Supporting Information

For

Isolation of Base Stabilized Boron(I)-Monofluoride and its Radical Cation

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(S1) Experimental Section:

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Hexane, toluene and THF were distilled over Na/K alloy (25:75). Deuterated NMR solvents C_6D_6 was dried by stirring for 2 days over Na/K alloy followed by distillation in vacuum and degassed. ^{1}H, ^{13}C, ^{11}B and ^{19}F NMR spectra were recorded on Bruker Avance 200, Bruker Avance 300, and Bruker Avance 500 MHz NMR spectrometers and were referenced to the resonances of the solvent used. Microanalyses were performed by the Analytisches Labor für Anorganische Chemie für Universität Göttingen. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. LIFDI measurements were performed on a Joel AccuTOF spectrometer under inert atmosphere. Continuous-wave (CW) EPR spectra were recorded at X-band microwave frequencies (9 GHz) using a Bruker ElexSys E500 spectrometer with a Bruker SuperX CW bridge. The spectrometer S12 was equipped with the Bruker SHQ rectangular microwave cavity (Bruker 4122SHQ) and a helium flow cryostat (Oxford Instruments) for low temperature experiments. CV experiments were performed using a Biologic SP300 potentiostat and a three electrodes setup consisting of a glassy carbon-working electrode, a platinum wire counter electrode and an Ag/AgCl reference electrode. Ferrocene was used as an internal standard with $E^{o}(Fc/Fc^{+})$ = 0.61 V *vs* Ag/AgCl. All studies were performed in deoxygenated THF containing NBu_4PF_6 (0.1M) as supporting electrode. The starting material Me-cAAC,[S1] were by following literature procedures, while all other reagents were used as received.

Synthesis of **Me-cAAC:BF_3**:

A mixture of Me-cAAC (286 mg, 1 mmol), $BF_3.OEt_2$ (156 mg, 1.1 mmol) were taken in a 100 mL round bottom flask and 30 mL of hexane was added at -78 °C. The reaction mixture was slowly warm to room temperature and stirred for 15 hours. The reaction mixture was filtered, and solvent was removed under high vacuum. The resultant white solid was characterized as Me-cAAC: BF_3 (Yield: 350 mg, 98 %). ^{1}H NMR (300 MHz, C_6D_6): δ = 7.11 (d, *J* = 6 Hz, 1H, Ar-CH), 7.08 (d, *J* = 6.0 Hz, 1H, Ar-CH), 6.98 (dd, *J*= 9 Hz, 2H, Ar-CH), 2.60 (m, *J* = 6 Hz, 2H, $CHMe_2$), 1.53 (s, 6H, $NCMe_2$), 1.41 (d, *J*= 6Hz, 6H, $CHMe_2$), 1.38 (s, 2H, CH_2), 1.09 (d, *J* = 6 Hz, 6H), 0.78 (s, 6H, CMe_2); ^{13}C NMR (126 MHz, C_6D_6): δ = 145.8 (o), 130.4 (p), 125.6 (m), 125.2 (ipso), 80.9 (Cq), 61.3 (Cq), 45.2 (CH2), 36.9 (CH2), 29.7 (CH3), 29.5 (CH), 26.5 (CH3), 25.2 (CH3), 24.7 (CH2),

23.1 (CH2); ^{19}F NMR (470 MHz, C_6D_6): δ = −137.602 (*J* = 37.6 Hz), ^{11}B NMR (160 MHz, C_6D_6): δ = −0.41 (*J* = 37.6 Hz).

Synthesis of **(Me-cAAC:)$_2$BF** (**1**):

A mixture of Me-cAAC:BF_3 (354 mg, 1.0 mmol), Me-cAAC (286 mg, 1.0 mmol) and KC_8 (270 mg, 2 mmol) were taken in a 100 mL round bottom flask and 40 mL of toluene was added at -78 °C. The reaction mixture was slowly warm to room temperature to give a violet solution of compound **1**. After filtration of insoluble residue, the solvent was concentrated to 3 mL under high vacuum. The dark red violet solution was stored at 0 °C for 24 hours to get X-ray quality dark red violet block shaped crystals of **1** (Yield: 320 mg, 53 %). ^{1}H NMR (500 MHz, C_6D_6): δ = 7.06 (m, *J* = 10 Hz, 2H, Ar-CH), 6.98 (m, *J* = 5.0 Hz, 4H, Ar-CH), 3.19 (m, *J*= 10 Hz, 2H), 2.94 (m, *J* = 10 Hz, 2H), 1.79 (d, *J*= 10 Hz, 8H), 1.70 (s, 4H), 1.44 (s, 4H), 1.33 (d, *J* = 5 Hz, 6H), 1.28 (d, *J*= 5Hz, 6H), 1.21 (d, *J*= 5Hz, 4H), 1.17 (d, *J*= 5Hz, 4H), 1.13 (s, 4H), 1.08 (d, *J*= 10Hz, 2H), 0.99 (s, 2H), 0.93 (s, 4H), 0.46 (d, *J*= 5Hz, 4H); ^{13}C NMR (126 MHz, C_6D_6): δ = 145.8 (o), 130.4 (p), 125.6 (m), 125.2 (ipso), 80.9 (Cq), 61.3 (Cq), 45.2 (CH2), 36.9 (CH2), 29.7 (CH3), 29.5 (CH), 26.5 (CH3), 25.2 (CH3), 24.7 (CH2), 23.1 (CH2); ^{19}F NMR (470 MHz, C_6D_6): δ = −139.35, ^{11}B NMR (160 MHz, C_6D_6): δ = 25.53.

