.037(3)
F4_15	0.8855(5)	0.3149(3)	0.5126(3)	0.044(2)
F5_15	0.9592(4)	0.3636(4)	0.5202(3)	0.046(2)
F6_15	0.9539(5)	0.3203(4)	0.4747(3)	0.054(3)
C4_15	0.8308(6)	0.3680(5)	0.4621(4)	0.043(3)
F7_15	0.7894(4)	0.3570(5)	0.4854(3)	0.052(3)
F8_15	0.8427(5)	0.3246(4)	0.4448(3)	0.047(3)
F9_15	0.8057(5)	0.4007(5)	0.4398(3)	0.052(3)
O1_16	1.2252(3)	0.5358(4)	0.3800(3)	0.061(3)
C1_16	1.2805(4)	0.5247(3)	0.3704(2)	0.032(2)
C2_16	1.2800(5)	0.4840(4)	0.3421(3)	0.047(3)
F1_16	1.2385(3)	0.4938(4)	0.3182(2)	0.076(3)
F2_16	1.3314(3)	0.4780(4)	0.3268(2)	0.067(2)
F3_16	1.2639(6)	0.4386(4)	0.3546(3)	0.093(3)
C3_16	1.3149(5)	0.5042(5)	0.4022(3)	0.052(3)
F4_16	1.3247(4)	0.5410(4)	0.4244(2)	0.075(3)
F5_16	1.2835(4)	0.4686(4)	0.4183(3)	0.079(3)
F6_16	1.3668(4)	0.4844(4)	0.3935(3)	0.075(3)
C4_16	1.3126(5)	0.5714(4)	0.3555(3)	0.050(3)
F7_16	1.3005(6)	0.6108(3)	0.3755(3)	0.100(4)
F8_16	1.3717(3)	0.5657(3)	0.3559(2)	0.062(2)
F9_16	1.2943(5)	0.5825(4)	0.3238(2)	0.083(3)
O1_17	1.1364(14)	0.6003(9)	0.3431(6)	0.062(7)
C1_17	1.1260(8)	0.6236(7)	0.3123(5)	0.040(4)
C2_17	1.1501(9)	0.6779(7)	0.3125(5)	0.045(4)
F1_17	1.1240(10)	0.7045(6)	0.3367(5)	0.067(4)
F2_17	1.141(2)	0.7027(15)	0.2827(8)	0.070(5)
F3_17	1.2081(11)	0.6796(17)	0.3182(10)	0.071(6)
C3_17	1.1450(7)	0.5948(7)	0.2801(4)	0.040(4)
F4_17	1.1345(16)	0.5458(7)	0.2827(11)	0.069(5)
F5_17	1.2019(6)	0.6021(9)	0.2730(5)	0.069(5)
F6_17	1.1194(9)	0.6100(7)	0.2509(4)	0.061(4)
C4_17	1.0575(8)	0.6261(8)	0.3132(6)	0.064(5)
F7_17	1.0341(11)	0.5818(9)	0.3045(9)	0.063(6)
F8_17	1.0371(9)	0.6594(7)	0.2908(7)	0.083(5)
F9_17	1.0411(14)	0.6337(13)	0.3461(6)	0.084(6)
O1_18	0.8494(6)	0.3949(5)	0.5708(3)	0.045(3)
C1_18	0.8616(5)	0.3753(4)	0.6022(3)	0.034(2)
C2_18	0.8165(6)	0.3339(5)	0.6091(3)	0.046(3)
F1_18	0.8076(6)	0.3061(4)	0.5806(3)	0.070(3)

F2_18	0.8343(7)	0.3030(5)	0.6347(4)	0.076(4)
F3_18	0.7642(5)	0.3533(5)	0.6186(4)	0.095(4)
C3_18	0.8557(5)	0.4158(4)	0.6304(3)	0.039(3)
F4_18	0.9039(4)	0.4457(3)	0.6312(2)	0.060(3)
F5_18	0.8113(5)	0.4456(4)	0.6230(3)	0.060(2)
F6_18	0.8504(7)	0.3989(4)	0.6622(2)	0.081(4)
C4_18	0.9256(6)	0.3538(6)	0.6037(4)	0.073(4)
F7_18	0.9654(5)	0.3842(5)	0.5912(5)	0.108(5)
F8_18	0.9425(7)	0.3428(6)	0.6356(4)	0.111(5)
F9_18	0.9275(7)	0.3113(4)	0.5854(4)	0.093(4)
C1_19	0.3362(6)	0.7604(4)	0.7159(3)	0.053(3)
C2_19	0.3648(7)	0.7969(5)	0.7370(3)	0.059(3)
C3_19	0.3879(6)	0.8342(4)	0.7146(3)	0.053(3)
C4_19	0.3725(6)	0.8222(5)	0.6811(3)	0.056(3)
C5_19	0.3373(7)	0.7779(5)	0.6815(3)	0.064(3)
C6_19	0.3164(8)	0.7501(7)	0.6499(4)	0.074(4)
H6A_19	0.316759	0.772715	0.629980	0.110
H6B_19	0.276137	0.737734	0.653683	0.110
H6C_19	0.342869	0.721727	0.645415	0.110
C7_19	0.3990(8)	0.8444(7)	0.6485(4)	0.073(5)
H7A_19	0.429135	0.821681	0.639337	0.109
H7B_19	0.417104	0.876848	0.653837	0.109
H7C_19	0.367745	0.849116	0.631247	0.109
C8_19	0.4294(7)	0.8756(6)	0.7259(5)	0.071(4)
H8A_19	0.442254	0.894745	0.705659	0.107
H8B_19	0.464040	0.860979	0.737295	0.107
H8C_19	0.408874	0.897911	0.741983	0.107
C9_19	0.3765(11)	0.7924(7)	0.7757(4)	0.086(6)
H9A_19	0.415908	0.778223	0.779417	0.129
H9B_19	0.346639	0.770514	0.786084	0.129
H9C_19	0.374299	0.825671	0.786267	0.129
C10_19	0.3173(8)	0.7081(5)	0.7254(5)	0.068(4)
H10A_19	0.279056	0.700666	0.714718	0.102
H10B_19	0.313708	0.705479	0.750548	0.102
H10C_19	0.346955	0.684097	0.717225	0.102
O1_20	0.1660(7)	0.5863(5)	0.6785(4)	0.057(3)
C1_20	0.1385(5)	0.6252(5)	0.6611(3)	0.059(3)
C2_20	0.1843(6)	0.6470(6)	0.6350(4)	0.071(4)
F1_20	0.2396(5)	0.6482(5)	0.6490(3)	0.072(3)
F2_20	0.1708(7)	0.6930(6)	0.6247(5)	0.100(5)
F3_20	0.1875(7)	0.6183(5)	0.6073(3)	0.095(4)
C3_20	0.0829(6)	0.6068(6)	0.6410(4)	0.080(4)
F4_20	0.0379(4)	0.6003(5)	0.6624(4)	0.095(4)
F5_20	0.0961(6)	0.5632(5)	0.6273(3)	0.100(4)
F6_20	0.0684(6)	0.6389(6)	0.6174(4)	0.117(7)
C4_20	0.1208(6)	0.6680(5)	0.6866(4)	0.069(4)
F7_20	0.0950(5)	0.6455(4)	0.7134(4)	0.085(4)
F8_20	0.0843(5)	0.7014(5)	0.6733(4)	0.088(4)
F9_20	0.1685(4)	0.6927(4)	0.6982(3)	0.073(3)
O1_21	1.1227(12)	0.5687(11)	0.4111(5)	0.044(5)
C1_21	1.1281(7)	0.5954(6)	0.4409(4)	0.051(4)
C2_21	1.0766(8)	0.5791(6)	0.4644(4)	0.062(4)
F1_21	1.0256(8)	0.5746(8)	0.4467(8)	0.080(5)
F2_21	1.0708(16)	0.6079(8)	0.4922(5)	0.104(6)
F3_21	1.0847(11)	0.5324(7)	0.4760(8)	0.088(5)

C3_21	1.1865(8)	0.5822(7)	0.4601(4)	0.071(5)
F4_21	1.2306(6)	0.6063(7)	0.4441(4)	0.076(4)
F5_21	1.1965(7)	0.5327(6)	0.4584(5)	0.069(4)
F6_21	1.1822(10)	0.5948(9)	0.4934(4)	0.111(7)
C4_21	1.1236(10)	0.6521(6)	0.4342(5)	0.085(6)
F7_21	1.1608(10)	0.6648(5)	0.4093(4)	0.087(6)
F8_21	1.1424(11)	0.6786(8)	0.4622(6)	0.114(8)
F9_21	1.0692(10)	0.6667(8)	0.4271(7)	0.115(7)
C1_22	0.4833(6)	0.6977(5)	0.7173(3)	0.063(3)
C2_22	0.4696(5)	0.6965(5)	0.6826(3)	0.054(3)
C3_22	0.4581(8)	0.6526(5)	0.6656(4)	0.079(5)
H3_22	0.448059	0.652500	0.641839	0.095
C4_22	0.4614(11)	0.6078(6)	0.6843(4)	0.094(6)
H4_22	0.457893	0.576597	0.672723	0.113
C5_22	0.4698(9)	0.6091(6)	0.7196(4)	0.073(4)
H5_22	0.468570	0.578943	0.732534	0.088
C6_22	0.4801(9)	0.6545(5)	0.7364(4)	0.079(5)
H6_22	0.484854	0.655530	0.760744	0.095
F1_22	0.4892(7)	0.7423(4)	0.7335(3)	0.107(4)
F2_22	0.4685(5)	0.7416(4)	0.6649(3)	0.085(3)
O1_23	0.7732(6)	0.4495(9)	0.5420(6)	0.045(5)
C1_23	0.7208(8)	0.4754(7)	0.5389(5)	0.033(4)
C2_23	0.7177(11)	0.5240(9)	0.5597(7)	0.062(6)
F1_23	0.7284(11)	0.5667(10)	0.5421(11)	0.080(6)
F2_23	0.6663(10)	0.5311(11)	0.5766(8)	0.075(6)
F3_23	0.7594(13)	0.5224(16)	0.5849(8)	0.079(6)
C3_23	0.6730(10)	0.4398(8)	0.5537(6)	0.048(5)
F4_23	0.6824(10)	0.3925(8)	0.5464(7)	0.063(5)
F5_23	0.6723(11)	0.4439(12)	0.5884(5)	0.075(6)
F6_23	0.6195(8)	0.4521(9)	0.5427(7)	0.067(5)
C4_23	0.7123(9)	0.4818(8)	0.4996(5)	0.051(5)
F7_23	0.6990(12)	0.4364(8)	0.4866(7)	0.062(5)
F8_23	0.6665(8)	0.5113(7)	0.4916(5)	0.061(4)
F9_23	0.7598(8)	0.5000(8)	0.4837(5)	0.066(5)
O1_24	0.1020(8)	0.5031(8)	0.6966(5)	0.0375(18)
C1_24	0.0581(6)	0.4726(5)	0.7085(3)	0.029(3)
C2_24	0.0848(6)	0.4221(5)	0.7198(3)	0.041(3)
F1_24	0.0986(8)	0.3937(6)	0.6923(3)	0.061(4)
F2_24	0.0461(13)	0.3941(7)	0.7384(5)	0.046(4)
F3_24	0.1324(8)	0.4286(12)	0.7397(6)	0.048(3)
C3_24	0.0261(6)	0.4976(5)	0.7397(3)	0.042(3)
F4_24	0.0246(7)	0.5472(5)	0.7354(4)	0.051(3)
F5_24	0.0559(5)	0.4888(5)	0.7691(3)	0.045(3)
F6_24	-0.0281(5)	0.4821(5)	0.7431(3)	0.049(3)
C4_24	0.0130(6)	0.4652(5)	0.6789(3)	0.044(3)
F7_24	-0.0194(9)	0.5065(7)	0.6735(4)	0.060(4)
F8_24	-0.0221(5)	0.4270(5)	0.6850(3)	0.057(3)
F9_24	0.0410(8)	0.4569(7)	0.6488(3)	0.060(4)
O1_25	0.1600(14)	0.5592(13)	0.7483(5)	0.045(7)
C1_25	0.1868(8)	0.5729(7)	0.7785(5)	0.034(4)
C2_25	0.2511(8)	0.5890(7)	0.7696(5)	0.040(4)
F1_25	0.2519(18)	0.6097(14)	0.7381(6)	0.052(5)
F2_25	0.2744(13)	0.6220(12)	0.7916(7)	0.049(6)
F3_25	0.2896(7)	0.5505(7)	0.7681(5)	0.044(4)
C3_25	0.1892(9)	0.5299(8)	0.8054(5)	0.044(4)

F4_25	0.1375(10)	0.5203(11)	0.8202(8)	0.064(6)
F5_25	0.2062(15)	0.4860(9)	0.7916(9)	0.046(5)
F6_25	0.2287(15)	0.5413(15)	0.8303(7)	0.056(7)
C4_25	0.1502(10)	0.6180(8)	0.7920(6)	0.063(5)
F7_25	0.0930(10)	0.6072(15)	0.7907(14)	0.078(6)
F8_25	0.1641(17)	0.6291(11)	0.8246(6)	0.083(7)
F9_25	0.1595(12)	0.6589(9)	0.7730(8)	0.083(6)
O1_26	1.4075(5)	0.5827(4)	0.1996(4)	0.041(3)
C1_26	1.3687(5)	0.5449(4)	0.2039(3)	0.037(3)
C2_26	1.3702(7)	0.5289(6)	0.2422(3)	0.062(4)
F1_26	1.4143(6)	0.4984(5)	0.2491(3)	0.078(3)
F2_26	1.3207(6)	0.5016(5)	0.2498(3)	0.084(4)
F3_26	1.3728(7)	0.5675(4)	0.2635(3)	0.070(3)
C3_26	1.3052(6)	0.5632(5)	0.1949(4)	0.059(4)
F4_26	1.3054(6)	0.5917(5)	0.1666(3)	0.073(3)
F5_26	1.2799(5)	0.5911(5)	0.2186(4)	0.080(4)
F6_26	1.2687(5)	0.5235(4)	0.1894(3)	0.068(3)
C4_26	1.3836(7)	0.5004(5)	0.1805(4)	0.058(4)
F7_26	1.3681(8)	0.5090(6)	0.1479(3)	0.083(5)
F8_26	1.3594(7)	0.4571(4)	0.1895(4)	0.074(4)
F9_26	1.4428(6)	0.4924(4)	0.1794(4)	0.074(3)
C1_27	0.2762(5)	0.9091(5)	0.7221(3)	0.048(3)
C2_27	0.2256(7)	0.8804(6)	0.7334(3)	0.066(4)
C3_27	0.2014(6)	0.8549(5)	0.7041(4)	0.064(3)
C4_27	0.2348(6)	0.8702(6)	0.6750(3)	0.059(3)
C5_27	0.2783(5)	0.9040(5)	0.6858(3)	0.046(3)
C6_27	0.3131(9)	0.9385(6)	0.6627(5)	0.078(5)
H6A_27	0.329095	0.919407	0.643232	0.117
H6B_27	0.345701	0.953410	0.675801	0.117
H6C_27	0.287126	0.965034	0.654052	0.117
C7_27	0.2203(12)	0.8576(10)	0.6376(4)	0.109(8)
H7A_27	0.193633	0.883163	0.628206	0.163
H7B_27	0.200952	0.824802	0.636531	0.163
H7C_27	0.256815	0.856820	0.624027	0.163
C8_27	0.1447(7)	0.8246(7)	0.7020(9)	0.121(10)
H8A_27	0.126632	0.822457	0.724886	0.181
H8B_27	0.153794	0.790763	0.693649	0.181
H8C_27	0.117215	0.840848	0.685998	0.181
C9_27	0.2007(13)	0.8865(7)	0.7688(5)	0.116(9)
H9A_27	0.194711	0.922197	0.773644	0.173
H9B_27	0.228240	0.872418	0.785715	0.173
H9C_27	0.162676	0.868979	0.770327	0.173
C10_27	0.3095(8)	0.9479(6)	0.7426(5)	0.076(5)
H10A_27	0.343248	0.959953	0.729107	0.114
H10B_27	0.323766	0.932922	0.764140	0.114
H10C_27	0.283142	0.975971	0.747915	0.114
O1_28	0.4198(3)	0.7096(3)	0.5217(2)	0.0373(17)
C1_28	0.3623(4)	0.7203(4)	0.5247(3)	0.047(2)
C2_28	0.3308(5)	0.6923(4)	0.5559(3)	0.052(3)
F1_28	0.3172(3)	0.6452(3)	0.5478(2)	0.060(2)
F2_28	0.2816(4)	0.7159(4)	0.5664(3)	0.080(3)
F3_28	0.3671(3)	0.6914(3)	0.58210(18)	0.0562(19)
C3_28	0.3556(6)	0.7772(5)	0.5302(4)	0.079(4)
F4_28	0.3889(6)	0.8017(4)	0.5080(4)	0.112(5)
F5_28	0.3719(6)	0.7892(4)	0.5627(3)	0.098(3)

F6_28	0.3011(5)	0.7948(5)	0.5260(4)	0.136(6)
C4_28	0.3281(6)	0.7047(6)	0.4919(3)	0.077(4)
F7_28	0.3411(5)	0.7358(6)	0.4650(2)	0.113(5)
F8_28	0.2691(4)	0.7052(5)	0.4950(3)	0.100(4)
F9_28	0.3435(4)	0.6588(4)	0.4816(3)	0.082(3)
O1_29	0.2294(3)	0.5035(3)	0.70423(19)	0.0386(16)
C1_29	0.2710(4)	0.4849(4)	0.6828(3)	0.052(3)
C2_29	0.2791(6)	0.4286(5)	0.6911(4)	0.088(4)
F1_29	0.2323(5)	0.4031(5)	0.6793(5)	0.126(5)
F2_29	0.3282(5)	0.4086(4)	0.6803(5)	0.126(6)
F3_29	0.2765(6)	0.4207(4)	0.7254(3)	0.110(4)
C3_29	0.3322(5)	0.5109(5)	0.6890(3)	0.062(3)
F4_29	0.3223(5)	0.5603(4)	0.6887(3)	0.082(3)
F5_29	0.3539(4)	0.4986(4)	0.7193(2)	0.076(3)
F6_29	0.3701(4)	0.5023(4)	0.6637(3)	0.085(3)
C4_29	0.2557(6)	0.4907(7)	0.6437(3)	0.099(5)
F7_29	0.2651(5)	0.5375(6)	0.6326(3)	0.120(5)
F8_29	0.2851(5)	0.4591(7)	0.6240(3)	0.140(6)
F9_29	0.1978(5)	0.4808(8)	0.6400(4)	0.142(7)
O1_30	0.5394(5)	0.6872(5)	0.5296(4)	0.031(3)
C1_30	0.5712(5)	0.7165(5)	0.5511(3)	0.046(3)
C2_30	0.5588(7)	0.7027(7)	0.5897(4)	0.070(4)
F1_30	0.5843(6)	0.6604(6)	0.5982(3)	0.093(4)
F2_30	0.5763(9)	0.7370(8)	0.6117(4)	0.104(5)
F3_30	0.4993(5)	0.6978(6)	0.5943(3)	0.070(4)
C3_30	0.5541(7)	0.7719(5)	0.5462(4)	0.062(4)
F4_30	0.5455(8)	0.7815(6)	0.5120(3)	0.077(4)
F5_30	0.5019(6)	0.7837(5)	0.5618(4)	0.095(5)
F6_30	0.5981(8)	0.8025(6)	0.5572(5)	0.084(5)
C4_30	0.6389(5)	0.7080(6)	0.5434(3)	0.058(3)
F7_30	0.6514(5)	0.7339(6)	0.5144(3)	0.076(4)
F8_30	0.6753(6)	0.7238(6)	0.5684(3)	0.079(4)
F9_30	0.6488(5)	0.6592(5)	0.5400(4)	0.078(4)
O1_31	1.4678(14)	0.6612(12)	0.1675(5)	0.042(5)
C1_31	1.4755(7)	0.6614(6)	0.1332(5)	0.053(4)
C2_31	1.4986(7)	0.6090(6)	0.1219(5)	0.049(4)
F1_31	1.4522(6)	0.5772(5)	0.1203(3)	0.058(4)
F2_31	1.5221(14)	0.6105(12)	0.0903(5)	0.061(4)
F3_31	1.5382(8)	0.5907(7)	0.1447(4)	0.074(4)
C3_31	1.5221(11)	0.7007(8)	0.1232(6)	0.107(7)
F4_31	1.5103(19)	0.7443(8)	0.1397(9)	0.185(17)
F5_31	1.5776(9)	0.6874(9)	0.1319(6)	0.140(8)
F6_31	1.5188(14)	0.7099(13)	0.0891(5)	0.125(9)
C4_31	1.4155(8)	0.6725(8)	0.1154(6)	0.068(5)
F7_31	1.3935(10)	0.7178(7)	0.1181(5)	0.094(5)
F8_31	1.4192(16)	0.6639(14)	0.0813(5)	0.099(7)
F9_31	1.3722(5)	0.6449(7)	0.1294(3)	0.066(4)
O1_10	1.1178(10)	0.5002(7)	0.3580(7)	0.042(6)
C1_10	1.0790(7)	0.4630(6)	0.3627(4)	0.032(3)
C2_10	1.0723(8)	0.4321(7)	0.3289(4)	0.059(4)
F1_10	1.1264(7)	0.4270(6)	0.3142(4)	0.073(4)
F2_10	1.0516(11)	0.3855(8)	0.3344(7)	0.069(6)
F3_10	1.0381(9)	0.4562(6)	0.3065(4)	0.088(6)
C3_10	1.0180(7)	0.4812(6)	0.3753(5)	0.052(4)
F4_10	1.0185(5)	0.4923(5)	0.4084(4)	0.064(4)