Exact Mass: 600.49, Found: 600.50

Melting range: 223-225 °C to a red violet liquid.

Anal (%). calcd for $C_{40}H_{62}B_1F_1N_2$ (600.49): C, 79.97; H, 10.40; N, 4.66 Found: C, 78.95; H, 10.01; N, 4.58.

Synthesis of **[(Me-cAAC:)$_2$BF]$^{+}$[B(C$_6$F$_5$)$_4$]$^{-}$** (**2**):

A mixture of (Me-cAAC:)$_2$BF (60 mg, 0.1 mmol) and $LiB(C_6F_5)_4$ (87 mg, 0.1 mmol) were taken in a 100 mL round bottom flask and 20 mL of toluene was added at -78 °C. The reaction mixture was slowly warm to room temperature to give a reddish-brown solution of compound **2**. After filtration of insoluble residue, the solvent was concentrated to 3 mL under high vacuum. The dark reddish-brown solution was stored at 0 °C for 48 hours to get X-ray quality brown block shaped crystals of **2** (Yield: 73 mg, 50 %).

Exact Mass: 1279.48, but experimentally mass was not found. Mass was found for $(cAAC)_2BF$ and $B(C_6F_5)_4$ with Na.

Melting range: 171-174 °C to a red brown liquid.

Anal (%). calcd for $C_{64}H_{62}B_2F_{21}N_2$ (1279.48): C, 60.06; H, 4.88; N, 2.19 Found: C, 59.25; H, 4.44; N, 2.31.

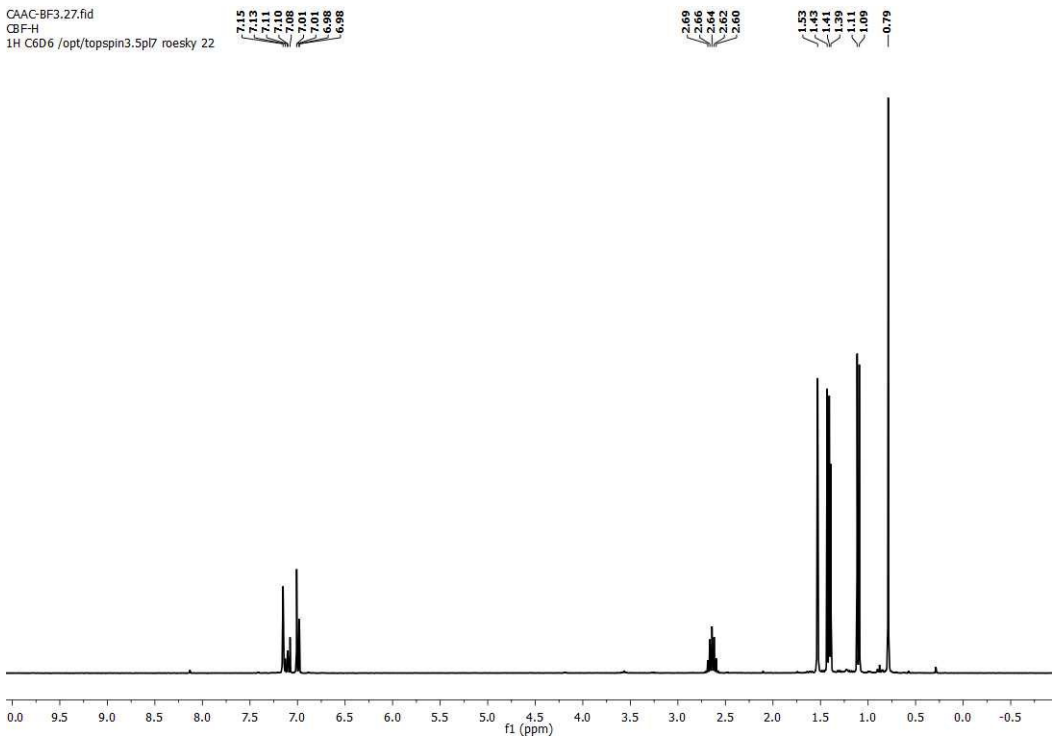


Figure S1. ^{1}H-NMR spectrum of **Me-cAAC:BF_3**.

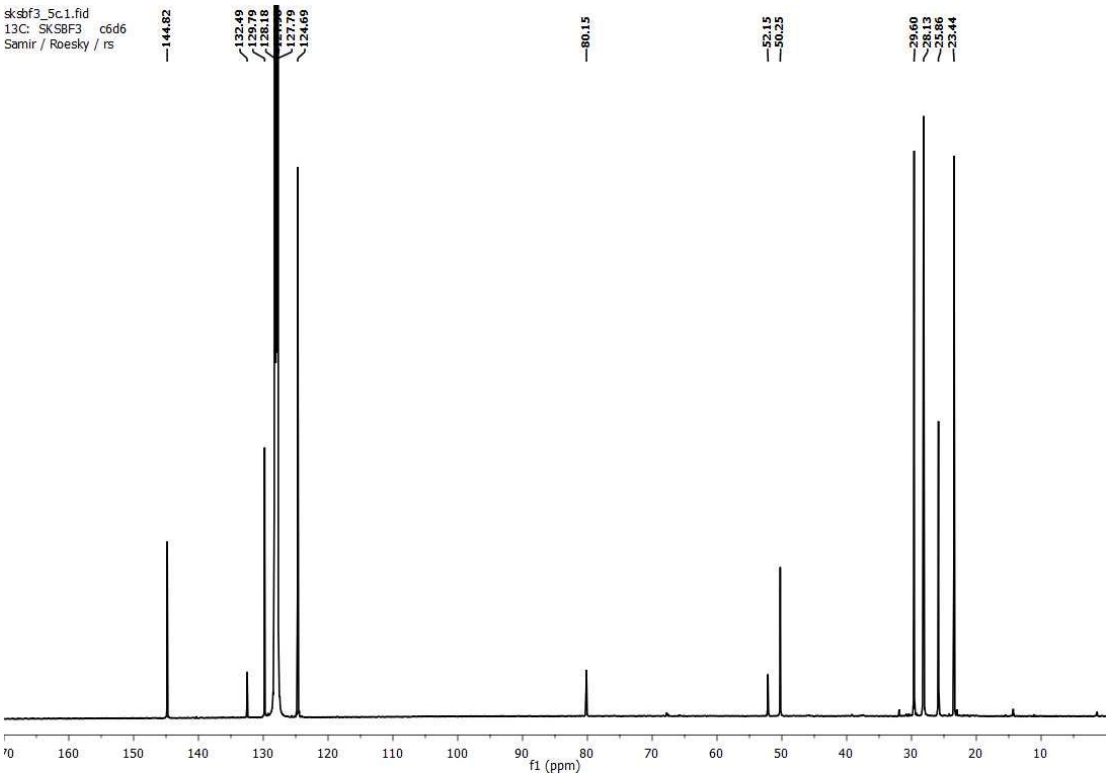


Figure S2. ^{13}C-NMR spectrum of **Me-cAAC:BF$_3$**.