F5_10	0.9999(8)	0.5214(7)	0.3581(7)	0.092(6)
F6_10	0.9769(12)	0.4456(11)	0.3708(9)	0.066(5)
C4_10	1.1044(7)	0.4277(5)	0.3905(4)	0.035(3)
F7_10	1.1230(7)	0.4550(5)	0.4177(3)	0.056(3)
F8_10	1.0657(10)	0.3949(7)	0.4038(4)	0.049(4)
F9_10	1.1503(5)	0.4016(5)	0.3779(4)	0.064(4)
O1_32	0.1562(11)	0.5543(9)	0.7502(3)	0.032(5)
C1_32	0.1841(7)	0.5700(6)	0.7797(4)	0.034(4)
C2_32	0.2242(7)	0.5266(6)	0.7932(4)	0.037(4)
F1_32	0.2760(5)	0.5256(6)	0.7768(3)	0.043(3)
F2_32	0.2376(12)	0.5292(11)	0.8267(5)	0.048(5)
F3_32	0.1969(13)	0.4830(8)	0.7858(9)	0.057(6)
C3_32	0.1372(7)	0.5806(7)	0.8079(4)	0.048(4)
F4_32	0.0924(10)	0.6078(13)	0.7966(10)	0.078(6)
F5_32	0.1175(10)	0.5367(7)	0.8206(6)	0.068(5)
F6_32	0.1610(12)	0.6062(8)	0.8343(5)	0.077(6)
C4_32	0.2223(8)	0.6178(6)	0.7740(5)	0.051(4)
F7_32	0.1874(10)	0.6580(7)	0.7718(7)	0.076(5)
F8_32	0.2604(12)	0.6252(11)	0.7992(6)	0.064(7)
F9_32	0.2500(15)	0.6163(12)	0.7437(6)	0.063(5)
O1_33	0.4790(3)	0.6413(3)	0.47601(17)	0.0287(14)
C1_33	0.5060(4)	0.6460(4)	0.4443(2)	0.037(2)
C2_33	0.5208(5)	0.7017(4)	0.4366(3)	0.044(2)
F1_33	0.5696(3)	0.7163(3)	0.45364(18)	0.0413(15)
F2_33	0.5305(4)	0.7102(3)	0.40352(18)	0.059(2)
F3_33	0.4771(3)	0.7320(3)	0.44705(19)	0.0483(16)
C3_33	0.4620(5)	0.6265(5)	0.4166(2)	0.050(3)
F4_33	0.4370(4)	0.5837(3)	0.42662(19)	0.061(2)
F5_33	0.4183(3)	0.6600(4)	0.4119(2)	0.066(2)
F6_33	0.4890(4)	0.6183(4)	0.38629(19)	0.068(2)
C4_33	0.5631(4)	0.6147(4)	0.4435(3)	0.039(2)
F7_33	0.5516(3)	0.5657(3)	0.4419(2)	0.0548(19)
F8_33	0.5975(3)	0.6259(3)	0.4159(2)	0.056(2)
F9_33	0.5957(3)	0.6217(3)	0.47166(18)	0.0437(15)
O1_34	1.1585(7)	0.6006(9)	0.3420(6)	0.033(4)
C1_34	1.1248(8)	0.6274(7)	0.3191(5)	0.044(4)
C2_34	1.0952(10)	0.5931(8)	0.2917(5)	0.064(5)
F1_34	1.0461(11)	0.5729(10)	0.3048(8)	0.070(5)
F2_34	1.0852(11)	0.6170(8)	0.2622(5)	0.078(5)
F3_34	1.1306(16)	0.5541(9)	0.2846(11)	0.074(5)
C3_34	1.1720(9)	0.6617(7)	0.3016(5)	0.050(4)
F4_34	1.2069(13)	0.6816(18)	0.3255(10)	0.078(6)
F5_34	1.2022(8)	0.6337(7)	0.2796(5)	0.062(4)
F6_34	1.149(2)	0.6992(13)	0.2833(9)	0.068(5)
C4_34	1.0771(8)	0.6606(6)	0.3366(5)	0.056(5)
F7_34	1.0993(9)	0.6993(7)	0.3530(6)	0.075(5)
F8_34	1.0392(9)	0.6777(8)	0.3129(6)	0.082(5)
F9_34	1.0453(11)	0.6341(10)	0.3587(6)	0.075(6)
O1_35	1.1248(19)	0.5752(18)	0.4108(7)	0.037(8)
C1_35	1.1292(10)	0.5915(9)	0.4441(6)	0.051(6)
C2_35	1.1808(13)	0.6294(10)	0.4473(8)	0.081(7)
F1_35	1.2043(18)	0.6486(11)	0.4184(9)	0.098(10)
F2_35	1.168(2)	0.6667(16)	0.4687(12)	0.118(10)
F3_35	1.2248(14)	0.6023(14)	0.4603(9)	0.095(7)
C3_35	1.1376(12)	0.5459(10)	0.4696(6)	0.060(6)

F4_35	1.0866(16)	0.5218(16)	0.4737(15)	0.088(7)
F5_35	1.1766(15)	0.5139(12)	0.4555(9)	0.080(7)
F6_35	1.1581(15)	0.5596(19)	0.5005(6)	0.126(14)
C4_35	1.0712(12)	0.6185(10)	0.4542(7)	0.073(7)
F7_35	1.0236(15)	0.5926(14)	0.4454(14)	0.080(7)
F8_35	1.071(3)	0.6241(17)	0.4892(7)	0.105(8)
F9_35	1.066(2)	0.6648(13)	0.4424(12)	0.114(9)
O1_36	0.8828(17)	0.4276(17)	0.5052(8)	0.031(7)
C1_36	0.8807(10)	0.4010(8)	0.4748(6)	0.043(5)
C2_36	0.8878(10)	0.3444(8)	0.4834(6)	0.044(5)
F1_36	0.8493(9)	0.3310(8)	0.5082(5)	0.046(4)
F2_36	0.8773(13)	0.3140(9)	0.4571(5)	0.058(5)
F3_36	0.9429(9)	0.3360(9)	0.4946(7)	0.048(4)
C3_36	0.9341(12)	0.4198(12)	0.4529(8)	0.038(6)
F4_36	0.9251(14)	0.4656(12)	0.4397(11)	0.047(6)
F5_36	0.9816(15)	0.424(2)	0.4730(9)	0.033(6)
F6_36	0.947(2)	0.389(2)	0.4271(12)	0.051(8)
C4_36	0.8217(10)	0.4106(9)	0.4557(6)	0.059(5)
F7_36	0.8074(10)	0.4597(8)	0.4569(5)	0.056(5)
F8_36	0.8248(13)	0.3968(11)	0.4227(6)	0.071(6)
F9_36	0.7749(11)	0.3866(10)	0.4687(7)	0.068(7)
O1_37	0.1033(18)	0.5006(19)	0.6965(13)	0.0375(18)
C1_37	0.0595(11)	0.4678(9)	0.7055(6)	0.031(5)
C2_37	0.0005(11)	0.4965(10)	0.7109(7)	0.049(6)
F1_37	0.0091(17)	0.5387(11)	0.7291(11)	0.054(6)
F2_37	-0.0373(12)	0.4694(11)	0.7289(8)	0.046(5)
F3_37	-0.026(2)	0.510(2)	0.6814(9)	0.060(7)
C3_37	0.0529(12)	0.4272(10)	0.6769(6)	0.047(6)
F4_37	0.0975(18)	0.3946(15)	0.6798(10)	0.066(7)
F5_37	0.054(2)	0.4466(19)	0.6454(8)	0.064(7)
F6_37	0.0029(12)	0.4011(12)	0.6811(8)	0.058(6)
C4_37	0.0781(12)	0.4407(10)	0.7393(6)	0.031(5)
F7_37	0.1351(16)	0.428(3)	0.7387(15)	0.043(6)
F8_37	0.046(3)	0.3991(16)	0.7450(14)	0.044(6)
F9_37	0.0694(16)	0.4693(12)	0.7671(6)	0.046(6)
O1_38	0.5419(17)	0.683(3)	0.5305(18)	0.036(11)
C1_38	0.5760(14)	0.7111(15)	0.5519(10)	0.046(7)
C2_38	0.589(2)	0.7631(16)	0.5357(10)	0.065(8)
F1_38	0.629(2)	0.759(2)	0.5104(12)	0.070(8)
F2_38	0.610(4)	0.796(3)	0.5583(18)	0.081(8)
F3_38	0.538(3)	0.782(3)	0.5226(18)	0.067(8)
C3_38	0.5417(19)	0.7183(18)	0.5864(11)	0.065(8)
F4_38	0.517(3)	0.674(2)	0.5946(15)	0.068(8)
F5_38	0.499(2)	0.752(2)	0.5838(17)	0.096(14)
F6_38	0.578(3)	0.731(4)	0.6122(16)	0.101(8)
C4_38	0.6354(14)	0.6849(16)	0.5607(11)	0.066(8)
F7_38	0.628(2)	0.6462(18)	0.5823(15)	0.082(14)
F8_38	0.672(3)	0.717(3)	0.5767(19)	0.076(8)
F9_38	0.663(2)	0.668(3)	0.5328(15)	0.074(8)
O1_39	0.7799(5)	0.4695(7)	0.5337(6)	0.052(5)
C1_39	0.7209(7)	0.4795(6)	0.5382(4)	0.032(4)
C2_39	0.6906(7)	0.4358(7)	0.5565(4)	0.035(4)
F1_39	0.7079(8)	0.3927(6)	0.5438(6)	0.058(4)
F2_39	0.6309(7)	0.4372(7)	0.5539(5)	0.057(4)
F3_39	0.7013(9)	0.4360(10)	0.5904(4)	0.079(6)

C3_39	0.7178(10)	0.5311(8)	0.5566(6)	0.059(5)
F4_39	0.7489(10)	0.5634(10)	0.5369(9)	0.082(6)
F5_39	0.7425(12)	0.5313(14)	0.5879(6)	0.086(6)
F6_39	0.6623(8)	0.5450(8)	0.5600(6)	0.066(5)
C4_39	0.6887(8)	0.4893(7)	0.5035(5)	0.052(4)
F7_39	0.7233(8)	0.5191(8)	0.4847(5)	0.079(5)
F8_39	0.6364(7)	0.5129(7)	0.5085(5)	0.066(4)
F9_39	0.6772(9)	0.4488(7)	0.4852(6)	0.063(5)
O1_40	0.863(3)	0.3972(18)	0.5705(12)	0.052(11)
C1_40	0.8681(14)	0.3770(11)	0.6021(9)	0.046(7)
C2_40	0.8483(17)	0.3215(11)	0.6030(9)	0.044(7)
F1_40	0.7916(17)	0.3191(19)	0.5934(13)	0.050(6)
F2_40	0.851(3)	0.305(2)	0.6356(11)	0.066(8)
F3_40	0.883(2)	0.2929(15)	0.5835(14)	0.069(12)
C3_40	0.9323(14)	0.3818(14)	0.6161(11)	0.076(8)
F4_40	0.961(2)	0.4220(19)	0.604(2)	0.108(5)
F5_40	0.9653(18)	0.3420(17)	0.6101(16)	0.069(8)
F6_40	0.926(3)	0.389(2)	0.6503(11)	0.099(14)
C4_40	0.8297(17)	0.4050(14)	0.6294(11)	0.059(8)
F7_40	0.850(2)	0.4513(13)	0.6322(12)	0.056(6)
F8_40	0.835(3)	0.384(2)	0.6607(11)	0.081(8)
F9_40	0.7725(17)	0.403(3)	0.6209(19)	0.116(19)
O1_41	1.469(2)	0.6661(18)	0.1697(8)	0.048(8)
C1_41	1.4815(9)	0.6614(8)	0.1359(7)	0.054(5)
C2_41	1.5133(11)	0.7105(8)	0.1252(7)	0.068(6)
F1_41	1.4725(13)	0.7462(10)	0.1228(6)	0.081(9)
F2_41	1.5474(17)	0.7065(16)	0.0969(9)	0.110(10)
F3_41	1.5501(12)	0.7266(10)	0.1503(8)	0.081(7)
C3_41	1.5210(11)	0.6156(9)	0.1284(7)	0.068(5)
F4_41	1.5040(12)	0.5749(8)	0.1455(7)	0.074(5)
F5_41	1.5761(10)	0.6260(13)	0.1382(7)	0.102(9)
F6_41	1.521(2)	0.604(2)	0.0947(7)	0.067(6)
C4_41	1.4223(10)	0.6568(9)	0.1155(8)	0.064(6)
F7_41	1.3967(13)	0.6112(9)	0.1193(7)	0.087(8)
F8_41	1.432(2)	0.665(2)	0.0819(8)	0.102(8)
F9_41	1.3829(11)	0.6893(11)	0.1268(6)	0.074(5)
O1_42	1.427(2)	0.5818(8)	0.1947(12)	0.045(9)
C1_42	1.3976(12)	0.5401(9)	0.2053(7)	0.051(6)
C2_42	1.4165(15)	0.5275(13)	0.2430(7)	0.073(7)
F1_42	1.421(3)	0.5683(13)	0.2625(8)	0.088(12)
F2_42	1.3776(19)	0.4979(15)	0.2589(9)	0.073(7)
F3_42	1.4681(17)	0.5034(18)	0.2412(11)	0.101(15)
C3_42	1.4179(16)	0.4960(10)	0.1820(8)	0.065(6)
F4_42	1.393(2)	0.499(2)	0.1509(10)	0.079(8)
F5_42	1.4760(16)	0.4973(15)	0.1760(13)	0.079(7)
F6_42	1.404(3)	0.4514(11)	0.1956(11)	0.088(13)
C4_42	1.3298(13)	0.5460(11)	0.2040(9)	0.062(7)
F7_42	1.3113(18)	0.5695(18)	0.1756(10)	0.071(6)
F8_42	1.304(2)	0.5009(13)	0.2070(17)	0.124(18)
F9_42	1.3096(19)	0.5703(15)	0.2319(10)	0.081(11)
O1_43	0.172(3)	0.5892(19)	0.6816(19)	0.044(11)
C1_43	0.150(2)	0.6322(16)	0.6675(11)	0.067(8)
C2_43	0.141(2)	0.6723(19)	0.6961(12)	0.072(7)
F1_43	0.090(3)	0.662(3)	0.712(2)	0.082(8)
F2_43	0.138(4)	0.7182(19)	0.6824(16)	0.09(2)

F3_43	0.182(3)	0.674(3)	0.7209(13)	0.077(18)
C3_43	0.197(3)	0.651(2)	0.6414(14)	0.072(8)
F4_43	0.211(4)	0.617(3)	0.6173(18)	0.092(8)
F5_43	0.248(3)	0.660(4)	0.659(2)	0.074(8)
F6_43	0.180(5)	0.693(3)	0.626(3)	0.100(8)
C4_43	0.090(2)	0.624(2)	0.6496(14)	0.080(9)
F7_43	0.094(3)	0.605(3)	0.6180(15)	0.079(8)
F8_43	0.061(3)	0.668(3)	0.648(2)	0.099(18)
F9_43	0.054(3)	0.594(3)	0.668(2)	0.094(9)
O1_13	1.4773(17)	0.6650(18)	0.2357(11)	0.038(10)
C1_13	1.5270(13)	0.6549(11)	0.2534(7)	0.065(7)
C2_13	1.5507(15)	0.7047(12)	0.2697(9)	0.093(8)
F1_13	1.569(2)	0.7327(18)	0.2435(13)	0.113(8)
F2_13	1.590(2)	0.6937(17)	0.2941(12)	0.091(4)
F3_13	1.5108(19)	0.7330(14)	0.2858(13)	0.092(11)
C3_13	1.5116(17)	0.6223(14)	0.2853(9)	0.098(11)
F4_13	1.471(2)	0.5861(17)	0.2841(10)	0.101(13)
F5_13	1.494(3)	0.657(2)	0.3086(11)	0.102(8)
F6_13	1.561(2)	0.602(2)	0.2978(18)	0.17(2)
C4_13	1.5777(13)	0.6349(14)	0.2303(8)	0.082(9)
F7_13	1.5660(19)	0.5900(15)	0.2177(12)	0.077(8)
F8_13	1.6278(13)	0.629(2)	0.2486(9)	0.106(17)
F9_13	1.5864(19)	0.6650(19)	0.2023(11)	0.096(8)
O1_44	1.1087(18)	0.5076(13)	0.3544(11)	0.037(7)
C1_44	1.0758(11)	0.4656(10)	0.3588(5)	0.037(5)
C2_44	1.0838(12)	0.4291(10)	0.3280(6)	0.056(6)
F1_44	1.1358(10)	0.4049(8)	0.3287(8)	0.061(5)
F2_44	1.0421(17)	0.3931(14)	0.3266(12)	0.065(7)
F3_44	1.0842(10)	0.4542(8)	0.2982(5)	0.054(5)
C3_44	1.0106(11)	0.4841(11)	0.3597(7)	0.069(7)
F4_44	1.0077(13)	0.5227(11)	0.3815(9)	0.088(7)
F5_44	0.9968(13)	0.4978(16)	0.3275(8)	0.121(13)
F6_44	0.972(2)	0.4500(18)	0.3697(14)	0.065(6)
C4_44	1.0887(11)	0.4395(10)	0.3935(6)	0.050(6)
F7_44	1.0673(15)	0.4640(10)	0.4215(6)	0.090(9)
F8_44	1.067(2)	0.3928(12)	0.3931(9)	0.062(7)
F9_44	1.1471(10)	0.4368(14)	0.3973(9)	0.096(12)

*Table S 14 Atomic coordinates and U_{eq} [Å^2] for **8***

Atom	***x***	***y***	***z***	U_{eq}
Fe1	0.30894(2)	0.54158(2)	0.90033(3)	0.01789(10)
N1	0.17548(16)	0.49320(16)	0.85168(16)	0.0233(6)
C1	0.22631(18)	0.51224(16)	0.87017(16)	0.0192(6)
Al1	0.50277(5)	0.23865(5)	0.12331(5)	0.01865(19)
C2	0.11014(19)	0.4684(2)	0.8300(2)	0.0266(8)
Al2	0.41778(5)	0.24841(5)	0.65875(5)	0.01705(19)
C3	0.0583(2)	0.5048(2)	0.8698(2)	0.0328(8)
H3A	0.065677	0.553427	0.867202	0.049
H3B	0.062026	0.490249	0.913874	0.049
H3C	0.013736	0.494149	0.853945	0.049
C4	0.1023(2)	0.4877(3)	0.7600(2)	0.0406(10)
H4A	0.139464	0.469034	0.735680	0.061
H4B	0.102180	0.536766	0.755919	0.061

H4C	0.060393	0.469535	0.743765	0.061
C5	0.1088(2)	0.3934(2)	0.8405(3)	0.0446(12)
H5A	0.065218	0.375696	0.828191	0.067
H5B	0.116811	0.383784	0.885194	0.067
H5C	0.143414	0.372113	0.814830	0.067
O1_13	0.5721(12)	0.2820(13)	0.0962(9)	0.030(2)
C1_13	0.6059(5)	0.3071(5)	0.0465(5)	0.0228(19)
C2_13	0.5601(4)	0.3441(4)	0.0003(4)	0.0375(18)
F1_13	0.5396(3)	0.4020(2)	0.0244(3)	0.0561(16)
F2_13	0.5867(8)	0.3552(7)	-0.0566(5)	0.045(2)
F3_13	0.5059(3)	0.3054(3)	-0.0111(3)	0.0472(14)
C3_13	0.6448(5)	0.2503(6)	0.0116(5)	0.043(3)
F4_13	0.6710(3)	0.2071(3)	0.0521(3)	0.0595(18)
F5_13	0.6037(3)	0.2179(3)	-0.0270(3)	0.0552(15)
F6_13	0.6937(5)	0.2762(7)	-0.0236(5)	0.073(3)
C4_13	0.6581(4)	0.3575(5)	0.0748(5)	0.0387(18)
F7_13	0.7061(2)	0.3255(3)	0.1036(3)	0.0498(14)
F8_13	0.6810(8)	0.3978(8)	0.0291(7)	0.073(4)
F9_13	0.6271(4)	0.3979(3)	0.1165(3)	0.0514(14)
O1_12	0.48123(17)	0.17574(16)	0.07179(15)	0.0346(6)
C1_12	0.4341(2)	0.1326(2)	0.05121(19)	0.0317(8)
C2_12	0.4106(3)	0.0855(3)	0.1041(3)	0.0540(14)
F1_12	0.4579(2)	0.03886(17)	0.11654(18)	0.0669(11)
F2_12	0.3537(2)	0.0539(2)	0.0908(2)	0.0746(12)
F3_12	0.40056(19)	0.12061(18)	0.15747(15)	0.0566(8)
C3_12	0.3726(3)	0.1724(3)	0.0245(2)	0.0445(11)
F4_12	0.39228(17)	0.22429(18)	-0.00916(17)	0.0542(8)
F5_12	0.33516(16)	0.1947(2)	0.07215(18)	0.0598(9)
F6_12	0.33426(18)	0.1343(2)	-0.01174(17)	0.0572(8)
C4_12	0.4652(3)	0.0909(3)	-0.0035(2)	0.0469(11)
F7_12	0.4725(2)	0.12869(19)	-0.05493(14)	0.0558(8)
F8_12	0.4284(2)	0.03718(18)	-0.01843(19)	0.0670(10)
F9_12	0.5249(2)	0.06949(19)	0.01265(18)	0.0600(9)
O1_3	0.52579(14)	0.20855(15)	0.19647(14)	0.0299(6)
C1_3	0.57314(19)	0.18197(19)	0.23377(19)	0.0277(7)
C2_3	0.6357(2)	0.2276(2)	0.2384(2)	0.0346(9)
F1_3	0.67455(13)	0.22008(17)	0.18835(14)	0.0447(7)
F2_3	0.67275(16)	0.21407(18)	0.28918(16)	0.0512(8)
F3_3	0.61865(14)	0.29187(13)	0.24126(14)	0.0399(6)
C3_3	0.5423(3)	0.1740(3)	0.3011(2)	0.0445(11)
F4_3	0.47999(16)	0.15312(18)	0.29769(15)	0.0506(7)
F5_3	0.54223(19)	0.23330(19)	0.33050(15)	0.0556(8)
F6_3	0.5759(2)	0.1319(2)	0.33767(18)	0.0677(11)
C4_3	0.5941(3)	0.1111(2)	0.2099(3)	0.0478(12)
F7_3	0.5461(2)	0.06648(15)	0.2221(2)	0.0620(10)
F8_3	0.64955(19)	0.08932(18)	0.2361(2)	0.0711(12)
F9_3	0.60321(19)	0.11343(18)	0.14719(18)	0.0601(9)
O1_4	0.43386(15)	0.29000(15)	0.13143(15)	0.0315(6)
C1_4	0.39989(18)	0.33575(19)	0.16441(19)	0.0267(7)
C2_4	0.3467(2)	0.3690(3)	0.1219(3)	0.0471(11)
F1_4	0.29554(16)	0.3292(2)	0.1130(2)	0.0676(11)
F2_4	0.3240(2)	0.42671(19)	0.1456(2)	0.0692(11)
F3_4	0.3725(2)	0.3831(2)	0.06551(17)	0.0653(10)
C3_4	0.4473(2)	0.3914(2)	0.1908(2)	0.0380(9)
F4_4	0.50313(15)	0.36278(17)	0.21250(18)	0.0512(8)

F5_4	0.46512(18)	0.43339(15)	0.14527(18)	0.0542(8)
F6_4	0.42160(17)	0.42756(16)	0.23655(17)	0.0536(8)
C4_4	0.3644(2)	0.3016(2)	0.2221(3)	0.0427(11)
F7_4	0.40798(19)	0.28799(19)	0.26771(15)	0.0570(8)
F8_4	0.31748(17)	0.3396(2)	0.24707(18)	0.0600(9)
F9_4	0.3362(2)	0.24462(17)	0.2040(2)	0.0618(9)
O1_5	0.46102(13)	0.20480(13)	0.60109(13)	0.0235(5)
C1_5	0.45890(19)	0.17919(19)	0.54223(18)	0.0260(7)
C2_5	0.4444(2)	0.2352(2)	0.4926(2)	0.0345(9)
F1_5	0.38043(15)	0.25123(14)	0.49126(12)	0.0382(6)
F2_5	0.46144(19)	0.21650(16)	0.43421(13)	0.0513(8)
F3_5	0.47884(16)	0.29043(13)	0.50701(14)	0.0427(6)
C3_5	0.5271(2)	0.1453(2)	0.5277(2)	0.0327(9)
F4_5	0.54834(13)	0.11027(14)	0.57660(14)	0.0394(6)
F5_5	0.57318(14)	0.19184(15)	0.51516(16)	0.0459(7)
F6_5	0.52354(15)	0.10419(15)	0.47786(15)	0.0448(7)
C4_5	0.4031(2)	0.1250(2)	0.53777(19)	0.0286(8)
F7_5	0.42156(14)	0.06871(13)	0.56659(13)	0.0370(6)
F8_5	0.38769(14)	0.10901(14)	0.47793(12)	0.0379(6)
F9_5	0.34821(12)	0.14674(14)	0.56547(13)	0.0350(5)
O1_6	0.3613(7)	0.2001(6)	0.7015(6)	0.0210(19)
C1_6	0.3525(3)	0.1537(4)	0.7472(3)	0.0218(14)
C2_6	0.3163(3)	0.1863(3)	0.8053(2)	0.0289(11)
F1_6	0.2530(4)	0.1972(3)	0.7926(3)	0.0367(14)
F2_6	0.3200(3)	0.1481(2)	0.85667(17)	0.0409(10)
F3_6	0.3431(5)	0.2452(4)	0.8177(7)	0.041(2)
C3_6	0.4193(3)	0.1227(3)	0.7703(3)	0.0384(14)
F4_6	0.4595(4)	0.1109(6)	0.7221(6)	0.047(2)
F5_6	0.4506(3)	0.1638(4)	0.8093(4)	0.0503(18)
F6_6	0.4107(5)	0.0640(5)	0.8000(4)	0.047(2)
C4_6	0.3077(3)	0.0969(2)	0.7203(2)	0.0269(11)
F7_6	0.3425(3)	0.0571(2)	0.6818(2)	0.0419(11)
F8_6	0.2818(5)	0.0580(3)	0.7648(3)	0.0374(14)
F9_6	0.2580(5)	0.1223(6)	0.6866(3)	0.0324(17)
O1_7	0.47696(12)	0.28046(13)	0.70978(12)	0.0223(5)
C1_7	0.53709(16)	0.31006(18)	0.71501(17)	0.0216(7)
C2_7	0.55576(19)	0.31280(19)	0.78607(19)	0.0271(7)
F1_7	0.57771(14)	0.25341(13)	0.80620(14)	0.0388(6)
F2_7	0.60322(13)	0.35784(14)	0.79849(14)	0.0388(6)
F3_7	0.50329(13)	0.32843(14)	0.82053(12)	0.0357(6)
C3_7	0.5339(2)	0.3835(2)	0.6887(2)	0.0292(8)
F4_7	0.50375(13)	0.38386(14)	0.63225(13)	0.0390(6)
F5_7	0.49891(13)	0.42252(12)	0.72690(15)	0.0375(6)
F6_7	0.59341(13)	0.41115(14)	0.68115(15)	0.0415(6)
C4_7	0.59204(19)	0.2704(2)	0.6789(2)	0.0313(8)
F7_7	0.58953(13)	0.28309(15)	0.61662(13)	0.0403(6)
F8_7	0.65252(12)	0.28701(15)	0.69807(16)	0.0460(8)
F9_7	0.58402(12)	0.20491(13)	0.68668(15)	0.0390(6)
O1_8	0.37037(12)	0.30909(12)	0.62131(12)	0.0210(5)
C1_8	0.31654(18)	0.34970(17)	0.62492(18)	0.0237(7)
C2_8	0.2570(2)	0.3172(2)	0.5879(2)	0.0322(8)
F1_8	0.26580(15)	0.32168(16)	0.52630(14)	0.0442(6)
F2_8	0.19930(13)	0.34694(16)	0.60297(16)	0.0456(7)
F3_8	0.25195(13)	0.25240(13)	0.60215(13)	0.0365(6)
C3_8	0.29458(19)	0.36241(19)	0.6941(2)	0.0280(7)

F4_8	0.34780(12)	0.36862(13)	0.73140(12)	0.0322(5)
F5_8	0.25870(12)	0.31206(12)	0.71694(12)	0.0327(5)
F6_8	0.25873(14)	0.41869(13)	0.70099(15)	0.0414(6)
C4_8	0.3352(2)	0.4182(2)	0.5935(2)	0.0318(8)
F7_8	0.37327(14)	0.45395(12)	0.63273(14)	0.0390(6)
F8_8	0.28191(16)	0.45491(15)	0.57947(19)	0.0523(8)
F9_8	0.36988(16)	0.40842(14)	0.54104(13)	0.0408(6)
C1_9	0.3468(3)	0.4767(3)	0.3918(3)	0.0491(12)
C2_9	0.3350(3)	0.4100(3)	0.3904(2)	0.0480(11)
C3_9	0.2723(3)	0.3849(3)	0.3958(3)	0.0516(12)
H3_9	0.264461	0.337789	0.394272	0.062
C4_9	0.2203(3)	0.4298(3)	0.4037(3)	0.0566(13)
H4_9	0.176005	0.413554	0.407167	0.068
C5_9	0.2325(3)	0.4976(3)	0.4064(3)	0.0517(12)
H5_9	0.197062	0.528171	0.413718	0.062
C6_9	0.2969(3)	0.5213(3)	0.3985(3)	0.0497(12)
H6_9	0.305574	0.568274	0.397815	0.060
F1_9	0.41083(19)	0.4972(2)	0.3857(3)	0.0833(14)
F2_9	0.3870(2)	0.3665(2)	0.3836(2)	0.0746(12)
O1_10	0.370(2)	0.201(2)	0.7048(19)	0.023(7)
C1_10	0.3609(8)	0.1540(10)	0.7498(9)	0.020(4)
C2_10	0.2865(7)	0.1319(8)	0.7510(7)	0.030(3)
F1_10	0.2649(18)	0.1240(18)	0.6926(10)	0.040(7)
F2_10	0.2775(14)	0.0749(9)	0.7816(10)	0.041(5)
F3_10	0.2495(10)	0.1785(11)	0.7793(12)	0.039(4)
C3_10	0.3798(7)	0.1852(7)	0.8152(6)	0.025(3)
F4_10	0.4459(8)	0.1866(8)	0.8192(10)	0.026(3)
F5_10	0.3586(16)	0.2476(11)	0.821(2)	0.030(5)
F6_10	0.3564(8)	0.1475(7)	0.8615(6)	0.037(3)
C4_10	0.4053(8)	0.0916(7)	0.7347(7)	0.029(3)
F7_10	0.4630(14)	0.114(2)	0.713(2)	0.050(8)
F8_10	0.416(2)	0.0544(18)	0.7849(13)	0.054(9)
F9_10	0.3763(10)	0.0543(7)	0.6903(7)	0.039(3)
O1_11	0.568(2)	0.279(2)	0.0896(16)	0.030(2)
C1_11	0.5997(9)	0.3053(8)	0.0390(9)	0.030(4)
C2_11	0.5490(8)	0.3208(9)	-0.0141(8)	0.054(4)
F1_11	0.5323(6)	0.2655(6)	-0.0443(4)	0.071(3)
F2_11	0.5759(16)	0.3646(15)	-0.0545(13)	0.073(8)
F3_11	0.4948(4)	0.3485(8)	0.0108(5)	0.069(4)
C3_11	0.6336(8)	0.3716(8)	0.0598(7)	0.055(4)
F4_11	0.6643(7)	0.3634(8)	0.1151(5)	0.075(5)
F5_11	0.5876(7)	0.4202(5)	0.0628(7)	0.081(4)
F6_11	0.6851(8)	0.3900(14)	0.0222(11)	0.063(7)
C4_11	0.6516(9)	0.2535(9)	0.0140(9)	0.057(5)
F7_11	0.7030(5)	0.2537(8)	0.0532(6)	0.085(4)
F8_11	0.6716(11)	0.2688(9)	-0.0444(7)	0.079(5)
F9_11	0.6236(7)	0.1931(5)	0.0101(8)	0.081(5)
C1_1	0.3078(2)	0.43881(19)	0.93060(19)	0.0257(7)
C2_1	0.3745(2)	0.46108(19)	0.92826(19)	0.0270(8)
C3_1	0.3816(2)	0.5145(2)	0.97312(18)	0.0284(8)
C4_1	0.31783(19)	0.5276(2)	1.00111(18)	0.0257(7)
C5_1	0.27279(19)	0.47968(19)	0.97721(18)	0.0231(7)
C6_1	0.2836(2)	0.37544(19)	0.9006(2)	0.0351(9)
H6A_1	0.235009	0.373357	0.903598	0.053
H6B_1	0.302975	0.336668	0.922377	0.053

H6C_1	0.296806	0.374716	0.856050	0.053
C9_1	0.3043(2)	0.5743(2)	1.0549(2)	0.0352(9)
H9A_1	0.335317	0.612239	1.053136	0.053
H9B_1	0.310139	0.550208	1.094906	0.053
H9C_1	0.258610	0.591026	1.051966	0.053
C8_1	0.4457(2)	0.5411(3)	1.0004(2)	0.0401(10)
H8A_1	0.482147	0.532429	0.970775	0.060
H8B_1	0.454909	0.518567	1.040568	0.060
H8C_1	0.441658	0.589636	1.007439	0.060
C7_1	0.4287(2)	0.4278(2)	0.8920(2)	0.0371(10)
H7A_1	0.413574	0.419023	0.848771	0.056
H7B_1	0.440430	0.385183	0.912405	0.056
H7C_1	0.467733	0.457212	0.890914	0.056
C10_1	0.2053(2)	0.4652(2)	1.0038(2)	0.0306(8)
H10A_1	0.186278	0.506624	1.021131	0.046
H10B_1	0.209157	0.431538	1.037435	0.046
H10C_1	0.176395	0.447911	0.970317	0.046
C1_2	0.2761(2)	0.63709(19)	0.86438(18)	0.0260(7)
C2_2	0.3359(2)	0.64722(19)	0.8976(2)	0.0291(7)
C3_2	0.3877(2)	0.6089(2)	0.8665(2)	0.0308(8)
C4_2	0.3585(2)	0.57459(19)	0.81548(19)	0.0272(8)
C5_2	0.2927(2)	0.59401(18)	0.81104(18)	0.0256(7)
C6_2	0.2129(2)	0.6744(2)	0.8750(3)	0.0391(10)
H6A_2	0.212215	0.714686	0.848365	0.059
H6B_2	0.209821	0.687594	0.919483	0.059
H6C_2	0.175207	0.645468	0.864132	0.059
C7_2	0.3475(2)	0.6972(2)	0.9497(2)	0.0371(9)
H7A_2	0.385798	0.683080	0.974969	0.056
H7B_2	0.307996	0.699667	0.976611	0.056
H7C_2	0.356313	0.741584	0.931300	0.056
C11_2	0.2491(3)	0.5856(3)	0.7538(2)	0.0384(10)
H11A_2	0.265259	0.614635	0.719703	0.058
H11B_2	0.203300	0.598021	0.764435	0.058
H11C_2	0.250271	0.538585	0.739878	0.058
C9_2	0.3938(2)	0.5328(2)	0.7665(2)	0.0354(9)
H9A_2	0.398410	0.558867	0.727487	0.053
H9B_2	0.367979	0.491994	0.757992	0.053
H9C_2	0.437912	0.520349	0.782196	0.053
C8_2	0.4612(2)	0.6165(2)	0.8745(2)	0.0373(9)
H8A_2	0.482500	0.572331	0.870810	0.056
H8B_2	0.470611	0.635463	0.916284	0.056
H8C_2	0.478555	0.646535	0.841818	0.056

*Table S 15 Atomic coordinates and U_{eq} [Å^2] for **S1***

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.24066(5)	0.57875(3)	0.77546(3)	0.01127(11)
N1	0.78940(16)	0.73189(8)	0.54999(8)	0.0173(3)
O1_1	0.17863(13)	0.58373(7)	0.84690(6)	0.0167(3)
C1_1	0.07063(19)	0.58535(10)	0.87294(10)	0.0191(4)
C2_1	-0.0052(2)	0.52274(11)	0.86082(11)	0.0260(5)
F1_1	-0.07683(12)	0.52105(7)	0.80025(6)	0.0312(3)

F2_1	-0.08400(12)	0.51392(7)	0.90342(7)	0.0332(3)
F3_1	0.07406(13)	0.47442(6)	0.86549(8)	0.0390(4)
C3_1	0.1116(2)	0.59671(12)	0.94818(11)	0.0297(5)
F4_1	0.20105(14)	0.64072(8)	0.96106(7)	0.0435(4)
F5_1	0.16125(14)	0.54472(8)	0.97840(7)	0.0430(4)
F6_1	0.01358(13)	0.61369(8)	0.97663(7)	0.0393(4)
C4_1	-0.0183(2)	0.64007(11)	0.84254(11)	0.0266(5)
F7_1	0.02545(14)	0.69558(6)	0.86837(8)	0.0382(3)
F8_1	-0.13853(12)	0.63417(7)	0.85243(7)	0.0323(3)
F9_1	-0.02108(13)	0.64452(7)	0.77838(7)	0.0330(3)
O1_2	0.26916(12)	0.65151(6)	0.74341(7)	0.0155(3)
C1_2	0.34598(19)	0.70239(9)	0.74849(10)	0.0173(4)
C2_2	0.3179(2)	0.74620(10)	0.80436(12)	0.0301(5)
F1_2	0.20404(15)	0.77404(7)	0.78673(8)	0.0431(4)
F2_2	0.40654(17)	0.79082(7)	0.82037(8)	0.0460(4)
F3_2	0.31349(16)	0.71322(7)	0.85866(7)	0.0380(3)
C3_2	0.4906(2)	0.68389(10)	0.76286(12)	0.0263(5)
F4_2	0.51257(12)	0.63674(6)	0.72452(7)	0.0326(3)
F5_2	0.52644(13)	0.66593(6)	0.82547(7)	0.0359(3)
F6_2	0.56672(13)	0.73115(7)	0.75235(9)	0.0449(4)
C4_2	0.3163(2)	0.73851(10)	0.68174(11)	0.0233(4)
F7_2	0.36866(13)	0.71032(7)	0.63597(6)	0.0329(3)
F8_2	0.36011(13)	0.79744(6)	0.68701(7)	0.0338(3)
F9_2	0.19030(12)	0.74122(7)	0.65921(7)	0.0333(3)
O1_3	0.38510(13)	0.53971(6)	0.79293(7)	0.0185(3)
C1_3	0.45523(19)	0.49356(9)	0.82703(10)	0.0210(4)
C2_3	0.5943(2)	0.49855(11)	0.81340(14)	0.0336(6)
F1_3	0.65396(13)	0.54740(7)	0.84548(10)	0.0484(4)
F2_3	0.66394(13)	0.44711(6)	0.83333(9)	0.0409(4)
F3_3	0.59415(14)	0.50660(7)	0.74978(9)	0.0426(4)
C3_3	0.3981(2)	0.42831(10)	0.80376(11)	0.0244(4)
F4_3	0.27143(12)	0.42872(6)	0.79720(7)	0.0273(3)
F5_3	0.42636(13)	0.41281(6)	0.74553(7)	0.0320(3)
F6_3	0.44305(13)	0.38240(6)	0.84616(7)	0.0331(3)
C4_3	0.4584(2)	0.50027(11)	0.90228(11)	0.0299(5)
F7_3	0.35094(14)	0.47786(7)	0.91862(7)	0.0350(3)
F8_3	0.55708(15)	0.46902(7)	0.93839(7)	0.0444(4)
F9_3	0.46915(15)	0.55994(7)	0.92036(7)	0.0386(3)
O1_4	0.12877(13)	0.54181(6)	0.71641(7)	0.0181(3)
C1_4	0.0872(2)	0.52560(10)	0.65292(10)	0.0205(4)
C2_4	0.1790(2)	0.54885(13)	0.60767(11)	0.0368(6)
F1_4	0.16546(16)	0.60954(8)	0.59574(7)	0.0504(4)
F2_4	0.15864(17)	0.51894(11)	0.54974(7)	0.0616(5)
F3_4	0.30129(14)	0.53918(9)	0.63630(7)	0.0454(4)
C3_4	0.0771(2)	0.45285(11)	0.64820(12)	0.0302(5)
F4_4	0.03270(13)	0.42949(6)	0.69854(7)	0.0355(3)
F5_4	0.19170(14)	0.42688(7)	0.64839(8)	0.0443(4)
F6_4	-0.00133(15)	0.43432(7)	0.59245(8)	0.0457(4)
C4_4	-0.0490(2)	0.55403(10)	0.62904(10)	0.0247(5)
F7_4	-0.13578(12)	0.52476(7)	0.65666(7)	0.0306(3)
F8_4	-0.08819(14)	0.55045(7)	0.56354(6)	0.0361(3)
F9_4	-0.05067(14)	0.61433(6)	0.64507(7)	0.0367(3)
C1_5	0.69105(19)	0.68931(9)	0.52445(10)	0.0177(4)
Br1_5	0.36682(2)	0.54783(2)	0.44513(2)	0.03149(7)
C2_5	0.6605(2)	0.67704(10)	0.45660(10)	0.0224(4)

H2_5	0.705458	0.697844	0.427111	0.027
C3_5	0.5647(2)	0.63453(11)	0.43294(10)	0.0242(5)
H3_5	0.544022	0.625358	0.387120	0.029
C4_5	0.4988(2)	0.60522(10)	0.47681(11)	0.0222(4)
C5_5	0.5273(2)	0.61739(10)	0.54395(11)	0.0225(4)
H5_5	0.480970	0.596941	0.573075	0.027
C6_5	0.6235(2)	0.65951(10)	0.56802(10)	0.0203(4)
H6_5	0.643957	0.668282	0.613933	0.024
C1_6	0.77991(19)	0.76494(9)	0.60885(10)	0.0166(4)
Br1_6	0.75254(2)	0.86650(2)	0.80282(2)	0.03014(6)
C2_6	0.66858(19)	0.79878(9)	0.61260(10)	0.0186(4)
H2_6	0.599253	0.800315	0.575972	0.022
C3_6	0.6607(2)	0.83000(9)	0.67040(11)	0.0203(4)
H3_6	0.587155	0.854450	0.673642	0.024
C4_6	0.7622(2)	0.82504(9)	0.72368(10)	0.0187(4)
C5_6	0.87210(19)	0.79095(10)	0.72043(10)	0.0197(4)
H5_6	0.939751	0.788042	0.757746	0.024
C6_6	0.88199(19)	0.76123(9)	0.66222(10)	0.0188(4)
H6_6	0.957543	0.738508	0.658590	0.023
C1_7	0.90104(19)	0.73958(10)	0.52358(9)	0.0173(4)
Br1_7	1.29272(2)	0.76267(2)	0.45726(2)	0.03286(7)
C2_7	0.9543(2)	0.68893(10)	0.49459(10)	0.0201(4)
H2_7	0.911037	0.649723	0.489126	0.024
C3_7	1.0700(2)	0.69670(10)	0.47413(10)	0.0224(4)
H3_7	1.107478	0.662720	0.454753	0.027
C4_7	1.1315(2)	0.75444(10)	0.48199(10)	0.0212(4)
C5_7	1.0776(2)	0.80561(10)	0.50828(10)	0.0214(4)
H5_7	1.119483	0.845184	0.511657	0.026
C6_7	0.96264(19)	0.79815(10)	0.52939(10)	0.0189(4)
H6_7	0.924971	0.832612	0.547886	0.023