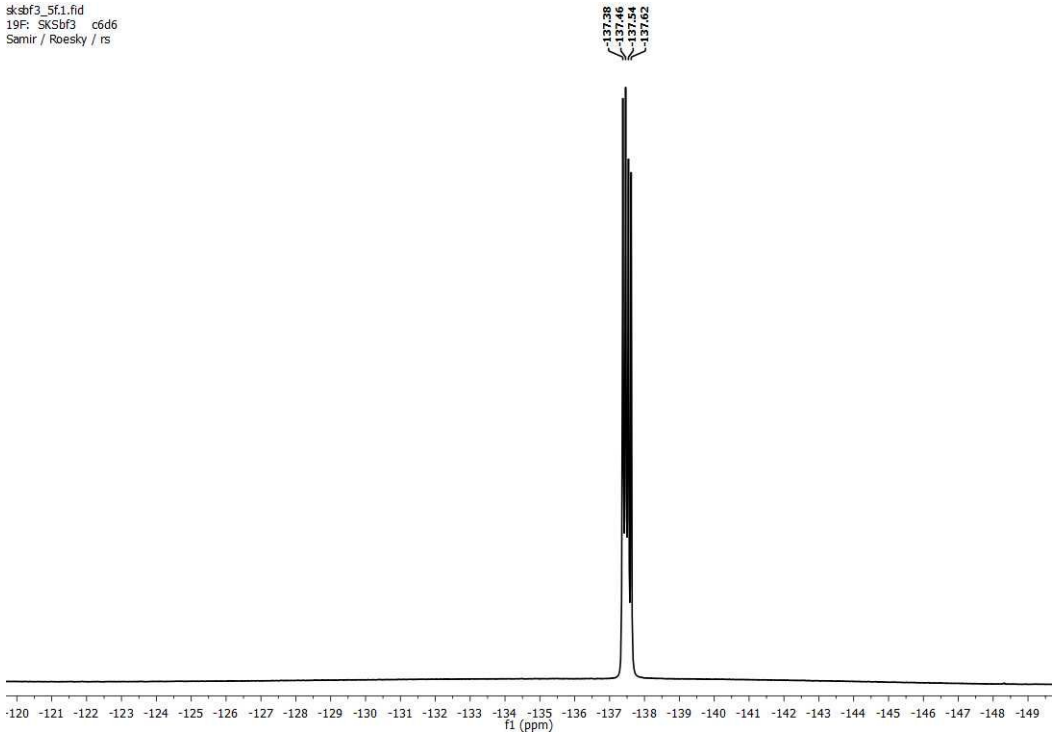


Figure S3. ^{19}F-NMR spectrum of **Me-cAAC:BF$_3$**.

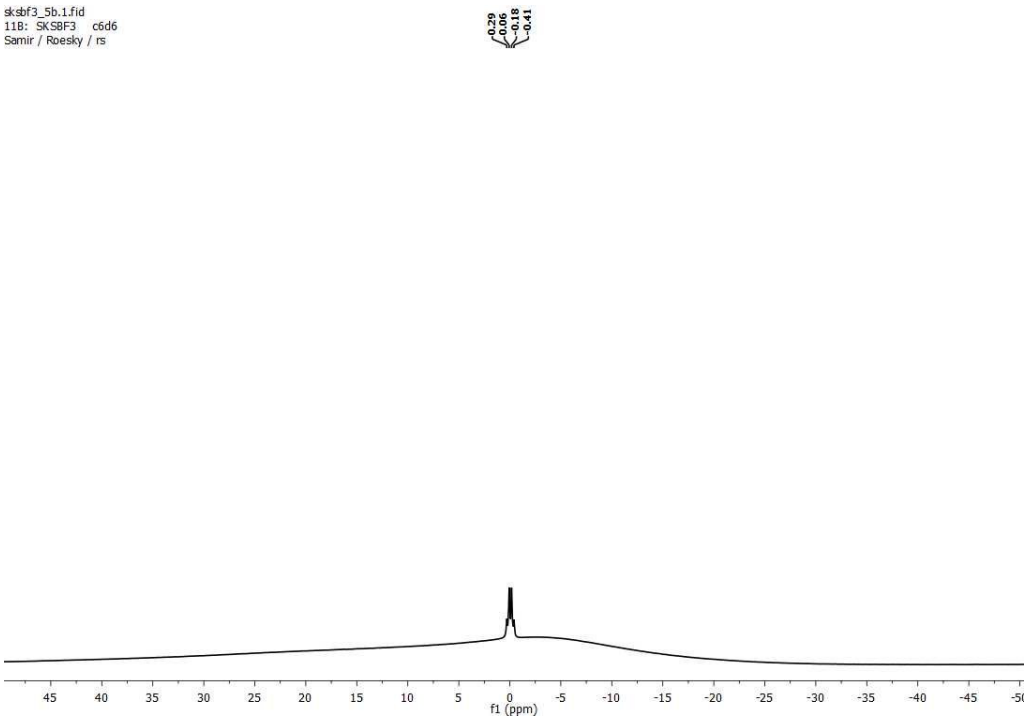


Figure S4. ^{11}B-NMR spectrum of **Me-cAAC:BF$_3$**.