*Table S 16 Atomic coordinates and U_{eq} [Å²] for **S2***

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.06641(18)	0.44463(11)	0.32194(10)	0.0150(3)
Al2	-0.01161(18)	0.90039(11)	0.67600(10)	0.0145(3)
N1	0.7873(5)	0.3556(3)	0.7898(3)	0.0158(10)
N2	0.2774(5)	-0.0130(3)	0.2079(3)	0.0167(10)
O1_1	0.1448(4)	0.4620(3)	0.4335(2)	0.0210(8)
C1_1	0.2406(6)	0.4465(4)	0.4987(4)	0.0191(12)
C2_1	0.3590(7)	0.4274(5)	0.4631(4)	0.0309(14)
F1_1	0.3149(5)	0.3341(3)	0.4260(3)	0.0439(11)
F2_1	0.4703(4)	0.4378(3)	0.5266(3)	0.0336(9)
F3_1	0.3937(5)	0.4807(4)	0.4020(3)	0.0523(13)
C3_1	0.3050(7)	0.5387(4)	0.5695(4)	0.0298(14)
F4_1	0.2092(5)	0.5719(3)	0.5846(3)	0.0403(10)
F5_1	0.3962(5)	0.6080(3)	0.5385(3)	0.0435(11)
F6_1	0.3733(4)	0.5229(3)	0.6460(2)	0.0353(9)
C4_1	0.1673(7)	0.3602(4)	0.5446(4)	0.0301(14)
F7_1	0.0900(5)	0.3843(3)	0.5960(3)	0.0405(10)
F8_1	0.2559(4)	0.3283(3)	0.5979(3)	0.0346(9)
F9_1	0.0787(5)	0.2871(3)	0.4864(3)	0.0454(11)
O1_2	-0.0881(4)	0.4651(3)	0.3127(2)	0.0201(8)
C1_2	-0.2010(6)	0.4604(4)	0.3443(4)	0.0173(11)

C2_2	-0.2854(6)	0.5110(4)	0.2832(4)	0.0243(12)
F1_2	-0.2235(5)	0.6061(3)	0.2995(3)	0.0364(9)
F2_2	-0.4155(4)	0.4882(3)	0.2916(3)	0.0380(9)
F3_2	-0.2915(4)	0.4857(3)	0.1980(2)	0.0298(8)
C3_2	-0.2942(7)	0.3529(4)	0.3432(4)	0.0243(13)
F4_2	-0.2158(4)	0.3025(2)	0.3756(2)	0.0316(9)
F5_2	-0.3614(4)	0.3118(3)	0.2602(2)	0.0348(9)
F6_2	-0.3897(4)	0.3448(3)	0.3912(2)	0.0328(9)
C4_2	-0.1583(7)	0.5119(4)	0.4413(4)	0.0241(13)
F7_2	-0.1215(4)	0.4565(3)	0.4999(2)	0.0304(8)
F8_2	-0.2629(4)	0.5340(3)	0.4637(2)	0.0326(9)
F9_2	-0.0517(4)	0.5931(2)	0.4507(2)	0.0332(9)
O1_3	0.1620(5)	0.5193(3)	0.2581(3)	0.0203(9)
C1_3	0.2014(6)	0.6066(4)	0.2286(4)	0.0215(12)
C2_3	0.3407(8)	0.6235(5)	0.2015(5)	0.0441(18)
F1_3	0.4467(5)	0.6474(4)	0.2754(4)	0.0624(14)
F2_3	0.3697(5)	0.6961(3)	0.1516(3)	0.0475(12)
F3_3	0.3462(6)	0.5479(3)	0.1607(4)	0.0597(15)
C3_3	0.0918(7)	0.6109(4)	0.1479(4)	0.0318(14)
F4_3	-0.0353(4)	0.5684(3)	0.1565(3)	0.0457(11)
F5_3	0.1013(6)	0.5610(3)	0.0744(3)	0.0533(13)
F6_3	0.1054(4)	0.6987(2)	0.1273(2)	0.0308(8)
C4_3	0.2251(8)	0.6883(4)	0.3040(4)	0.0356(16)
F7_3	0.0957(5)	0.6890(3)	0.3128(3)	0.0442(11)
F8_3	0.2915(4)	0.7763(2)	0.2857(3)	0.0345(9)
F9_3	0.2811(6)	0.6742(3)	0.3810(3)	0.0581(15)
O1_4	0.0455(10)	0.3277(4)	0.2831(6)	0.0158(17)
C1_4	0.0188(10)	0.2610(5)	0.2125(5)	0.0192(17)
C2_4	-0.0631(12)	0.1622(6)	0.2384(6)	0.029(3)
F1_4	-0.1935(6)	0.1536(3)	0.2377(5)	0.0388(13)
F2_4	-0.0678(8)	0.0879(3)	0.1818(4)	0.0453(17)
F3_4	-0.0028(5)	0.1514(3)	0.3192(3)	0.0355(12)
C3_4	0.1582(10)	0.2603(5)	0.1924(6)	0.0270(17)
F4_4	0.2441(6)	0.3474(3)	0.1933(3)	0.0381(14)
F5_4	0.2194(6)	0.2169(4)	0.2511(3)	0.0375(13)
F6_4	0.1363(7)	0.2104(5)	0.1119(3)	0.0419(14)
C4_4	-0.0708(11)	0.2838(5)	0.1293(5)	0.0295(17)
F7_4	0.0073(6)	0.3586(3)	0.0956(3)	0.0410(15)
F8_4	-0.1268(9)	0.2097(6)	0.0644(5)	0.0416(18)
F9_4	-0.1740(6)	0.3081(4)	0.1492(3)	0.0408(14)
O1_5	-0.1224(4)	0.9200(3)	0.5862(2)	0.0190(8)
C1_5	-0.1787(6)	0.9001(4)	0.4981(3)	0.0183(11)
C2_5	-0.1077(6)	0.9883(4)	0.4519(4)	0.0208(12)
F1_5	-0.1467(4)	1.0628(2)	0.4724(2)	0.0269(8)
F2_5	-0.1417(4)	0.9675(2)	0.3634(2)	0.0310(9)
F3_5	0.0300(4)	1.0179(2)	0.4787(2)	0.0274(8)
C3_5	-0.1584(7)	0.8093(4)	0.4551(4)	0.0231(12)
F4_5	-0.1689(4)	0.7442(2)	0.5111(2)	0.0304(9)
F5_5	-0.0339(4)	0.8307(2)	0.4367(2)	0.0286(8)
F6_5	-0.2536(4)	0.7692(2)	0.3793(2)	0.0297(8)
C4_5	-0.3370(6)	0.8812(4)	0.4824(4)	0.0233(12)
F7_5	-0.4038(4)	0.7950(2)	0.5022(3)	0.0309(8)
F8_5	-0.3952(4)	0.8872(3)	0.3989(2)	0.0317(8)
F9_5	-0.3607(4)	0.9470(2)	0.5341(2)	0.0267(8)
O1_6	0.0313(5)	0.9955(3)	0.7589(3)	0.0239(9)

C1_6	0.0258(6)	1.0828(4)	0.7829(3)	0.0194(11)
C2_6	0.1231(7)	1.1621(4)	0.7396(4)	0.0232(13)
F1_6	0.2569(4)	1.1829(3)	0.7776(3)	0.0315(9)
F2_6	0.0970(4)	1.2447(2)	0.7442(2)	0.0269(8)
F3_6	0.1065(4)	1.1324(3)	0.6540(2)	0.0331(9)
C3_6	-0.1237(7)	1.0844(4)	0.7560(4)	0.0221(12)
F4_6	-0.2153(4)	1.0029(2)	0.7702(3)	0.0329(9)
F5_6	-0.1582(4)	1.0933(2)	0.6701(2)	0.0264(8)
F6_6	-0.1410(4)	1.1571(2)	0.8021(2)	0.0274(8)
C4_6	0.0779(7)	1.1054(4)	0.8861(3)	0.0232(12)
F7_6	-0.0197(4)	1.0542(3)	0.9252(2)	0.0325(9)
F8_6	0.1106(4)	1.1984(2)	0.9154(2)	0.0312(9)
F9_6	0.1915(4)	1.0828(3)	0.9144(2)	0.0306(8)
O1_7	0.1317(4)	0.8960(3)	0.6393(3)	0.0218(8)
C1_7	0.2583(6)	0.8881(4)	0.6572(4)	0.0225(12)
C2_7	0.3705(7)	0.9902(4)	0.6806(5)	0.0335(15)
F1_7	0.3796(5)	1.0295(3)	0.7620(3)	0.0414(10)
F2_7	0.4978(5)	0.9925(3)	0.6763(4)	0.0508(12)
F3_7	0.3379(5)	1.0495(3)	0.6252(3)	0.0444(11)
C3_7	0.2759(7)	0.8358(4)	0.5725(4)	0.0271(13)
F4_7	0.1646(4)	0.7592(3)	0.5396(3)	0.0342(9)
F5_7	0.2911(5)	0.8943(3)	0.5098(3)	0.0407(10)
F6_7	0.3864(4)	0.8081(3)	0.5896(3)	0.0409(10)
C4_7	0.2777(7)	0.8291(4)	0.7372(4)	0.0293(13)
F7_7	0.2005(5)	0.7362(3)	0.7121(3)	0.0408(10)
F8_7	0.4082(5)	0.8358(3)	0.7674(3)	0.0459(11)
F9_7	0.2344(5)	0.8603(3)	0.8040(2)	0.0378(9)
O1_8	-0.0790(5)	0.7950(3)	0.7190(3)	0.0233(9)
C1_8	-0.1668(6)	0.7314(3)	0.7583(3)	0.0187(11)
C2_8	-0.0844(7)	0.7214(4)	0.8508(4)	0.0280(13)
F1_8	-0.0027(5)	0.6704(3)	0.8423(2)	0.0352(9)
F2_8	-0.1694(5)	0.6766(3)	0.9021(2)	0.0371(10)
F3_8	-0.0027(5)	0.8075(3)	0.8939(2)	0.0346(9)
C3_8	-0.2907(7)	0.7629(4)	0.7707(4)	0.0257(13)
F4_8	-0.3356(4)	0.7998(3)	0.6992(2)	0.0323(8)
F5_8	-0.2497(5)	0.8310(3)	0.8403(2)	0.0331(9)
F6_8	-0.3970(5)	0.6900(3)	0.7841(3)	0.0407(10)
C4_8	-0.2260(7)	0.6324(4)	0.6978(4)	0.0235(12)
F7_8	-0.3244(4)	0.6312(2)	0.6295(2)	0.0302(8)
F8_8	-0.2768(5)	0.5582(2)	0.7422(3)	0.0392(11)
F9_8	-0.1244(4)	0.6160(2)	0.6659(2)	0.0304(8)
C1_9	0.7105(7)	0.3491(4)	0.8570(4)	0.0195(12)
Br1_9	0.43590(7)	0.33134(5)	1.05977(4)	0.03289(17)
C2_9	0.6115(7)	0.2615(4)	0.8629(4)	0.0210(13)
H2_9	0.599956	0.205264	0.825181	0.025
C3_9	0.5298(7)	0.2560(4)	0.9238(4)	0.0244(13)
H3_9	0.459116	0.197104	0.927006	0.029
C4_9	0.5535(7)	0.3382(5)	0.9794(4)	0.0236(13)
C5_9	0.6544(7)	0.4252(4)	0.9770(4)	0.0231(13)
H5_9	0.668375	0.480201	1.017187	0.028
C6_9	0.7352(7)	0.4314(4)	0.9156(4)	0.0205(12)
H6_9	0.806073	0.490478	0.913080	0.025
C1_10	0.9350(6)	0.4019(4)	0.8153(4)	0.0163(12)
Br1_10	1.41136(8)	0.56180(6)	0.91205(5)	0.0451(2)
C2_10	1.0083(7)	0.3833(4)	0.8953(4)	0.0217(13)

H2_10	0.959655	0.338850	0.929885	0.026
C3_10	1.1488(7)	0.4288(4)	0.9232(4)	0.0260(14)
H3_10	1.198832	0.415775	0.976480	0.031
C4_10	1.2179(7)	0.4952(4)	0.8720(4)	0.0239(13)
C5_10	1.1470(7)	0.5141(4)	0.7927(4)	0.0255(14)
H5_10	1.195549	0.559122	0.758526	0.031
C6_10	1.0061(7)	0.4666(4)	0.7647(4)	0.0181(12)
H6_10	0.956831	0.478015	0.710244	0.022
C1_13	0.7197(7)	0.3143(4)	0.7052(4)	0.0170(12)
C2_13	0.7912(7)	0.2842(4)	0.6458(4)	0.0177(12)
H2_13	0.889607	0.301775	0.661845	0.021
C3_13	0.7180(6)	0.2306(4)	0.5669(4)	0.0178(12)
H3_13	0.766422	0.209455	0.529032	0.021
C4_13	0.5699(6)	0.2047(4)	0.5385(3)	0.0159(11)
C5_13	0.5040(7)	0.2447(4)	0.5948(4)	0.0201(12)
H5_13	0.407423	0.234053	0.575553	0.024
C6_13	0.5746(7)	0.2972(4)	0.6746(4)	0.0207(12)
H6_13	0.527490	0.322779	0.710318	0.025
C1_14	0.3447(6)	0.0325(4)	0.2912(4)	0.0171(12)
C2_14	0.4897(7)	0.0528(4)	0.3212(4)	0.0186(12)
H2_14	0.537712	0.029458	0.284509	0.022
C3_14	0.5613(6)	0.1050(4)	0.4015(4)	0.0179(12)
H3_14	0.657933	0.116040	0.420899	0.021
C4_14	0.4925(6)	0.1436(4)	0.4571(4)	0.0167(11)
C5_14	0.3453(7)	0.1173(4)	0.4284(4)	0.0198(12)
H5_14	0.296266	0.138102	0.466028	0.024
C6_14	0.2725(7)	0.0634(4)	0.3488(4)	0.0200(12)
H6_14	0.174199	0.046390	0.331881	0.024
Br1_11	-0.33799(8)	-0.24481(6)	0.08472(5)	0.0449(2)
C1_11	0.1308(6)	-0.0636(4)	0.1815(4)	0.0171(12)
C2_11	0.0599(6)	-0.0572(4)	0.0977(4)	0.0193(12)
H2_11	0.107726	-0.016664	0.060213	0.023
C3_11	-0.0811(7)	-0.1102(4)	0.0686(4)	0.0234(13)
H3_11	-0.131079	-0.106464	0.011289	0.028
C4_11	-0.1476(7)	-0.1690(5)	0.1255(4)	0.0257(14)
C5_11	-0.0790(7)	-0.1751(4)	0.2093(4)	0.0232(13)
H5_11	-0.127456	-0.215142	0.246836	0.028
C6_11	0.0630(7)	-0.1215(4)	0.2385(4)	0.0193(12)
H6_11	0.112496	-0.124498	0.296256	0.023
C1_12	0.3565(6)	-0.0109(4)	0.1409(3)	0.0171(12)
Br1_12	0.63200(7)	-0.00056(5)	-0.06009(4)	0.03654(18)
C2_12	0.3414(7)	-0.0966(4)	0.0922(4)	0.0249(14)
H2_12	0.277343	-0.156221	0.100764	0.030
C3_12	0.4218(7)	-0.0931(5)	0.0307(4)	0.0279(14)
H3_12	0.412177	-0.150392	-0.004654	0.033
C4_12	0.5180(7)	-0.0041(5)	0.0209(4)	0.0255(14)
C5_12	0.5292(7)	0.0800(5)	0.0683(4)	0.0261(14)
H5_12	0.592804	0.139642	0.059387	0.031
C6_12	0.4485(7)	0.0782(4)	0.1288(4)	0.0221(13)
H6_12	0.455064	0.136297	0.161617	0.026
O1_15	0.026(6)	0.330(2)	0.269(3)	0.032(17)
C1_15	-0.014(2)	0.2583(15)	0.1998(16)	0.017(12)
C2_15	-0.121(3)	0.2804(16)	0.1262(17)	0.018(10)
F1_15	-0.243(3)	0.2616(19)	0.1483(17)	0.039(7)
F2_15	-0.144(4)	0.227(2)	0.0493(18)	0.024(9)

F3_15	-0.073(2)	0.3742(12)	0.1172(14)	0.026(5)
C3_15	0.114(2)	0.2558(16)	0.1652(16)	0.016(10)
F4_15	0.219(2)	0.261(2)	0.2319(15)	0.027(6)
F5_15	0.158(2)	0.3308(13)	0.1207(14)	0.031(6)
F6_15	0.088(3)	0.1758(16)	0.1109(17)	0.031(8)
C4_15	-0.083(3)	0.1592(16)	0.2303(16)	0.012(12)
F7_15	0.014(2)	0.1291(16)	0.2774(17)	0.029(6)
F8_15	-0.150(3)	0.0905(14)	0.1616(12)	0.022(5)
F9_15	-0.169(3)	0.1633(17)	0.2817(17)	0.026(6)

*Table S 17 Atomic coordinates and U_{eq} [Å^2] for **S3***

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.62351(6)	0.25485(5)	0.38363(4)	0.01479(17)
N01A	0.10047(18)	0.35662(15)	0.73542(11)	0.0199(5)
O1_1	0.53969(14)	0.33396(12)	0.36608(9)	0.0198(4)
C1_1	0.4887(2)	0.39544(18)	0.38621(13)	0.0210(6)
C2_1	0.4330(2)	0.4444(2)	0.33277(15)	0.0320(7)
F1_1	0.49279(16)	0.49648(13)	0.31199(9)	0.0391(5)
F2_1	0.36067(16)	0.49068(14)	0.34565(10)	0.0470(6)
F3_1	0.39636(15)	0.39157(14)	0.29082(9)	0.0415(5)
C3_1	0.4159(2)	0.3574(2)	0.42090(16)	0.0326(7)
F4_1	0.45822(16)	0.29881(13)	0.45730(10)	0.0418(5)
F5_1	0.34264(14)	0.32078(14)	0.38505(11)	0.0463(6)
F6_1	0.37863(14)	0.41484(13)	0.45193(10)	0.0399(5)
C4_1	0.5569(2)	0.45750(18)	0.42540(13)	0.0247(6)
F7_1	0.58072(14)	0.42855(12)	0.47920(8)	0.0308(4)
F8_1	0.51570(15)	0.53316(11)	0.42843(9)	0.0354(5)
F9_1	0.63717(13)	0.46882(12)	0.40538(8)	0.0303(4)
O1_2	0.68685(14)	0.24533(12)	0.32783(8)	0.0185(4)
C1_2	0.7292(2)	0.28421(18)	0.28772(13)	0.0207(6)
C2_2	0.6627(2)	0.35282(18)	0.25408(13)	0.0244(6)
F1_2	0.66499(15)	0.42268(11)	0.28598(9)	0.0331(4)
F2_2	0.68799(15)	0.37366(12)	0.20417(8)	0.0349(5)
F3_2	0.57191(12)	0.32692(11)	0.24253(8)	0.0273(4)
C3_2	0.7494(2)	0.2162(2)	0.24422(14)	0.0294(7)
F4_2	0.78907(15)	0.14850(13)	0.27141(9)	0.0391(5)
F5_2	0.66866(15)	0.19249(12)	0.20957(8)	0.0341(4)
F6_2	0.80931(16)	0.24398(14)	0.21014(10)	0.0455(6)
C4_2	0.8244(2)	0.3267(2)	0.31780(16)	0.0348(8)
F7_2	0.89144(14)	0.26904(16)	0.33549(11)	0.0499(6)
F8_2	0.85990(16)	0.37918(16)	0.28236(10)	0.0522(6)
F9_2	0.81132(15)	0.37043(14)	0.36361(9)	0.0418(5)
O1_3	0.56818(15)	0.16019(12)	0.39213(9)	0.0206(4)
C1_3	0.5188(2)	0.09410(17)	0.36453(12)	0.0188(6)
C2_3	0.4422(2)	0.12408(18)	0.31222(13)	0.0243(6)
F1_3	0.36910(14)	0.16193(13)	0.33052(9)	0.0369(5)
F2_3	0.40585(14)	0.06129(12)	0.27760(8)	0.0319(4)
F3_3	0.48011(15)	0.17930(12)	0.28063(8)	0.0369(5)
C3_3	0.5895(2)	0.03151(19)	0.34331(13)	0.0245(6)
F4_3	0.66777(13)	0.02109(13)	0.38361(9)	0.0352(5)
F5_3	0.61742(15)	0.05981(13)	0.29596(8)	0.0355(5)
F6_3	0.55045(14)	-0.04467(11)	0.33085(9)	0.0311(4)
C4_3	0.4684(2)	0.04832(18)	0.40901(13)	0.0233(6)

F7_3	0.53214(15)	0.00723(12)	0.44763(8)	0.0326(4)
F8_3	0.40244(14)	-0.00729(12)	0.38401(9)	0.0329(4)
F9_3	0.42347(14)	0.10249(12)	0.43772(9)	0.0323(4)
O1_4	0.69725(14)	0.27979(12)	0.44836(9)	0.0202(4)
C1_4	0.7593(2)	0.25269(18)	0.49597(13)	0.0223(6)
C2_4	0.8486(2)	0.2105(2)	0.47947(14)	0.0302(7)
F1_4	0.90899(14)	0.26815(16)	0.46514(10)	0.0488(6)
F2_4	0.89903(14)	0.16517(13)	0.52278(9)	0.0383(5)
F3_4	0.82371(14)	0.16034(13)	0.43421(8)	0.0365(5)
C3_4	0.7092(2)	0.1880(2)	0.53052(14)	0.0304(7)
F4_4	0.61935(15)	0.21125(16)	0.53156(10)	0.0484(6)
F5_4	0.70511(15)	0.11257(12)	0.50655(9)	0.0358(5)
F6_4	0.75477(17)	0.18014(15)	0.58568(8)	0.0444(5)
C4_4	0.7911(3)	0.3307(2)	0.53485(16)	0.0423(9)
F7_4	0.7229(2)	0.35375(16)	0.56378(10)	0.0605(7)
F8_4	0.87114(18)	0.31467(14)	0.57432(10)	0.0558(7)
F9_4	0.80982(19)	0.39498(13)	0.50341(11)	0.0585(7)
C1_7	0.1132(2)	0.37335(18)	0.79629(13)	0.0194(6)
Br1_7	0.13326(3)	0.43835(2)	0.99137(2)	0.03388(10)
C2_7	0.1514(2)	0.45028(18)	0.81783(14)	0.0220(6)
H2_7	0.171550	0.490150	0.792351	0.026
C3_7	0.1601(2)	0.46877(19)	0.87595(14)	0.0226(6)
H3_7	0.185857	0.521317	0.890645	0.027
C4_7	0.1310(2)	0.41034(19)	0.91252(13)	0.0224(6)
C5_7	0.0965(2)	0.33267(19)	0.89216(14)	0.0265(7)
H5_7	0.078814	0.292132	0.918067	0.032
C6_7	0.0878(2)	0.31430(19)	0.83426(14)	0.0243(7)
H6_7	0.064255	0.260814	0.820136	0.029
C1_6	0.1002(2)	0.27138(17)	0.71607(12)	0.0179(6)
Br1_6	0.10710(2)	0.00141(2)	0.64049(2)	0.02557(8)
C2_6	0.1824(2)	0.22207(19)	0.73097(13)	0.0206(6)
H2_6	0.237493	0.243972	0.756001	0.025
C3_6	0.1842(2)	0.14122(18)	0.70939(13)	0.0200(6)
H3_6	0.240095	0.107299	0.719641	0.024
C4_6	0.1034(2)	0.11008(17)	0.67263(13)	0.0178(6)
C5_6	0.0206(2)	0.15712(18)	0.65867(13)	0.0189(6)
H5_6	-0.034808	0.134460	0.634357	0.023
C6_6	0.0190(2)	0.23804(18)	0.68058(13)	0.0200(6)
H6_6	-0.037853	0.270971	0.671292	0.024
C1_8	0.0492(2)	0.41578(18)	0.69617(13)	0.0180(6)
Br1_8	-0.12143(2)	0.59971(2)	0.55863(2)	0.03178(9)
C2_8	0.0729(2)	0.42650(17)	0.64166(13)	0.0181(6)
C3_8	0.0231(2)	0.48057(18)	0.60053(13)	0.0190(6)
H3_8	0.040416	0.486090	0.563453	0.023
C4_8	-0.0523(2)	0.52622(18)	0.61468(13)	0.0209(6)
C5_8	-0.0772(2)	0.51905(19)	0.66884(15)	0.0247(7)
H5_8	-0.128638	0.551565	0.678282	0.030
C6_8	-0.0266(2)	0.46404(19)	0.70922(14)	0.0225(6)
H6_8	-0.043745	0.459156	0.746369	0.027
N1_5	0.38327(18)	0.24390(16)	0.59101(11)	0.0215(5)
C1_5	0.2442(2)	0.39631(18)	0.65557(13)	0.0195(6)
H1_5	0.253886	0.439579	0.683980	0.023
N2_5	0.15299(17)	0.38002(14)	0.62694(10)	0.0165(5)
C3_5	0.3090(2)	0.28807(18)	0.60255(12)	0.0178(6)
C4_5	0.2127(2)	0.27247(18)	0.57342(12)	0.0188(6)

H4_5	0.200488	0.229712	0.544713	0.023
C5_5	0.1387(2)	0.31824(18)	0.58643(12)	0.0178(6)
H5_5	0.075068	0.306762	0.566660	0.021
C6_5	0.4812(2)	0.2583(2)	0.62220(15)	0.0301(7)
H6A_5	0.520909	0.208766	0.618393	0.045
H6B_5	0.480084	0.268321	0.663288	0.045
H6C_5	0.508468	0.307513	0.605884	0.045
C7_5	0.3689(2)	0.1801(2)	0.54567(15)	0.0273(7)
H7A_5	0.332824	0.204444	0.509783	0.041
H7B_5	0.332618	0.132816	0.557700	0.041
H7C_5	0.431638	0.160136	0.539014	0.041
C2_5	0.3207(2)	0.35307(18)	0.64484(13)	0.0199(6)
H2_5	0.383171	0.366038	0.665722	0.024

Table S 18 Atomic coordinates and U_{eq} *[Å²] for* ***S4a***

Atom	***x***	***y***	***z***	U_{eq}
Al04	0.13750(4)	0.46500(3)	0.64446(2)	0.01661(14)
N1	0.58600(10)	0.28456(7)	0.58272(5)	0.0149(4)
O1_1	0.2098(9)	0.5139(7)	0.6403(6)	0.031(3)
C1_1	0.2696(5)	0.5430(3)	0.6564(2)	0.0219(17)
C2_1	0.3307(3)	0.5515(2)	0.62257(15)	0.0306(12)
F1_1	0.3747(8)	0.5072(5)	0.6168(4)	0.045(3)
F2_1	0.3807(2)	0.59257(18)	0.63026(11)	0.0404(10)
F3_1	0.2958(6)	0.5631(4)	0.5882(2)	0.0434(18)
C3_1	0.2391(3)	0.5998(2)	0.67052(15)	0.0290(12)
F4_1	0.1726(6)	0.5950(6)	0.6910(4)	0.036(3)
F5_1	0.2221(4)	0.6327(3)	0.63989(15)	0.0365(13)
F6_1	0.2903(8)	0.6274(5)	0.6933(4)	0.034(2)
C4_1	0.3102(3)	0.51301(19)	0.69171(14)	0.0257(11)
F7_1	0.2673(4)	0.5167(2)	0.72449(17)	0.0353(12)
F8_1	0.3814(2)	0.53388(18)	0.69963(14)	0.0375(10)
F9_1	0.3179(7)	0.4600(3)	0.6835(3)	0.0371(16)
O1_2	0.06357(9)	0.47669(6)	0.61020(4)	0.0193(3)
C1_2	0.01284(12)	0.51341(9)	0.59397(6)	0.0179(4)
C2_2	0.05665(14)	0.55165(10)	0.56431(7)	0.0269(5)
F1_2	0.09772(9)	0.59062(6)	0.58366(5)	0.0387(4)
F2_2	0.00777(9)	0.57774(6)	0.53947(4)	0.0353(4)
F3_2	0.10780(9)	0.52338(6)	0.54245(4)	0.0363(4)
C3_2	-0.05181(14)	0.48030(10)	0.57129(7)	0.0243(5)
F4_2	-0.07820(8)	0.43878(6)	0.59343(4)	0.0305(3)
F5_2	-0.02224(9)	0.45878(6)	0.53817(4)	0.0346(4)
F6_2	-0.11414(8)	0.51125(6)	0.56156(5)	0.0368(4)
C4_2	-0.02707(13)	0.54917(9)	0.62655(7)	0.0219(5)
F7_2	-0.08083(8)	0.52066(6)	0.64671(4)	0.0293(3)
F8_2	-0.06345(8)	0.59367(6)	0.61148(4)	0.0316(3)
F9_2	0.02647(8)	0.56697(6)	0.65255(4)	0.0287(3)
O1_3	0.10127(9)	0.46566(6)	0.69265(4)	0.0227(3)
C1_3	0.06886(14)	0.43493(10)	0.72202(7)	0.0244(5)
C2_3	0.02328(17)	0.38447(12)	0.70561(7)	0.0368(6)
F1_3	0.07299(11)	0.34279(6)	0.69749(5)	0.0463(4)
F2_3	-0.03059(10)	0.36454(7)	0.73099(4)	0.0465(4)
F3_3	-0.01351(10)	0.39670(7)	0.67210(4)	0.0448(4)
C3_3	0.01128(16)	0.47194(11)	0.74594(7)	0.0336(6)

F4_3	0.04041(10)	0.52152(6)	0.75169(5)	0.0440(4)
F5_3	-0.05630(9)	0.47819(8)	0.72582(5)	0.0493(4)
F6_3	-0.00768(10)	0.45012(7)	0.78120(4)	0.0438(4)
C4_3	0.13574(17)	0.41473(10)	0.75017(7)	0.0324(6)
F7_3	0.16341(10)	0.45633(6)	0.77235(4)	0.0420(4)
F8_3	0.11016(10)	0.37599(6)	0.77579(4)	0.0398(4)
F9_3	0.19597(10)	0.39457(7)	0.73033(5)	0.0422(4)
O1_4	0.17363(9)	0.39971(6)	0.63598(5)	0.0237(4)
C1_4	0.20028(13)	0.36218(10)	0.60964(7)	0.0250(5)
C2_4	0.25742(15)	0.38887(11)	0.57924(8)	0.0320(6)
F1_4	0.32746(8)	0.39940(7)	0.59597(5)	0.0439(4)
F2_4	0.27067(9)	0.35694(7)	0.54748(5)	0.0409(4)
F3_4	0.22875(9)	0.43663(6)	0.56608(5)	0.0373(4)
C3_4	0.13010(15)	0.33602(11)	0.58683(7)	0.0309(6)
F4_4	0.07048(8)	0.32502(7)	0.61132(4)	0.0383(4)
F5_4	0.10271(8)	0.37067(6)	0.55904(4)	0.0346(3)
F6_4	0.14929(10)	0.28912(7)	0.56839(5)	0.0463(4)
C4_4	0.24496(16)	0.31661(11)	0.63312(8)	0.0373(6)
F7_4	0.19425(10)	0.28336(7)	0.65175(5)	0.0473(4)
F8_4	0.29046(10)	0.28563(7)	0.60936(5)	0.0534(5)
F9_4	0.29143(9)	0.33920(7)	0.66044(5)	0.0451(4)
O1_5	0.2051(9)	0.5182(6)	0.6380(5)	0.021(2)
C1_5	0.2655(5)	0.5504(3)	0.6510(2)	0.0233(17)
C2_5	0.2417(3)	0.5757(2)	0.69191(15)	0.0329(13)
F1_5	0.2506(4)	0.5380(2)	0.72068(16)	0.0396(13)
F2_5	0.2892(9)	0.6180(5)	0.7011(4)	0.040(2)
F3_5	0.1680(6)	0.5916(6)	0.6927(4)	0.037(3)
C3_5	0.2799(3)	0.5985(2)	0.62096(14)	0.0314(12)
F4_5	0.2787(5)	0.5800(3)	0.5841(2)	0.0374(15)
F5_5	0.2235(4)	0.6364(3)	0.62385(15)	0.0365(12)
F6_5	0.3493(2)	0.62368(19)	0.62696(11)	0.0425(10)
C4_5	0.3427(3)	0.5169(2)	0.65557(16)	0.0366(13)
F7_5	0.3746(7)	0.5061(6)	0.6204(4)	0.050(3)
F8_5	0.3964(3)	0.54281(19)	0.67862(16)	0.0502(12)
F9_5	0.3284(7)	0.4685(3)	0.6726(3)	0.0449(19)
C1_6	0.74579(12)	0.26848(9)	0.61982(6)	0.0146(4)
N1_6	0.77733(10)	0.25413(7)	0.65537(5)	0.0165(4)
N2_6	0.76447(10)	0.32189(7)	0.61365(5)	0.0152(4)
C3_6	0.80762(13)	0.34106(9)	0.64590(6)	0.0190(5)
H3_6	0.828298	0.377167	0.649095	0.023
C4_6	0.78993(13)	0.19876(9)	0.67136(6)	0.0188(5)
C5_6	0.72897(13)	0.17231(9)	0.69220(7)	0.0215(5)
C6_6	0.74623(16)	0.11993(10)	0.70637(8)	0.0296(6)
H6_6	0.706296	0.099791	0.719950	0.036
C7_6	0.81983(16)	0.09642(10)	0.70122(8)	0.0322(6)
H7_6	0.829868	0.060642	0.711469	0.039
C8_6	0.87851(15)	0.12402(10)	0.68154(8)	0.0283(6)
H8_6	0.928994	0.107252	0.678610	0.034
C9_6	0.86564(13)	0.17640(9)	0.66566(7)	0.0218(5)
C10_6	0.65008(13)	0.19982(9)	0.70106(7)	0.0230(5)
H10_6	0.632206	0.219419	0.676463	0.028
C11_6	0.58605(15)	0.15918(11)	0.71298(8)	0.0322(6)
H11A_6	0.535195	0.178403	0.715039	0.048
H11B_6	0.599424	0.142779	0.738775	0.048
H11C_6	0.582183	0.130130	0.692826	0.048

C12_6	0.65952(15)	0.24255(10)	0.73441(8)	0.0305(6)
H12A_6	0.608308	0.260080	0.739656	0.046
H12B_6	0.697946	0.270579	0.726212	0.046
H12C_6	0.678317	0.224271	0.758637	0.046
C13_6	0.93360(14)	0.20582(10)	0.64483(7)	0.0257(5)
H13_6	0.912861	0.241253	0.633823	0.031
C14_6	0.99900(15)	0.21948(11)	0.67487(8)	0.0333(6)
H14A_6	1.041417	0.239828	0.661461	0.050
H14B_6	1.020391	0.185275	0.686003	0.050
H14C_6	0.977019	0.242076	0.696373	0.050
C15_6	0.96822(15)	0.17247(13)	0.61035(8)	0.0380(7)
H15A_6	1.010571	0.193633	0.597562	0.057
H15B_6	0.926514	0.164667	0.590870	0.057
H15C_6	0.989754	0.137753	0.620536	0.057
C16_6	0.75368(13)	0.35542(9)	0.57799(6)	0.0158(4)
C17_6	0.79433(12)	0.34066(9)	0.54326(6)	0.0176(4)
C18_6	0.78677(13)	0.37607(9)	0.51065(7)	0.0206(5)
H18_6	0.813718	0.367641	0.486584	0.025
C19_6	0.74106(14)	0.42288(9)	0.51274(7)	0.0229(5)
H19_6	0.735825	0.445933	0.490043	0.027
C20_6	0.70282(13)	0.43646(9)	0.54766(7)	0.0199(5)
H20_6	0.670991	0.468691	0.548468	0.024
C21_6	0.70961(12)	0.40427(9)	0.58169(6)	0.0169(4)
C22_6	0.85015(13)	0.29178(9)	0.53985(7)	0.0205(5)
H22_6	0.845168	0.269604	0.564811	0.025
C23_6	0.82932(15)	0.25403(10)	0.50460(7)	0.0283(5)
H23A_6	0.864542	0.221966	0.504656	0.042
H23B_6	0.835874	0.274353	0.479609	0.042
H23C_6	0.774282	0.241729	0.507075	0.042
C24_6	0.93591(14)	0.31172(11)	0.53685(8)	0.0304(6)
H24A_6	0.971495	0.279883	0.535724	0.046
H24B_6	0.948795	0.334153	0.560216	0.046
H24C_6	0.942348	0.333878	0.512682	0.046
C25_6	0.67677(13)	0.42618(9)	0.62077(6)	0.0189(5)
H25_6	0.676047	0.395511	0.640628	0.023
C26_6	0.59312(14)	0.44959(10)	0.61712(7)	0.0260(5)
H26A_6	0.572294	0.457673	0.643718	0.039
H26B_6	0.558858	0.422590	0.603958	0.039
H26C_6	0.594560	0.483518	0.601345	0.039
C27_6	0.73177(14)	0.47222(9)	0.63642(7)	0.0237(5)
H27A_6	0.712582	0.485041	0.662347	0.036
H27B_6	0.731927	0.502991	0.617548	0.036
H27C_6	0.785665	0.457809	0.639286	0.036
C2_6	0.81481(13)	0.29928(9)	0.67177(7)	0.0199(5)
H2_6	0.840928	0.300531	0.696808	0.024
C1_9	0.55754(12)	0.31823(9)	0.55089(6)	0.0160(4)
Br1_9	0.49578(2)	0.45118(2)	0.45529(2)	0.02369(6)
C2_9	0.60009(13)	0.32178(9)	0.51545(6)	0.0188(5)
H2_9	0.643884	0.297963	0.511162	0.023
C3_9	0.57946(13)	0.35940(9)	0.48653(7)	0.0195(5)
H3_9	0.608887	0.361470	0.462477	0.023
C4_9	0.51571(13)	0.39415(9)	0.49270(6)	0.0190(5)
C5_9	0.46988(13)	0.38938(9)	0.52641(7)	0.0203(5)
H5_9	0.424827	0.412280	0.529934	0.024
C6_9	0.49001(12)	0.35080(9)	0.55525(6)	0.0186(5)

H6_9	0.457522	0.346562	0.578138	0.022
C1_10	0.53331(12)	0.27324(9)	0.61572(6)	0.0151(4)
Br1_10	0.36618(2)	0.23652(2)	0.72289(2)	0.02899(6)
C2_10	0.52691(13)	0.31073(9)	0.64658(6)	0.0201(5)
H2_10	0.557395	0.343591	0.646041	0.024
C3_10	0.47636(13)	0.30070(10)	0.67829(7)	0.0228(5)
H3_10	0.471374	0.326772	0.699218	0.027
C4_10	0.43346(13)	0.25247(10)	0.67907(7)	0.0207(5)
C5_10	0.43932(13)	0.21424(10)	0.64888(7)	0.0232(5)
H5_10	0.409961	0.180911	0.649976	0.028
C6_10	0.48874(13)	0.22519(9)	0.61689(7)	0.0212(5)
H6_10	0.492161	0.199601	0.595571	0.025
C1_11	0.63522(12)	0.23880(8)	0.57240(6)	0.0149(4)
Br1_11	0.78475(2)	0.08255(2)	0.54358(2)	0.02615(6)
C2_11	0.70787(12)	0.22977(8)	0.59170(6)	0.0141(4)
C3_11	0.75005(12)	0.18170(8)	0.58281(6)	0.0156(4)
H3_11	0.798567	0.174492	0.596140	0.019
C4_11	0.72241(13)	0.14484(9)	0.55514(6)	0.0179(5)
C5_11	0.65236(13)	0.15393(9)	0.53515(6)	0.0188(5)
H5_11	0.633992	0.128575	0.515698	0.023
C6_11	0.60961(12)	0.20063(9)	0.54403(6)	0.0180(5)
H6_11	0.561172	0.207110	0.530439	0.022

Table S 19 Atomic coordinates and U_{eq} [Å^2] for [FeCp$_2$][Al(OR^F)$_4$]*

Atom	***x***	***y***	***z***	U_{eq}
Fe1	0.64351(4)	0.96557(6)	1.06789(6)	0.0164(3)
Fe2	0.01267(4)	0.54253(6)	0.28800(7)	0.0200(3)
Fe3	0.31830(4)	0.00406(7)	0.38846(7)	0.0211(3)
Al1	0.49675(8)	0.69348(13)	0.80071(13)	0.0176(5)
Al2	0.17568(7)	0.78333(12)	0.60302(13)	0.0166(5)
Al06	0.16007(8)	0.26530(15)	0.50887(15)	0.0260(6)
C02H	0.7017(3)	0.9667(4)	1.1323(5)	0.0213(18)
C02M	0.5868(3)	0.9214(5)	1.0468(5)	0.0241(19)
C02Q	0.0271(3)	0.4789(6)	0.3708(6)	0.033(2)
C02U	0.6733(3)	0.9758(5)	1.1691(5)	0.0236(19)
C02Y	-0.0010(3)	0.6134(5)	0.2133(5)	0.027(2)
C032	0.6196(3)	0.9464(5)	0.9670(5)	0.0231(19)
C036	-0.0191(3)	0.5525(5)	0.1879(5)	0.027(2)
C038	0.6368(3)	0.8892(5)	1.0002(5)	0.0230(19)
C03D	0.6170(3)	0.8727(4)	1.0495(5)	0.0227(19)
C03G	-0.0176(3)	0.6325(5)	0.2659(5)	0.029(2)
C03J	0.6506(3)	1.0348(5)	1.1451(5)	0.025(2)
C03L	0.3792(3)	-0.0193(5)	0.4047(5)	0.025(2)
C03S	0.0670(3)	0.4912(6)	0.2993(6)	0.035(2)
C03T	0.7333(3)	0.9128(5)	1.1409(5)	0.029(2)
H03A	0.738869	0.904368	1.098393	0.044
H03B	0.723084	0.872682	1.156323	0.044
H03C	0.758172	0.926685	1.173478	0.044
C03V	0.3133(3)	0.0913(5)	0.4387(6)	0.034(2)
C03Y	0.2964(3)	0.1001(5)	0.3721(6)	0.031(2)
C040	0.5882(3)	0.9664(5)	0.9949(4)	0.0222(19)
C041	0.0738(3)	0.5461(5)	0.3421(5)	0.031(2)
C042	0.6973(3)	1.0196(5)	1.0847(5)	0.0216(18)

C043	0.6656(3)	1.0602(4)	1.0928(5)	0.025(2)
C044	0.0377(3)	0.4491(5)	0.3160(5)	0.031(2)
C045	0.6693(3)	0.8470(5)	0.9844(6)	0.030(2)
H04A	0.656562	0.811501	0.954406	0.046
H04B	0.686577	0.828190	1.025434	0.046
H04C	0.685738	0.873929	0.963211	0.046
C046	0.6306(3)	0.9785(5)	0.9098(5)	0.032(2)
H04D	0.609268	0.970287	0.868833	0.047
H04E	0.656198	0.960341	0.905780	0.047
H04F	0.633573	1.025901	0.917518	0.047
C047	0.0487(3)	0.5391(5)	0.3860(5)	0.030(2)
C048	-0.0462(3)	0.5328(6)	0.2249(5)	0.031(2)
C049	0.3603(3)	-0.0119(5)	0.3352(5)	0.028(2)
C04G	0.3592(4)	-0.0690(6)	0.4276(6)	0.039(3)
C04H	-0.0454(3)	0.5831(5)	0.2735(5)	0.028(2)
C04K	0.2640(3)	0.0543(6)	0.3500(6)	0.035(2)
C04L	0.6681(3)	0.9333(6)	1.2242(5)	0.036(3)
H04G	0.640278	0.936838	1.227123	0.054
H04H	0.686838	0.947544	1.266014	0.054
H04I	0.673865	0.887611	1.215453	0.054
C04P	0.3722(4)	0.0322(7)	0.2873(6)	0.043(3)
H04J	0.387718	0.007318	0.262744	0.064
H04K	0.388906	0.068112	0.311380	0.064
H04L	0.347926	0.050334	0.256272	0.064
C04Q	0.6256(3)	0.8146(5)	1.0946(6)	0.033(2)
H04M	0.625041	0.774661	1.068502	0.050
H04N	0.604964	0.811629	1.118681	0.050
H04O	0.652284	0.819514	1.126243	0.050
C04R	0.7220(3)	1.0284(6)	1.0375(6)	0.033(2)
H04P	0.729660	0.985357	1.024128	0.050
H04Q	0.746427	1.053412	1.058910	0.050
H04R	0.706236	1.052216	0.998398	0.050
C04T	0.3285(3)	-0.0587(6)	0.3149(6)	0.038(3)
C04U	0.5580(3)	0.9253(6)	1.0889(5)	0.033(2)
H04S	0.533753	0.899651	1.068334	0.049
H04T	0.550499	0.971191	1.092755	0.049
H04U	0.571091	0.907734	1.132969	0.049
C04Z	0.5603(3)	1.0240(6)	0.9725(6)	0.035(2)
H04V	0.573794	1.057109	0.952399	0.053
H04W	0.553282	1.043074	1.010716	0.053
H04X	0.535591	1.009228	0.939934	0.053
C050	0.1025(3)	0.6010(6)	0.3429(7)	0.043(3)
H05A	0.129601	0.588392	0.369348	0.064
H05B	0.093654	0.640052	0.362237	0.064
H05C	0.103101	0.610720	0.297480	0.064
C053	0.0288(3)	0.6534(6)	0.1892(6)	0.040(3)
H05D	0.046234	0.624090	0.172396	0.060
H05E	0.045325	0.679536	0.225837	0.060
H05F	0.014133	0.682629	0.153632	0.060
C054	0.2616(3)	0.0171(5)	0.4055(7)	0.038(3)
C056	0.6194(3)	1.0645(6)	1.1727(6)	0.039(3)
H05G	0.599510	1.087777	1.137614	0.059
H05H	0.632262	1.095425	1.207945	0.059
H05I	0.605819	1.029924	1.190932	0.059
C057	0.2922(4)	0.0390(6)	0.4609(6)	0.045(3)

C058	0.3287(4)	-0.0949(6)	0.3732(7)	0.044(3)
C059	0.0227(4)	0.3851(6)	0.2856(7)	0.045(3)
H05J	0.029907	0.380112	0.243954	0.067
H05K	-0.006776	0.383358	0.276902	0.067
H05L	0.034985	0.349653	0.315950	0.067
C05C	0.3095(4)	0.1513(6)	0.3302(7)	0.047(3)
H05M	0.296689	0.142300	0.283288	0.070
H05N	0.338935	0.149881	0.338728	0.070
H05O	0.301317	0.194824	0.341467	0.070
C05F	0.6517(3)	1.1237(5)	1.0564(6)	0.036(2)
H05P	0.651827	1.119049	1.010043	0.053
H05Q	0.670053	1.159203	1.077060	0.053
H05R	0.624269	1.133966	1.058459	0.053
C05H	0.0876(4)	0.4776(7)	0.2464(7)	0.045(3)
H05S	0.067257	0.467001	0.204851	0.067
H05T	0.106112	0.440441	0.259726	0.067
H05U	0.102844	0.516419	0.239920	0.067
C05J	-0.0113(4)	0.5145(6)	0.1312(6)	0.040(3)
H05V	-0.034218	0.519786	0.091811	0.060
H05W	-0.007857	0.467947	0.143034	0.060
H05X	0.013341	0.531014	0.121968	0.060
C05N	-0.0007(4)	0.4521(7)	0.4075(6)	0.045(3)
H05Y	-0.009293	0.487556	0.432024	0.067
H05Z	0.013351	0.418319	0.438524	0.067
H010	-0.024433	0.432872	0.376057	0.067
C05P	-0.0706(4)	0.5836(7)	0.3219(7)	0.048(3)
H011	-0.097047	0.603192	0.300842	0.072
H012	-0.056848	0.609334	0.360934	0.072
H013	-0.074377	0.538515	0.335286	0.072
C05R	0.4143(3)	0.0213(7)	0.4437(6)	0.041(3)
H014	0.439484	-0.003141	0.448877	0.062
H015	0.410786	0.031157	0.487371	0.062
H016	0.415453	0.062390	0.420030	0.062
C05S	-0.0719(4)	0.4730(6)	0.2136(6)	0.043(3)
H017	-0.098379	0.483285	0.183269	0.065
H018	-0.075424	0.457727	0.255897	0.065
H019	-0.058871	0.438552	0.194306	0.065
C05U	0.3471(5)	0.1316(7)	0.4821(8)	0.062(4)
H01A	0.369211	0.134994	0.461325	0.093
H01B	0.356942	0.110377	0.525438	0.093
H01C	0.337037	0.175533	0.487833	0.093
C05W	-0.0083(4)	0.6952(6)	0.3049(7)	0.049(3)
H01D	0.016847	0.714062	0.299661	0.073
H01E	-0.005206	0.686077	0.351776	0.073
H01F	-0.030473	0.726425	0.288569	0.073
C05X	0.0479(5)	0.5858(7)	0.4427(6)	0.053(3)
H01G	0.058444	0.628711	0.434693	0.079
H01H	0.064628	0.567891	0.484597	0.079
H01I	0.019994	0.590732	0.445182	0.079
C05Y	0.3015(4)	-0.0693(10)	0.2465(8)	0.069(5)
H01J	0.290752	-0.027099	0.227224	0.103
H01K	0.279030	-0.098128	0.248513	0.103
H01L	0.316942	-0.089773	0.219063	0.103
C05Z	0.2306(5)	-0.0354(8)	0.4078(15)	0.109(10)
H01M	0.208213	-0.015615	0.421370	0.163

H01N	0.243410	-0.069384	0.439757	0.163
H01O	0.220295	-0.055148	0.363879	0.163
C065	0.3715(5)	-0.0937(10)	0.5003(8)	0.078(6)
H06A	0.347129	-0.103849	0.513882	0.118
H06B	0.387034	-0.059581	0.529191	0.118
H06C	0.388076	-0.133307	0.503643	0.118
C067	0.2374(6)	0.0516(8)	0.2818(8)	0.075(6)
H06D	0.253612	0.057220	0.250540	0.113
H06E	0.217260	0.086714	0.275389	0.113
H06F	0.223657	0.009042	0.274265	0.113
C06A	0.3003(5)	-0.1526(7)	0.3729(10)	0.069(5)
H06G	0.272788	-0.136208	0.367009	0.104
H06H	0.309270	-0.176199	0.415021	0.104
H06I	0.300701	-0.182338	0.336463	0.104
C06G	0.3013(7)	0.0159(9)	0.5319(8)	0.087(7)
H06J	0.300342	-0.032114	0.532846	0.130
H06K	0.281129	0.033878	0.552136	0.130
H06L	0.328265	0.030935	0.556561	0.130
O1_2	0.4834(6)	0.7286(10)	0.8670(6)	0.025(3)
C1_2	0.4887(3)	0.7284(5)	0.9338(7)	0.028(3)
C2_2	0.5284(4)	0.6929(6)	0.9703(7)	0.037(3)
F1_2	0.5582(4)	0.7093(7)	0.9439(10)	0.047(3)
F2_2	0.5404(8)	0.7098(11)	1.0341(6)	0.052(3)
F3_2	0.5242(4)	0.6278(5)	0.9669(6)	0.056(3)
C3_2	0.4528(4)	0.6936(6)	0.9510(7)	0.041(3)
F4_2	0.4200(3)	0.7318(6)	0.9348(6)	0.054(3)
F5_2	0.4435(5)	0.6384(9)	0.9157(11)	0.053(3)
F6_2	0.4602(7)	0.6799(10)	1.0153(7)	0.053(4)
C4_2	0.4901(4)	0.8010(6)	0.9569(7)	0.040(3)
F7_2	0.4615(4)	0.8358(6)	0.9137(8)	0.053(3)
F8_2	0.4836(7)	0.8082(11)	1.0157(7)	0.053(4)
F9_2	0.5257(3)	0.8277(6)	0.9574(6)	0.053(3)
O1_3	0.54290(17)	0.7189(3)	0.7925(3)	0.0202(13)
C1_3	0.5641(2)	0.7676(3)	0.7732(4)	0.0190(15)
C2_3	0.5573(2)	0.8338(4)	0.8047(4)	0.0215(16)
F1_3	0.57741(17)	0.8359(3)	0.8694(3)	0.0276(12)
F2_3	0.56916(17)	0.8852(3)	0.7755(3)	0.0272(12)
F3_3	0.51836(15)	0.8427(3)	0.8001(3)	0.0258(12)
C3_3	0.5514(2)	0.7745(4)	0.6961(4)	0.0226(16)
F4_3	0.54632(17)	0.7153(3)	0.6679(3)	0.0291(12)
F5_3	0.51687(16)	0.8068(3)	0.6748(3)	0.0281(12)
F6_3	0.57966(17)	0.8061(3)	0.6747(3)	0.0294(12)
C4_3	0.6099(2)	0.7496(4)	0.7975(4)	0.0228(16)
F7_3	0.61883(16)	0.7037(3)	0.7588(3)	0.0304(13)
F8_3	0.63377(16)	0.8012(3)	0.7976(3)	0.0303(13)
F9_3	0.61928(16)	0.7258(3)	0.8592(3)	0.0276(12)
O1_4	0.50091(18)	0.6095(3)	0.8128(3)	0.0212(13)
C1_4	0.5160(2)	0.5524(3)	0.7964(4)	0.0187(15)
C2_4	0.5037(2)	0.4971(4)	0.8378(4)	0.0259(17)
F1_4	0.5264(2)	0.5002(3)	0.9007(3)	0.0397(15)
F2_4	0.5083(2)	0.4375(3)	0.8148(3)	0.0365(14)
F3_4	0.46542(16)	0.5037(3)	0.8379(3)	0.0332(13)
C3_4	0.4977(2)	0.5376(4)	0.7217(4)	0.0242(17)
F4_4	0.49926(19)	0.5909(3)	0.6855(3)	0.0305(13)
F5_4	0.45911(17)	0.5200(3)	0.7090(3)	0.0335(13)

F6_4	0.5171(2)	0.4900(3)	0.6995(3)	0.0361(14)
C4_4	0.5629(2)	0.5542(4)	0.8124(4)	0.0286(18)
F7_4	0.57474(18)	0.5860(3)	0.7660(3)	0.0341(13)
F8_4	0.5791(2)	0.4948(3)	0.8168(4)	0.0436(16)
F9_4	0.57874(17)	0.5856(3)	0.8691(3)	0.0369(14)
O1_1	0.4592(3)	0.7169(8)	0.7313(5)	0.023(2)
C1_1	0.4200(3)	0.7322(5)	0.7029(5)	0.023(2)
C2_1	0.4155(3)	0.8077(5)	0.6927(5)	0.034(2)
F1_1	0.4360(3)	0.8383(5)	0.7475(5)	0.048(3)
F2_1	0.3771(3)	0.8270(5)	0.6770(7)	0.042(3)
F3_1	0.4307(3)	0.8260(5)	0.6437(5)	0.049(2)
C3_1	0.4076(3)	0.6989(5)	0.6341(5)	0.035(3)
F4_1	0.4021(3)	0.6345(4)	0.6411(6)	0.056(3)
F5_1	0.4365(4)	0.7052(6)	0.6029(6)	0.049(3)
F6_1	0.3734(3)	0.7233(9)	0.5948(7)	0.047(3)
C4_1	0.3924(3)	0.7095(6)	0.7460(5)	0.036(3)
F7_1	0.4048(5)	0.6498(7)	0.7706(7)	0.060(3)
F8_1	0.3538(2)	0.7032(6)	0.7103(5)	0.046(3)
F9_1	0.3945(3)	0.7498(6)	0.7965(5)	0.054(3)
O1_5	0.19985(18)	0.7518(3)	0.5477(3)	0.0257(14)
C1_5	0.2348(2)	0.7316(4)	0.5365(4)	0.0280(17)
C2_5	0.2271(3)	0.7158(4)	0.4618(4)	0.035(2)
F1_5	0.1932(2)	0.6805(4)	0.4396(4)	0.055(2)
F2_5	0.2575(2)	0.6834(4)	0.4489(4)	0.0514(18)
F3_5	0.2222(3)	0.7710(4)	0.4262(4)	0.057(2)
C3_5	0.2676(3)	0.7866(4)	0.5548(5)	0.037(2)
F4_5	0.2839(2)	0.7911(4)	0.6201(3)	0.0503(18)
F5_5	0.2502(2)	0.8449(3)	0.5336(4)	0.056(2)
F6_5	0.2973(2)	0.7774(4)	0.5272(4)	0.057(2)
C4_5	0.2512(3)	0.6704(4)	0.5790(4)	0.036(2)
F7_5	0.2497(2)	0.6794(3)	0.6410(3)	0.0400(15)
F8_5	0.2893(2)	0.6564(4)	0.5805(4)	0.0471(17)
F9_5	0.2293(2)	0.6176(3)	0.5544(4)	0.0520(18)
O1_6	0.2061(5)	0.8438(8)	0.6465(8)	0.029(3)
C1_6	0.2167(4)	0.8812(6)	0.7019(6)	0.031(3)
C2_6	0.1799(4)	0.9213(6)	0.7104(7)	0.040(3)
F1_6	0.1716(5)	0.9710(6)	0.6669(7)	0.058(3)
F2_6	0.1861(8)	0.9465(8)	0.7705(8)	0.066(4)
F3_6	0.1472(4)	0.8824(12)	0.6983(12)	0.057(3)
C3_6	0.2336(4)	0.8390(7)	0.7647(7)	0.047(3)
F4_6	0.2568(7)	0.7896(8)	0.7538(15)	0.068(3)
F5_6	0.2041(4)	0.8113(8)	0.7847(7)	0.063(4)
F6_6	0.2557(7)	0.8749(14)	0.8148(8)	0.075(4)
C4_6	0.2495(3)	0.9295(6)	0.6932(6)	0.037(3)
F7_6	0.2865(3)	0.9038(7)	0.7083(7)	0.059(3)
F8_6	0.2518(7)	0.9830(9)	0.7311(10)	0.059(4)
F9_6	0.2398(5)	0.9503(12)	0.6307(7)	0.046(3)
O1_7	0.1668(5)	0.7256(7)	0.6573(7)	0.025(3)
C1_7	0.1428(3)	0.6787(5)	0.6706(5)	0.027(2)
C2_7	0.1154(3)	0.6473(5)	0.6064(6)	0.039(3)
F1_7	0.0828(3)	0.6842(6)	0.5827(7)	0.062(3)
F2_7	0.1033(4)	0.5870(5)	0.6146(7)	0.053(3)
F3_7	0.1352(6)	0.6459(9)	0.5594(7)	0.065(3)
C3_7	0.1711(3)	0.6246(6)	0.7105(6)	0.047(3)
F4_7	0.2010(4)	0.6522(9)	0.7577(9)	0.069(3)

F5_7	0.1883(4)	0.5911(7)	0.6707(7)	0.069(4)
F6_7	0.1524(3)	0.5818(6)	0.7390(7)	0.061(3)
C4_7	0.1162(4)	0.7069(6)	0.7133(6)	0.052(3)
F7_7	0.1379(4)	0.7156(8)	0.7760(5)	0.083(4)
F8_7	0.0852(4)	0.6678(6)	0.7119(7)	0.062(4)
F9_7	0.1015(4)	0.7648(5)	0.6863(8)	0.071(4)
O1_8	0.1295(4)	0.8109(10)	0.5543(8)	0.031(4)
C1_8	0.1086(3)	0.8435(6)	0.4985(6)	0.035(3)
C2_8	0.1219(5)	0.9164(6)	0.5039(7)	0.052(3)
F1_8	0.1061(5)	0.9469(7)	0.5477(7)	0.089(5)
F2_8	0.1100(8)	0.9486(10)	0.4462(10)	0.069(4)
F3_8	0.1620(5)	0.9193(11)	0.5214(11)	0.076(4)
C3_8	0.1161(4)	0.8130(6)	0.4346(6)	0.051(3)
F4_8	0.1166(5)	0.7471(6)	0.4407(7)	0.065(4)
F5_8	0.1511(4)	0.8340(8)	0.4269(7)	0.068(4)
F6_8	0.0860(4)	0.8275(7)	0.3811(6)	0.067(4)
C4_8	0.0631(4)	0.8367(7)	0.4940(7)	0.054(3)
F7_8	0.0506(4)	0.7773(6)	0.4691(9)	0.071(4)
F8_8	0.0411(4)	0.8813(7)	0.4533(7)	0.064(4)
F9_8	0.0573(6)	0.8455(11)	0.5533(8)	0.074(4)
O1_9	0.1610(3)	0.3512(4)	0.5012(5)	0.0238(19)
C1_9	0.1706(3)	0.4087(4)	0.5343(4)	0.022(2)
C2_9	0.2165(3)	0.4122(5)	0.5702(5)	0.030(2)
F1_9	0.2253(3)	0.3787(4)	0.6265(4)	0.038(2)
F2_9	0.2289(3)	0.4744(4)	0.5858(5)	0.047(2)
F3_9	0.2383(3)	0.3883(5)	0.5317(6)	0.039(2)
C3_9	0.1595(3)	0.4651(5)	0.4825(5)	0.036(2)
F4_9	0.1239(2)	0.4524(4)	0.4386(5)	0.046(2)
F5_9	0.1867(3)	0.4717(5)	0.4488(5)	0.044(2)
F6_9	0.1566(3)	0.5224(4)	0.5099(5)	0.051(2)
C4_9	0.1466(3)	0.4167(5)	0.5866(5)	0.032(2)
F7_9	0.1080(3)	0.4317(5)	0.5576(5)	0.044(2)
F8_9	0.1612(3)	0.4630(4)	0.6310(5)	0.049(2)
F9_9	0.1469(3)	0.3610(4)	0.6198(5)	0.039(2)
O1_11	0.1210(2)	0.2368(4)	0.5369(4)	0.0338(16)
C1_11	0.0818(2)	0.2182(4)	0.5245(4)	0.037(2)
C2_11	0.0743(3)	0.2004(5)	0.5916(5)	0.043(2)
F1_11	0.0908(2)	0.2439(4)	0.6380(3)	0.0505(18)
F2_11	0.0347(2)	0.1978(4)	0.5881(5)	0.061(2)
F3_11	0.0907(3)	0.1417(4)	0.6135(5)	0.067(2)
C3_11	0.0726(3)	0.1584(5)	0.4765(5)	0.053(3)
F4_11	0.0682(2)	0.1764(5)	0.4141(4)	0.066(2)
F5_11	0.1028(2)	0.1155(4)	0.4937(5)	0.071(3)
F6_11	0.0391(2)	0.1275(5)	0.4802(5)	0.075(3)
C4_11	0.0539(3)	0.2757(4)	0.4915(5)	0.039(2)
F7_11	0.0675(2)	0.3046(4)	0.4455(4)	0.0548(19)
F8_11	0.01608(19)	0.2561(5)	0.4628(4)	0.063(2)
F9_11	0.0522(2)	0.3208(4)	0.5373(4)	0.0497(18)
O1_13	0.4859(11)	0.7236(17)	0.8713(10)	0.023(5)
C1_13	0.4920(5)	0.7214(8)	0.9381(10)	0.026(3)
C2_13	0.5380(5)	0.7242(9)	0.9740(10)	0.034(4)
F1_13	0.5517(6)	0.7851(9)	0.9713(10)	0.051(5)
F2_13	0.5459(13)	0.7070(19)	1.0374(11)	0.048(4)
F3_13	0.5578(8)	0.6832(12)	0.9446(17)	0.044(5)
C3_13	0.4744(6)	0.6573(8)	0.9586(10)	0.035(4)

F4_13	0.4388(8)	0.6441(16)	0.915(2)	0.053(5)
F5_13	0.4989(7)	0.6062(9)	0.9599(10)	0.048(4)
F6_13	0.4680(12)	0.6619(17)	1.0182(12)	0.048(5)
C4_13	0.4711(5)	0.7815(9)	0.9597(10)	0.040(4)
F7_13	0.4315(5)	0.7718(12)	0.9481(12)	0.060(4)
F8_13	0.4861(11)	0.794(2)	1.0241(10)	0.051(5)
F9_13	0.4771(8)	0.8356(10)	0.9278(14)	0.047(4)
O1_14	0.4597(8)	0.714(2)	0.7291(14)	0.026(7)
C1_14	0.4205(7)	0.7263(10)	0.6973(10)	0.029(4)
C2_14	0.4061(7)	0.7912(11)	0.7218(12)	0.036(4)
F1_14	0.4328(10)	0.8386(14)	0.7225(18)	0.042(4)
F2_14	0.3706(8)	0.8110(17)	0.682(2)	0.043(6)
F3_14	0.4009(10)	0.7831(17)	0.7817(13)	0.057(5)
C3_14	0.3935(8)	0.6689(11)	0.7090(13)	0.045(5)
F4_14	0.3986(11)	0.6176(13)	0.6731(19)	0.063(6)
F5_14	0.4022(17)	0.652(2)	0.7722(15)	0.059(5)
F6_14	0.3546(7)	0.6860(19)	0.687(2)	0.051(6)
C4_14	0.4151(7)	0.7304(13)	0.6214(10)	0.042(5)
F7_14	0.4335(14)	0.6791(16)	0.6029(19)	0.052(5)
F8_14	0.3761(9)	0.728(3)	0.587(2)	0.050(5)
F9_14	0.4305(8)	0.7856(14)	0.6053(15)	0.058(7)
O1_15	0.2080(9)	0.8378(15)	0.6526(15)	0.038(7)
C1_15	0.2175(5)	0.8769(9)	0.7068(10)	0.035(4)
C2_15	0.2257(6)	0.9479(9)	0.6865(10)	0.041(4)
F1_15	0.1915(6)	0.9796(10)	0.6597(12)	0.052(4)
F2_15	0.2465(12)	0.9821(16)	0.7391(18)	0.061(6)
F3_15	0.2478(9)	0.947(2)	0.6436(15)	0.042(4)
C3_15	0.2565(6)	0.8491(11)	0.7557(11)	0.052(4)
F4_15	0.2557(12)	0.7837(12)	0.758(3)	0.067(5)
F5_15	0.2884(6)	0.8677(14)	0.7358(12)	0.064(4)
F6_15	0.2612(12)	0.872(3)	0.8167(13)	0.073(5)
C4_15	0.1829(6)	0.8784(10)	0.7411(11)	0.048(4)
F7_15	0.1825(8)	0.8238(11)	0.7762(12)	0.059(5)
F8_15	0.1871(15)	0.9290(13)	0.7830(17)	0.066(5)
F9_15	0.1467(7)	0.882(2)	0.697(2)	0.058(4)
O1_16	0.1297(7)	0.8133(19)	0.5568(15)	0.029(6)
C1_16	0.1075(5)	0.8479(10)	0.5038(9)	0.036(4)
C2_16	0.0736(6)	0.8843(11)	0.5254(10)	0.049(5)
F1_16	0.0898(10)	0.9253(15)	0.5751(14)	0.096(6)
F2_16	0.0502(8)	0.9173(15)	0.4753(13)	0.070(6)
F3_16	0.0504(12)	0.8416(18)	0.546(2)	0.073(5)
C3_16	0.0884(7)	0.8011(10)	0.4451(10)	0.055(5)
F4_16	0.1176(9)	0.7674(15)	0.4288(16)	0.064(4)
F5_16	0.0631(9)	0.7586(14)	0.4600(18)	0.080(6)
F6_16	0.0672(9)	0.8343(15)	0.3920(12)	0.072(6)
C4_16	0.1347(7)	0.8976(12)	0.4801(12)	0.045(4)
F7_16	0.1567(9)	0.8671(16)	0.4457(16)	0.072(5)
F8_16	0.1133(15)	0.943(2)	0.439(2)	0.068(5)
F9_16	0.1586(12)	0.929(2)	0.531(2)	0.074(6)
O1_17	0.1627(12)	0.7292(18)	0.6560(17)	0.029(7)
C1_17	0.1413(6)	0.6801(10)	0.6729(10)	0.031(4)
C2_17	0.1620(7)	0.6613(12)	0.7462(10)	0.045(5)
F1_17	0.1610(14)	0.7110(16)	0.7871(16)	0.090(6)
F2_17	0.1443(9)	0.6106(14)	0.7661(16)	0.059(6)
F3_17	0.2007(7)	0.646(3)	0.754(2)	0.066(5)

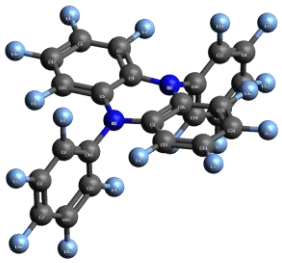
C3_17	0.1423(8)	0.6189(13)	0.6292(13)	0.050(5)
F4_17	0.1352(17)	0.634(3)	0.5653(13)	0.069(5)
F5_17	0.1788(9)	0.591(2)	0.647(2)	0.071(6)
F6_17	0.1146(10)	0.5757(15)	0.635(2)	0.058(6)
C4_17	0.0970(7)	0.7014(12)	0.6655(13)	0.048(5)
F7_17	0.0768(9)	0.7137(18)	0.6034(14)	0.070(6)
F8_17	0.0769(11)	0.6541(17)	0.687(2)	0.067(6)
F9_17	0.0965(12)	0.7555(15)	0.701(2)	0.076(6)
O1_18	0.2009(10)	0.2403(18)	0.5780(16)	0.039(8)
C1_18	0.2262(6)	0.2053(10)	0.6264(12)	0.044(4)
C2_18	0.2704(7)	0.2301(12)	0.6409(13)	0.062(5)
F1_18	0.2744(7)	0.2859(13)	0.6746(17)	0.061(7)
F2_18	0.2953(9)	0.1866(17)	0.6788(19)	0.063(6)
F3_18	0.2804(12)	0.238(2)	0.5845(16)	0.062(5)
C3_18	0.2257(8)	0.1317(11)	0.6067(14)	0.062(6)
F4_18	0.1881(8)	0.1109(16)	0.580(2)	0.069(5)
F5_18	0.2465(12)	0.1258(17)	0.5620(19)	0.087(10)
F6_18	0.2412(11)	0.0956(15)	0.6607(17)	0.073(6)
C4_18	0.2109(8)	0.2111(14)	0.6892(13)	0.070(5)
F7_18	0.1809(10)	0.168(2)	0.682(2)	0.109(12)
F8_18	0.2394(11)	0.200(2)	0.7451(14)	0.084(6)
F9_18	0.1976(13)	0.2720(16)	0.6921(19)	0.080(6)
O1_20	0.1527(13)	0.3368(13)	0.507(2)	0.034(7)
C1_20	0.1594(7)	0.4017(12)	0.5199(11)	0.032(4)
C2_20	0.1324(9)	0.4233(14)	0.5649(14)	0.045(4)
F1_20	0.1330(13)	0.3782(19)	0.6109(18)	0.049(5)
F2_20	0.1448(13)	0.4802(16)	0.595(2)	0.057(5)
F3_20	0.0945(9)	0.430(2)	0.527(2)	0.051(5)
C3_20	0.1472(8)	0.4430(14)	0.4554(13)	0.048(4)
F4_20	0.1767(10)	0.446(2)	0.4259(18)	0.054(5)
F5_20	0.1152(9)	0.4177(18)	0.4111(16)	0.053(5)
F6_20	0.1378(13)	0.5044(14)	0.469(2)	0.067(10)
C4_20	0.2044(7)	0.4139(14)	0.5568(14)	0.037(5)
F7_20	0.2285(11)	0.377(2)	0.531(3)	0.045(5)
F8_20	0.2151(12)	0.4767(15)	0.554(2)	0.052(5)
F9_20	0.2113(12)	0.398(2)	0.6205(14)	0.045(5)
O1_10	0.2054(3)	0.2444(5)	0.5616(5)	0.020(2)
C1_10	0.2263(3)	0.1992(5)	0.6041(5)	0.029(2)
C2_10	0.2705(3)	0.1998(6)	0.6003(6)	0.040(3)
F1_10	0.2724(4)	0.1717(7)	0.5438(5)	0.080(4)
F2_10	0.2960(3)	0.1682(6)	0.6495(5)	0.052(3)
F3_10	0.2833(4)	0.2616(5)	0.6006(7)	0.064(3)
C3_10	0.2249(4)	0.2146(6)	0.6754(5)	0.052(3)
F4_10	0.1886(3)	0.2337(6)	0.6767(5)	0.067(3)
F5_10	0.2497(4)	0.2640(6)	0.7006(5)	0.078(4)
F6_10	0.2365(4)	0.1624(6)	0.7156(5)	0.068(3)
C4_10	0.2087(4)	0.1293(5)	0.5852(6)	0.055(3)
F7_10	0.1764(3)	0.1204(6)	0.6087(7)	0.069(3)
F8_10	0.2356(3)	0.0835(5)	0.6124(7)	0.067(3)
F9_10	0.1968(4)	0.1203(5)	0.5198(5)	0.082(4)
O1_12	0.1537(2)	0.2356(4)	0.4290(4)	0.0379(18)
C1_12	0.1634(3)	0.2428(5)	0.3698(4)	0.043(2)
C2_12	0.1414(3)	0.1879(5)	0.3221(5)	0.058(3)
F1_12	0.1440(4)	0.1309(4)	0.3545(5)	0.085(3)
F2_12	0.1569(3)	0.1800(5)	0.2713(4)	0.074(3)

F3_12	0.1023(2)	0.2042(5)	0.2985(4)	0.074(3)
C3_12	0.1499(3)	0.3100(5)	0.3367(5)	0.046(2)
F4_12	0.1755(3)	0.3581(4)	0.3646(4)	0.067(2)
F5_12	0.1135(2)	0.3258(5)	0.3431(4)	0.069(2)
F6_12	0.1469(3)	0.3106(5)	0.2716(4)	0.069(2)
C4_12	0.2099(3)	0.2371(5)	0.3822(5)	0.047(2)
F7_12	0.2284(2)	0.2728(4)	0.4350(3)	0.0489(18)
F8_12	0.2222(2)	0.2551(5)	0.3303(4)	0.067(2)
F9_12	0.2216(3)	0.1755(4)	0.3951(5)	0.080(3)

S-4 Quantum chemical calculations

Table S 20 SCF energy, FreeH energy and FreeH entropy of presented compounds. (*BP86/def-SV(P)/D3(BJ))*

Compound	SCF /*Hartree*	FreeH energy [kJ/mol]	FreeH entropy [kJ/mol K]
[“phenazine^{F}”]$^{\cdot+}$ **4**$^{\cdot+}$	-2818.934205143	626.31	0.99143
[Sn(CHpz$_3$)$_2$]$^{2+}$ **6**$^{2+}$	-1433.226540258	1120.23	0.81621
[Fe(CO)Cp*$_2$]$^{2+}$ **7**$^{2+}$	-2156.281777383	1234.54	0.72132
[Fe(CN-^{t}Bu)Cp*$_2$]$^{2+}$ **8**$^{2+}$	-2293.574034725	1568.33	0.83216



Atomic coordinates of **4**$^{\cdot+}$

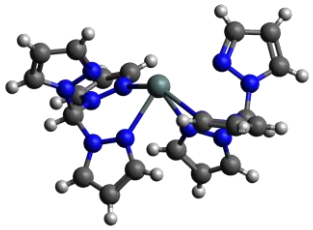
F	1.7130645	3.9362931	-0.3476610
F	0.6529156	-6.1481980	-1.1189093
F	2.9897374	0.8245089	4.0435074
F	-0.1081757	-2.3308300	-3.0339109
F	0.5194270	6.2310754	0.5853027
F	2.9920574	-1.8732722	3.6725205
F	-2.0192510	-1.6598090	0.5352365
F	1.8869580	2.4602759	2.2360497
F	-1.9308159	1.3756416	1.2523883
F	-1.8913803	6.0787153	1.8514531
F	-3.2406823	-4.1272778	0.6895670
F	-1.0202114	2.0157676	-4.5640157
F	-0.9446171	-0.6765502	-4.9648406
F	1.8595368	-3.6826415	-1.2701916
F	-3.1364329	3.6697105	2.1941383
F	1.8705029	-2.9679336	1.5091163
F	-1.8867622	-6.3501408	-0.1451176
F	-0.2883637	3.0833190	-2.2283329
N	0.4907140	1.4160108	-0.0281088
N	0.5232607	-1.3440316	-0.4301438
C	-0.0725659	5.0537522	0.7424581
C	0.5345417	3.8831424	0.2655789
C	-0.1762433	-1.0293824	-2.7651145
C	0.1781115	-0.5082898	-1.4953441
C	0.1522688	0.9154842	-1.2869690
C	-0.6148695	-0.1800032	-3.7879678
C	-1.3190855	4.9744281	1.3994154
C	0.0096428	-5.0594409	-0.7164652
C	1.1642473	0.6057815	0.8895702
C	-0.1051130	2.6436042	0.4366652
C	-0.2715333	1.7578014	-2.3455178
C	-1.3464581	2.5668456	1.0941853
C	1.8100124	1.1479435	2.0293792
C	2.3942516	0.3084218	2.9854718
C	-1.3051545	-5.1634394	-0.2143252
C	1.1759414	-0.8190009	0.6870618
C	-0.6478140	1.2179797	-3.5817428
C	-2.0048266	-4.0181113	0.2170113
C	-0.0672619	-2.6572943	-0.3597259
C	2.4005813	-1.0914953	2.7899536
C	1.7967146	-1.6473341	1.6553141
C	0.6249062	-3.8014818	-0.7917373
C	-1.9628688	3.7329065	1.5765629
C	-1.3789073	-2.7634509	0.1382344

vibrational spectrum of **4**$^{\cdot+}$

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.33	0.01498	YES	YES
8	a	11.66	0.06446	YES	YES
9	a	12.78	0.03181	YES	YES
10	a	19.66	0.12578	YES	YES
11	a	37.16	0.17248	YES	YES
12	a	41.48	0.04686	YES	YES
13	a	42.95	0.01057	YES	YES
14	a	44.57	0.00014	YES	YES
15	a	92.46	0.02716	YES	YES
16	a	100.32	0.03260	YES	YES
17	a	102.13	0.00343	YES	YES
18	a	103.05	0.02253	YES	YES
19	a	113.67	0.08079	YES	YES
20	a	116.30	0.02906	YES	YES
21	a	120.88	0.34221	YES	YES
22	a	125.64	0.01312	YES	YES
23	a	125.79	0.02862	YES	YES
24	a	131.17	0.11993	YES	YES
25	a	131.36	0.03661	YES	YES
26	a	146.85	0.00272	YES	YES
27	a	149.85	0.08585	YES	YES
28	a	203.63	0.43307	YES	YES
29	a	206.39	3.14897	YES	YES
30	a	214.20	1.44387	YES	YES
31	a	240.80	0.00708	YES	YES
32	a	246.64	0.68496	YES	YES
33	a	247.69	2.88501	YES	YES
34	a	251.88	0.00513	YES	YES
35	a	261.26	0.00788	YES	YES
36	a	261.55	0.00778	YES	YES
37	a	264.42	0.00628	YES	YES
38	a	265.23	0.00663	YES	YES
39	a	272.37	0.36552	YES	YES
40	a	274.55	0.10726	YES	YES
41	a	294.43	0.01285	YES	YES
42	a	296.61	0.04292	YES	YES
43	a	297.38	0.55470	YES	YES
44	a	299.80	0.32318	YES	YES
45	a	316.07	5.01787	YES	YES
46	a	323.01	0.06805	YES	YES
47	a	325.49	2.74161	YES	YES
48	a	335.44	0.00546	YES	YES
49	a	341.95	1.24026	YES	YES
50	a	347.71	1.87806	YES	YES
51	a	355.21	0.74904	YES	YES
52	a	357.38	1.67042	YES	YES
53	a	365.58	0.21651	YES	YES

54	a	375.96	0.92916	YES	YES
55	a	376.99	0.32829	YES	YES
56	a	382.50	1.07189	YES	YES
57	a	397.42	0.01182	YES	YES
58	a	423.08	0.12915	YES	YES
59	a	426.50	0.12251	YES	YES
60	a	428.29	0.90412	YES	YES
61	a	435.82	1.21866	YES	YES
62	a	438.26	1.64197	YES	YES
63	a	453.98	6.75224	YES	YES
64	a	460.08	4.42443	YES	YES
65	a	465.70	1.36143	YES	YES
66	a	468.01	0.80040	YES	YES
67	a	482.06	0.13627	YES	YES
68	a	494.20	0.00778	YES	YES
69	a	500.81	0.02925	YES	YES
70	a	508.55	1.82888	YES	YES
71	a	569.46	0.32519	YES	YES
72	a	570.57	0.00497	YES	YES
73	a	596.52	0.20922	YES	YES
74	a	607.06	11.22418	YES	YES
75	a	608.12	0.77165	YES	YES
76	a	610.09	0.03652	YES	YES
77	a	617.91	6.42916	YES	YES
78	a	617.99	2.26693	YES	YES
79	a	621.57	0.07198	YES	YES
80	a	621.86	0.41392	YES	YES
81	a	650.50	5.81310	YES	YES
82	a	690.20	42.00695	YES	YES
83	a	691.62	0.06389	YES	YES
84	a	702.83	12.66038	YES	YES
85	a	776.90	1.87711	YES	YES
86	a	777.28	1.84314	YES	YES
87	a	806.60	0.02110	YES	YES
88	a	819.51	79.16072	YES	YES
89	a	924.19	0.88044	YES	YES
90	a	930.71	37.47515	YES	YES
91	a	1007.16	86.36385	YES	YES
92	a	1007.65	4.61522	YES	YES
93	a	1009.62	231.83250	YES	YES
94	a	1040.32	61.46722	YES	YES
95	a	1090.10	531.48731	YES	YES
96	a	1105.46	164.39094	YES	YES
97	a	1133.83	12.44582	YES	YES
98	a	1159.35	12.42098	YES	YES
99	a	1182.61	2.54163	YES	YES
100	a	1185.47	2.79433	YES	YES
101	a	1197.51	2.82546	YES	YES
102	a	1217.12	40.31775	YES	YES
103	a	1244.10	40.60787	YES	YES
104	a	1250.17	0.00278	YES	YES
105	a	1334.42	3.56014	YES	YES
106	a	1335.83	0.23828	YES	YES
107	a	1343.30	82.94054	YES	YES
108	a	1348.44	9.75844	YES	YES

109	a	1348.75	8.16220	YES	YES
110	a	1352.55	0.11243	YES	YES
111	a	1360.08	25.47553	YES	YES
112	a	1360.70	1.53164	YES	YES
113	a	1374.62	1.64479	YES	YES
114	a	1444.64	2.58713	YES	YES
115	a	1461.86	0.82946	YES	YES
116	a	1469.17	2.63544	YES	YES
117	a	1499.08	0.75851	YES	YES
118	a	1510.56	1080.00889	YES	YES
119	a	1512.84	1312.28351	YES	YES
120	a	1520.05	107.36750	YES	YES
121	a	1522.60	156.27418	YES	YES
122	a	1529.85	178.80025	YES	YES
123	a	1530.69	550.66542	YES	YES
124	a	1531.25	29.59570	YES	YES
125	a	1584.43	116.30715	YES	YES
126	a	1604.29	0.27823	YES	YES
127	a	1609.88	2.90293	YES	YES
128	a	1610.94	23.71197	YES	YES
129	a	1628.02	7.54722	YES	YES
130	a	1628.55	0.65429	YES	YES
131	a	1634.74	20.66096	YES	YES
132	a	1635.27	22.14161	YES	YES



Atomic coordinates of **6**$^{2+}$

N	-0.6932924	1.2008177	0.3240209
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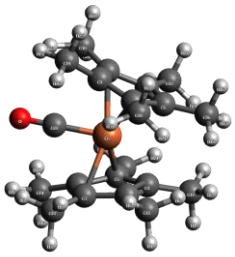
N	1.3865849	0.0000000	0.3240209
H	0.0000000	0.0000000	1.8710950
N	-0.8414994	1.4575197	-1.0108798
N	1.6829987	0.0000000	-1.0108798
N	-0.8414994	-1.4575197	-1.0108798
C	-1.2671842	-2.1948275	1.0728234
C	-1.8032929	-3.1233949	0.1845323
C	-1.5151309	-2.6242837	-1.1035633
C	2.5343685	0.0000000	1.0728234
C	3.0302618	0.0000000	-1.1035633
C	3.6065857	0.0000000	0.1845323
C	-1.2671842	2.1948275	1.0728234
C	-1.8032929	3.1233949	0.1845323
C	-1.5151309	2.6242837	-1.1035633
H	-1.2525984	2.1695641	2.1711318
H	-2.3372793	4.0482866	0.4368446
H	-1.7619439	3.0517763	-2.0859216
H	3.5238878	0.0000000	-2.0859216

H	4.6745587	0.0000000	0.4368446
H	2.5051969	0.0000000	2.1711318
H	-1.7619439	-3.0517763	-2.0859216
H	-1.2525984	-2.1695641	2.1711318
H	-2.3372793	-4.0482866	0.4368446
Sn	0.0000000	0.0000000	-2.6041702

vibrational spectrum of **6**$^{2+}$

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e	53.54	0.93990	YES	YES
8	e	53.54	0.93990	YES	YES
9	a2	75.59	0.00000	NO	NO
10	e	140.49	1.99384	YES	YES
11	e	140.49	1.99384	YES	YES
12	a2	147.67	0.00000	NO	NO
13	e	181.11	11.04866	YES	YES
14	e	181.11	11.04866	YES	YES
15	a1	187.07	7.41178	YES	YES
16	a1	240.76	11.24162	YES	YES
17	e	310.76	3.83937	YES	YES
18	e	310.76	3.83937	YES	YES
19	e	362.72	3.73333	YES	YES
20	e	362.72	3.73333	YES	YES
21	a1	378.70	7.74882	YES	YES
22	a2	577.49	0.00000	NO	NO
23	e	590.18	10.59376	YES	YES
24	e	590.18	10.59376	YES	YES
25	a2	615.06	0.00000	NO	NO
26	e	641.09	1.16428	YES	YES
27	e	641.09	1.16428	YES	YES
28	a2	753.99	0.00000	NO	NO
29	e	757.25	84.56668	YES	YES
30	e	757.25	84.56668	YES	YES
31	e	781.97	59.14281	YES	YES
32	e	781.97	59.14281	YES	YES
33	a2	849.37	0.00000	NO	NO
34	a1	849.88	27.74844	YES	YES
35	e	851.01	6.07813	YES	YES
36	e	851.01	6.07813	YES	YES
37	e	899.10	1.70390	YES	YES
38	e	899.10	1.70390	YES	YES
39	a1	906.48	0.26203	YES	YES
40	a2	908.59	0.00000	NO	NO
41	e	908.83	0.02775	YES	YES
42	e	908.83	0.02775	YES	YES
43	a1	983.41	20.08434	YES	YES
44	e	985.46	33.25617	YES	YES
45	e	985.46	33.25617	YES	YES

46	e	1053.86	102.53560	YES	YES
47	e	1053.86	102.53560	YES	YES
48	a1	1065.91	59.70486	YES	YES
49	a1	1098.97	4.69630	YES	YES
50	e	1101.97	8.40485	YES	YES
51	e	1101.97	8.40485	YES	YES
52	e	1163.04	7.69938	YES	YES
53	e	1163.04	7.69938	YES	YES
54	a1	1207.04	2.48079	YES	YES
55	e	1240.11	65.65646	YES	YES
56	e	1240.11	65.65646	YES	YES
57	e	1277.59	193.90484	YES	YES
58	e	1277.59	193.90484	YES	YES
59	a1	1278.38	5.02503	YES	YES
60	a1	1341.33	0.42495	YES	YES
61	e	1360.98	3.06977	YES	YES
62	e	1360.98	3.06977	YES	YES
63	e	1400.77	56.22018	YES	YES
64	e	1400.77	56.22018	YES	YES
65	a1	1425.87	153.17992	YES	YES
66	e	1448.74	9.62944	YES	YES
67	e	1448.74	9.62944	YES	YES
68	a1	1455.43	37.17109	YES	YES
69	e	1517.09	42.32759	YES	YES
70	e	1517.09	42.32759	YES	YES
71	a1	1522.58	0.24003	YES	YES
72	a1	3093.38	5.96843	YES	YES
73	e	3170.51	0.55375	YES	YES
74	e	3170.51	0.55375	YES	YES
75	a1	3170.67	18.85665	YES	YES
76	e	3177.14	1.96618	YES	YES
77	e	3177.14	1.96618	YES	YES
78	a1	3177.67	57.42276	YES	YES
79	e	3196.34	62.35600	YES	YES
80	e	3196.34	62.35600	YES	YES
81	a1	3196.70	11.03316	YES	YES



Atomic coordinates of **7**$^{2+}$

Fe	0.28014	-0.25475	0.01408
O	2.44986	-2.22779	0.12510
C	-1.02231	0.63403	-1.52176
C	0.31932	1.19565	-1.59953
C	1.22679	0.12950	-1.88305
C	0.43088	-1.11813	-1.97098
C	-0.93657	-0.80295	-1.66451
C	-0.82033	1.02372	1.42806
C	-1.24324	-0.36407	1.55459

C	-0.10582	-1.13629	1.94294
C	1.04683	-0.20908	2.04328
C	0.60824	1.09903	1.64525
C	-2.28953	1.41154	-1.59784
H	-2.57823	1.44733	-2.67666
H	-2.18725	2.46027	-1.26447
H	-3.13608	0.92937	-1.07003
C	0.66486	2.64802	-1.61416
H	0.64154	3.01132	-2.66863
H	1.68663	2.84129	-1.23102
H	-0.05552	3.26822	-1.04596
C	2.66817	0.27442	-2.24667
H	2.74324	0.47894	-3.34074
H	3.26004	-0.64080	-2.04457
H	3.14502	1.12642	-1.72129
C	0.89445	-2.42159	-2.53276
H	0.61781	-2.43060	-3.61418
H	0.38943	-3.29012	-2.06300
H	1.99079	-2.56275	-2.47286
C	-2.08059	-1.75946	-1.76488
H	-2.33530	-1.91995	-2.83866
H	-2.99415	-1.38133	-1.26806
H	-1.83091	-2.75355	-1.34007
C	-1.72811	2.20314	1.39433
H	-1.85279	2.54065	2.45218
H	-2.74066	1.97277	1.01601
H	-1.30820	3.06846	0.84427
C	-2.65016	-0.86192	1.51627
H	-3.07233	-0.82479	2.54810
H	-2.71385	-1.91633	1.18121
H	-3.30926	-0.24151	0.87824
C	-0.12171	-2.56281	2.38512
H	-0.37835	-2.59811	3.47020
H	0.85921	-3.06487	2.26543
H	-0.88979	-3.15544	1.84820
C	2.36055	-0.50221	2.68964
H	2.28561	-0.17191	3.75327
H	3.19489	0.06791	2.23246
H	2.61794	-1.57892	2.69746
C	1.43411	2.34197	1.72770
H	1.51240	2.66338	2.79272
H	0.98878	3.18517	1.16657
H	2.46924	2.17952	1.36281
C	1.59429	-1.45000	0.08087

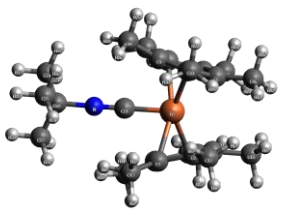
Vibrational spectrum of **7**$^{2+}$

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	29.06	0.46965	YES	YES
8	a	38.32	0.00631	YES	YES

9	a	115.09	0.03389	YES	YES
10	a	132.44	0.04924	YES	YES
11	a	136.11	0.41303	YES	YES
12	a	137.95	0.29730	YES	YES
13	a	139.56	0.23366	YES	YES
14	a	144.44	1.05610	YES	YES
15	a	146.40	0.20095	YES	YES
16	a	148.62	0.21976	YES	YES
17	a	158.73	1.30004	YES	YES
18	a	164.74	1.40604	YES	YES
19	a	165.30	3.33657	YES	YES
20	a	171.17	0.14519	YES	YES
21	a	179.28	0.91068	YES	YES
22	a	182.33	0.70547	YES	YES
23	a	190.84	2.54574	YES	YES
24	a	194.81	2.44351	YES	YES
25	a	199.60	6.39035	YES	YES
26	a	202.95	0.81361	YES	YES
27	a	217.68	7.87970	YES	YES
28	a	222.46	5.64760	YES	YES
29	a	228.68	7.35166	YES	YES
30	a	259.99	4.38791	YES	YES
31	a	267.88	0.69861	YES	YES
32	a	282.92	0.31124	YES	YES
33	a	287.58	0.34175	YES	YES
34	a	290.84	1.64798	YES	YES
35	a	292.92	0.78908	YES	YES
36	a	299.18	4.25805	YES	YES
37	a	300.21	1.54428	YES	YES
38	a	307.43	1.13052	YES	YES
39	a	320.80	10.82935	YES	YES
40	a	352.53	0.98709	YES	YES
41	a	397.23	5.10772	YES	YES
42	a	403.88	0.23512	YES	YES
43	a	418.76	1.72963	YES	YES
44	a	424.31	6.45335	YES	YES
45	a	471.54	8.58538	YES	YES
46	a	479.11	24.72951	YES	YES
47	a	516.94	0.20886	YES	YES
48	a	518.33	43.40861	YES	YES
49	a	524.35	13.08123	YES	YES
50	a	529.72	2.05303	YES	YES
51	a	531.19	5.59121	YES	YES
52	a	540.21	0.60805	YES	YES
53	a	541.10	0.26251	YES	YES
54	a	548.71	31.25708	YES	YES
55	a	590.14	0.00666	YES	YES
56	a	595.69	1.07824	YES	YES
57	a	596.23	0.23225	YES	YES
58	a	600.45	2.70894	YES	YES
59	a	606.52	3.05063	YES	YES
60	a	607.35	9.06640	YES	YES
61	a	789.21	0.95709	YES	YES
62	a	791.00	0.14487	YES	YES
63	a	805.11	0.84432	YES	YES

64	a	806.45	0.12415	YES	YES
65	a	930.47	0.19296	YES	YES
66	a	934.53	1.59251	YES	YES
67	a	937.91	0.63830	YES	YES
68	a	938.80	0.25474	YES	YES
69	a	971.82	60.05853	YES	YES
70	a	974.87	34.75253	YES	YES
71	a	981.22	52.81647	YES	YES
72	a	983.59	17.99517	YES	YES
73	a	988.38	2.38024	YES	YES
74	a	989.89	42.87003	YES	YES
75	a	993.07	5.05425	YES	YES
76	a	995.77	11.63808	YES	YES
77	a	995.81	0.52430	YES	YES
78	a	996.98	20.21081	YES	YES
79	a	1058.71	0.00912	YES	YES
80	a	1063.87	21.00914	YES	YES
81	a	1065.45	7.56463	YES	YES
82	a	1069.23	15.67131	YES	YES
83	a	1084.87	0.13376	YES	YES
84	a	1085.31	0.14683	YES	YES
85	a	1151.35	0.00167	YES	YES
86	a	1157.17	0.73248	YES	YES
87	a	1166.67	0.29982	YES	YES
88	a	1169.89	0.16435	YES	YES
89	a	1332.47	0.94220	YES	YES
90	a	1338.06	2.83136	YES	YES
91	a	1344.68	4.82094	YES	YES
92	a	1345.43	3.62488	YES	YES
93	a	1348.47	9.09367	YES	YES
94	a	1352.24	1.56251	YES	YES
95	a	1354.92	3.87046	YES	YES
96	a	1356.21	57.74589	YES	YES
97	a	1361.09	58.99204	YES	YES
98	a	1363.15	3.50108	YES	YES
99	a	1363.90	45.54358	YES	YES
100	a	1365.34	7.07047	YES	YES
101	a	1376.34	0.28085	YES	YES
102	a	1385.47	11.95542	YES	YES
103	a	1386.49	5.02770	YES	YES
104	a	1392.17	1.96318	YES	YES
105	a	1395.53	28.08286	YES	YES
106	a	1396.22	2.82207	YES	YES
107	a	1397.22	0.30861	YES	YES
108	a	1401.88	0.34417	YES	YES
109	a	1406.86	9.80479	YES	YES
110	a	1408.20	0.74044	YES	YES
111	a	1416.00	107.74436	YES	YES
112	a	1417.20	22.44785	YES	YES
113	a	1418.92	4.59489	YES	YES
114	a	1422.47	42.91637	YES	YES
115	a	1423.30	6.01810	YES	YES
116	a	1424.36	0.72761	YES	YES
117	a	1428.11	47.47421	YES	YES
118	a	1431.28	7.76701	YES	YES

119	a	1439.11	58.38195	YES	YES
120	a	1439.90	62.19115	YES	YES
121	a	1447.50	0.02311	YES	YES
122	a	1452.60	1.32973	YES	YES
123	a	1458.27	44.73375	YES	YES
124	a	1460.67	4.67593	YES	YES
125	a	1469.98	16.83700	YES	YES
126	a	1472.09	20.87544	YES	YES
127	a	1494.75	111.31982	YES	YES
128	a	1497.19	0.69000	YES	YES
129	a	2057.93	380.07304	YES	YES
130	a	2939.21	18.13025	YES	YES
131	a	2939.35	18.00180	YES	YES
132	a	2945.86	17.64658	YES	YES
133	a	2946.23	11.38949	YES	YES
134	a	2948.69	14.53422	YES	YES
135	a	2948.98	8.86764	YES	YES
136	a	2950.65	4.69882	YES	YES
137	a	2950.91	3.98211	YES	YES
138	a	2951.16	4.00631	YES	YES
139	a	2951.33	4.01845	YES	YES
140	a	3035.25	2.90520	YES	YES
141	a	3035.46	1.87425	YES	YES
142	a	3037.72	4.25285	YES	YES
143	a	3037.81	0.50357	YES	YES
144	a	3037.88	3.23667	YES	YES
145	a	3038.75	9.84227	YES	YES
146	a	3038.79	0.76083	YES	YES
147	a	3038.99	3.35749	YES	YES
148	a	3039.44	6.13131	YES	YES
149	a	3040.56	7.36174	YES	YES
150	a	3078.12	0.30620	YES	YES
151	a	3078.38	0.31044	YES	YES
152	a	3084.02	1.12621	YES	YES
153	a	3084.47	2.07141	YES	YES
154	a	3088.41	1.62627	YES	YES
155	a	3088.77	1.58357	YES	YES
156	a	3090.10	0.88439	YES	YES
157	a	3090.20	0.39211	YES	YES
158	a	3104.00	1.10310	YES	YES
159	a	3105.12	0.78396	YES	YES



Atomic coordinates of **8**$^{2+}$

Fe	-0.50962	0.43430	-0.03382
N	1.73099	-1.60020	0.06291
C	-1.82025	1.36323	-1.53871
C	-0.45826	1.85513	-1.66479

C	0.38346	0.74109	-1.95625
C	-0.47324	-0.46463	-1.99483
C	-1.80961	-0.07757	-1.66629
C	-1.54834	1.77810	1.36433
C	-2.02522	0.41178	1.51715
C	-0.91584	-0.40179	1.89314
C	0.26433	0.48161	1.98432
C	-0.11931	1.79884	1.57478
C	-3.05135	2.20042	-1.60697
H	-3.36660	2.21849	-2.67818
H	-2.88989	3.25184	-1.30744
H	-3.90578	1.77833	-1.04199
C	-0.03924	3.28876	-1.70913
H	-0.06950	3.64362	-2.76579
H	0.99935	3.43263	-1.34979
H	-0.71118	3.95081	-1.12866
C	1.81574	0.81805	-2.37499
H	1.86599	1.05299	-3.46359
H	2.35530	-0.13639	-2.21737
H	2.36069	1.62193	-1.83930
C	-0.10062	-1.80426	-2.53682
H	-0.48434	-1.86913	-3.58200
H	-0.56789	-2.63357	-1.96722
H	0.99237	-1.96284	-2.57386
C	-3.00174	-0.97835	-1.73127
H	-3.27361	-1.15821	-2.79745
H	-3.89137	-0.54263	-1.23875
H	-2.79751	-1.97020	-1.27764
C	-2.40562	2.99705	1.33304
H	-2.48386	3.36128	2.38575
H	-3.43747	2.80507	0.98743
H	-1.96624	3.83103	0.75070
C	-3.45318	-0.02641	1.50640
H	-3.85892	0.04681	2.54251
H	-3.56658	-1.08237	1.19012
H	-4.09463	0.60922	0.86537
C	-0.97856	-1.82829	2.33332
H	-1.19568	-1.86987	3.42597
H	-0.02379	-2.36472	2.16415
H	-1.78658	-2.38395	1.81568
C	1.56166	0.15895	2.64796
H	1.51476	0.55893	3.68817
H	2.42380	0.64775	2.15073
H	1.74816	-0.92884	2.72011
C	0.75703	3.00918	1.63859
H	0.84722	3.35180	2.69569
H	0.34913	3.85735	1.05643
H	1.78405	2.79651	1.27644
C	0.85674	-0.80876	0.02707
C	2.85629	-2.52680	0.15493
C	2.99326	-3.26101	-1.19388
C	2.55048	-3.52812	1.28746
C	4.12183	-1.69904	0.45984
H	1.61894	-4.09630	1.08188
H	2.45960	-3.01848	2.27024

H	3.38683	-4.25421	1.36227
H	4.31565	-0.95264	-0.33956
H	4.99574	-2.38152	0.51277
H	4.03839	-1.17378	1.43386
H	2.08047	-3.84528	-1.43301
H	3.84507	-3.96968	-1.12938
H	3.20810	-2.55304	-2.02277

Vibrational spectrum of **8**$^{2+}$

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.51	0.04283	YES	YES
8	a	30.89	0.01479	YES	YES
9	a	45.99	0.01066	YES	YES
10	a	77.96	0.38181	YES	YES
11	a	85.91	0.33218	YES	YES
12	a	116.04	0.04339	YES	YES
13	a	127.71	0.10370	YES	YES
14	a	134.93	0.09922	YES	YES
15	a	136.21	0.08399	YES	YES
16	a	138.04	0.24824	YES	YES
17	a	145.05	1.15884	YES	YES
18	a	146.81	0.00905	YES	YES
19	a	149.81	0.43839	YES	YES
20	a	158.71	1.62656	YES	YES
21	a	160.01	0.52142	YES	YES
22	a	164.59	3.25638	YES	YES
23	a	175.97	0.13361	YES	YES
24	a	178.49	0.36981	YES	YES
25	a	186.90	2.31365	YES	YES
26	a	189.03	1.11642	YES	YES
27	a	197.85	1.67647	YES	YES
28	a	198.91	1.02461	YES	YES
29	a	203.15	0.26581	YES	YES
30	a	211.87	3.44384	YES	YES
31	a	220.09	7.17265	YES	YES
32	a	228.97	0.95035	YES	YES
33	a	235.41	3.09406	YES	YES
34	a	263.02	4.40842	YES	YES
35	a	269.86	1.52673	YES	YES
36	a	277.32	3.04344	YES	YES
37	a	279.20	0.42873	YES	YES
38	a	282.83	0.38047	YES	YES
39	a	288.39	0.53354	YES	YES
40	a	290.19	0.96804	YES	YES
41	a	292.95	0.62397	YES	YES
42	a	300.02	0.30602	YES	YES
43	a	305.62	6.72753	YES	YES
44	a	306.84	0.28001	YES	YES
45	a	311.18	2.00474	YES	YES

46	a	317.96	14.74224	YES	YES
47	a	346.37	0.06824	YES	YES
48	a	350.05	3.96100	YES	YES
49	a	367.21	12.97708	YES	YES
50	a	391.66	5.87133	YES	YES
51	a	401.49	0.12205	YES	YES
52	a	413.23	2.29165	YES	YES
53	a	414.23	7.85622	YES	YES
54	a	419.01	4.85359	YES	YES
55	a	442.42	0.26795	YES	YES
56	a	475.13	8.71882	YES	YES
57	a	479.79	42.46444	YES	YES
58	a	502.03	13.33937	YES	YES
59	a	520.45	1.20469	YES	YES
60	a	525.15	0.71849	YES	YES
61	a	530.16	2.00211	YES	YES
62	a	533.38	0.76090	YES	YES
63	a	537.58	17.69667	YES	YES
64	a	540.92	1.46168	YES	YES
65	a	541.77	3.98483	YES	YES
66	a	589.83	0.16387	YES	YES
67	a	595.51	1.04408	YES	YES
68	a	597.89	0.16164	YES	YES
69	a	598.80	0.03077	YES	YES
70	a	604.90	0.55782	YES	YES
71	a	606.72	10.41458	YES	YES
72	a	732.57	2.25074	YES	YES
73	a	790.61	0.23842	YES	YES
74	a	792.52	0.07979	YES	YES
75	a	808.23	0.83152	YES	YES
76	a	809.34	0.00880	YES	YES
77	a	839.29	2.91448	YES	YES
78	a	908.32	0.97643	YES	YES
79	a	909.54	0.73640	YES	YES
80	a	932.29	0.58075	YES	YES
81	a	936.05	1.39215	YES	YES
82	a	941.45	1.37697	YES	YES
83	a	942.29	0.11443	YES	YES
84	a	943.08	0.03671	YES	YES
85	a	977.33	44.30748	YES	YES
86	a	980.18	37.22249	YES	YES
87	a	985.00	32.45477	YES	YES
88	a	988.11	17.89487	YES	YES
89	a	993.12	1.95242	YES	YES
90	a	994.31	36.58988	YES	YES
91	a	998.62	1.43657	YES	YES
92	a	1000.07	3.66361	YES	YES
93	a	1001.51	12.00849	YES	YES
94	a	1002.56	7.84657	YES	YES
95	a	1015.83	0.38670	YES	YES
96	a	1017.71	0.19501	YES	YES
97	a	1059.49	0.99348	YES	YES
98	a	1064.77	14.04467	YES	YES
99	a	1066.79	7.91709	YES	YES
100	a	1070.60	22.55749	YES	YES

101	a	1086.69	0.07303	YES	YES
102	a	1087.72	0.10063	YES	YES
103	a	1154.59	0.00970	YES	YES
104	a	1158.71	0.67103	YES	YES
105	a	1165.17	121.23028	YES	YES
106	a	1169.17	0.48246	YES	YES
107	a	1172.59	3.38267	YES	YES
108	a	1213.63	6.69828	YES	YES
109	a	1214.27	6.08564	YES	YES
110	a	1335.72	0.91639	YES	YES
111	a	1342.42	2.34756	YES	YES
112	a	1346.81	2.79755	YES	YES
113	a	1347.48	5.03845	YES	YES
114	a	1349.02	3.05167	YES	YES
115	a	1350.58	13.40545	YES	YES
116	a	1350.98	9.73100	YES	YES
117	a	1355.43	0.99282	YES	YES
118	a	1356.72	15.40074	YES	YES
119	a	1358.43	21.43083	YES	YES
120	a	1365.72	73.57461	YES	YES
121	a	1368.18	8.12871	YES	YES
122	a	1369.96	7.72064	YES	YES
123	a	1372.47	3.53131	YES	YES
124	a	1380.23	7.77330	YES	YES
125	a	1381.82	0.45097	YES	YES
126	a	1390.42	8.75413	YES	YES
127	a	1392.89	9.08165	YES	YES
128	a	1398.59	0.76171	YES	YES
129	a	1400.62	11.62381	YES	YES
130	a	1402.99	5.86776	YES	YES
131	a	1404.67	9.99868	YES	YES
132	a	1406.26	1.11211	YES	YES
133	a	1408.26	9.91512	YES	YES
134	a	1409.89	0.31813	YES	YES
135	a	1411.88	5.37176	YES	YES
136	a	1417.80	1.92287	YES	YES
137	a	1419.75	4.24565	YES	YES
138	a	1422.23	26.18947	YES	YES
139	a	1422.88	14.96104	YES	YES
140	a	1423.65	17.76947	YES	YES
141	a	1425.56	64.54860	YES	YES
142	a	1427.44	0.85004	YES	YES
143	a	1428.64	11.02295	YES	YES
144	a	1431.75	23.66732	YES	YES
145	a	1433.55	4.22520	YES	YES
146	a	1438.66	50.10805	YES	YES
147	a	1439.47	9.73828	YES	YES
148	a	1441.65	50.23077	YES	YES
149	a	1445.40	38.32128	YES	YES
150	a	1450.96	1.42649	YES	YES
151	a	1455.57	0.80680	YES	YES
152	a	1458.12	36.84105	YES	YES
153	a	1460.12	23.59590	YES	YES
154	a	1465.12	5.43653	YES	YES
155	a	1478.11	15.81024	YES	YES

156	a	1481.69	21.42583	YES	YES
157	a	1503.24	82.32146	YES	YES
158	a	1506.06	3.55927	YES	YES
159	a	2195.33	470.78371	YES	YES
160	a	2942.70	10.00558	YES	YES
161	a	2943.71	9.34728	YES	YES
162	a	2950.31	3.50753	YES	YES
163	a	2951.13	1.90124	YES	YES
164	a	2951.59	0.19950	YES	YES
165	a	2952.03	2.46177	YES	YES
166	a	2952.11	3.32054	YES	YES
167	a	2952.31	1.28930	YES	YES
168	a	2952.55	1.95875	YES	YES
169	a	2952.67	1.71701	YES	YES
170	a	2963.09	8.06681	YES	YES
171	a	2964.49	4.26875	YES	YES
172	a	2968.52	2.44161	YES	YES
173	a	3033.79	2.15848	YES	YES
174	a	3034.12	1.84931	YES	YES
175	a	3037.52	3.69175	YES	YES
176	a	3038.30	1.81060	YES	YES
177	a	3038.40	2.04733	YES	YES
178	a	3038.49	4.79894	YES	YES
179	a	3038.87	2.27582	YES	YES
180	a	3039.36	3.34071	YES	YES
181	a	3039.83	5.48225	YES	YES
182	a	3041.17	8.13431	YES	YES
183	a	3054.31	5.35610	YES	YES
184	a	3055.49	6.01860	YES	YES
185	a	3060.12	8.66219	YES	YES
186	a	3062.41	0.34971	YES	YES
187	a	3065.49	6.99287	YES	YES
188	a	3068.61	2.01764	YES	YES
189	a	3077.72	0.87433	YES	YES
190	a	3077.93	3.14731	YES	YES
191	a	3081.01	1.97794	YES	YES
192	a	3083.25	2.15489	YES	YES
193	a	3084.90	2.71118	YES	YES
194	a	3087.79	2.71884	YES	YES
195	a	3095.31	2.01864	YES	YES
196	a	3103.28	1.36078	YES	YES
197	a	3105.10	1.57750	YES	YES
198	a	3105.96	1.55903	YES	YES

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