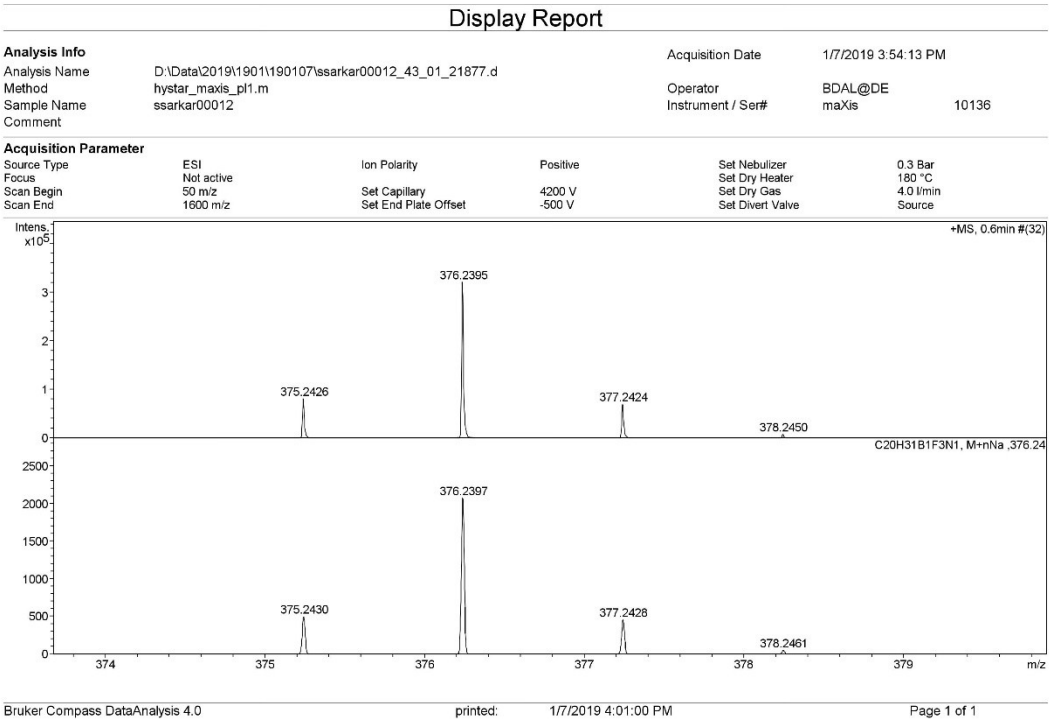


Figure S5. Mass distribution spectrum of **M+Na**.

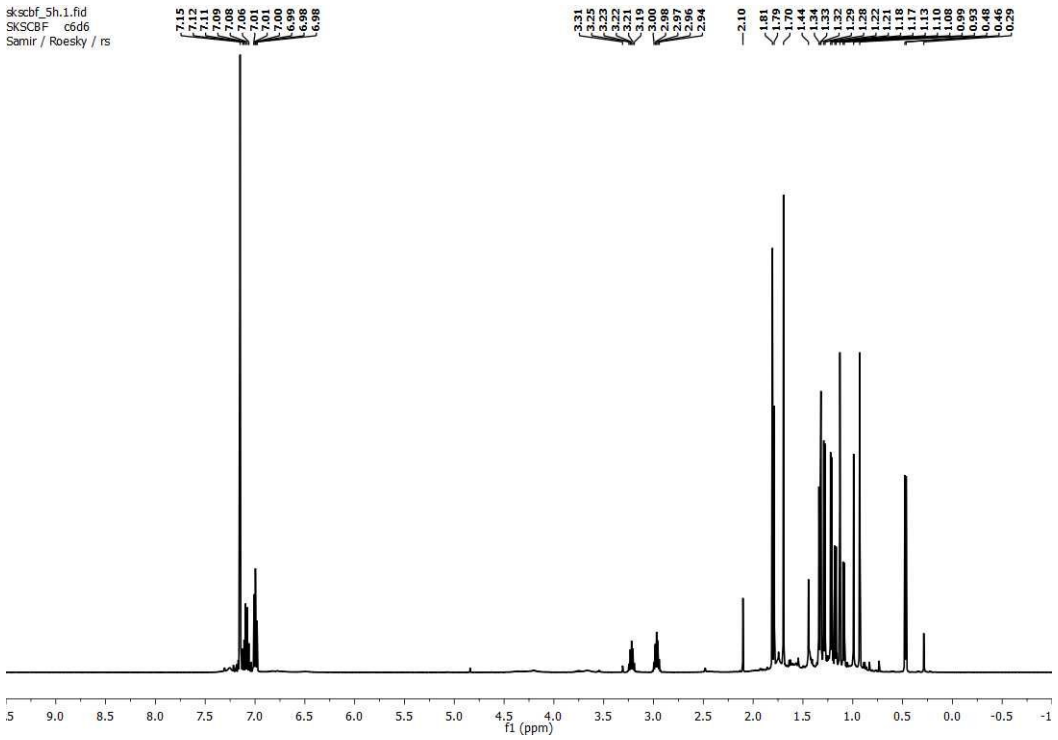


Figure S6. ^{1}H-NMR spectrum of **1**.

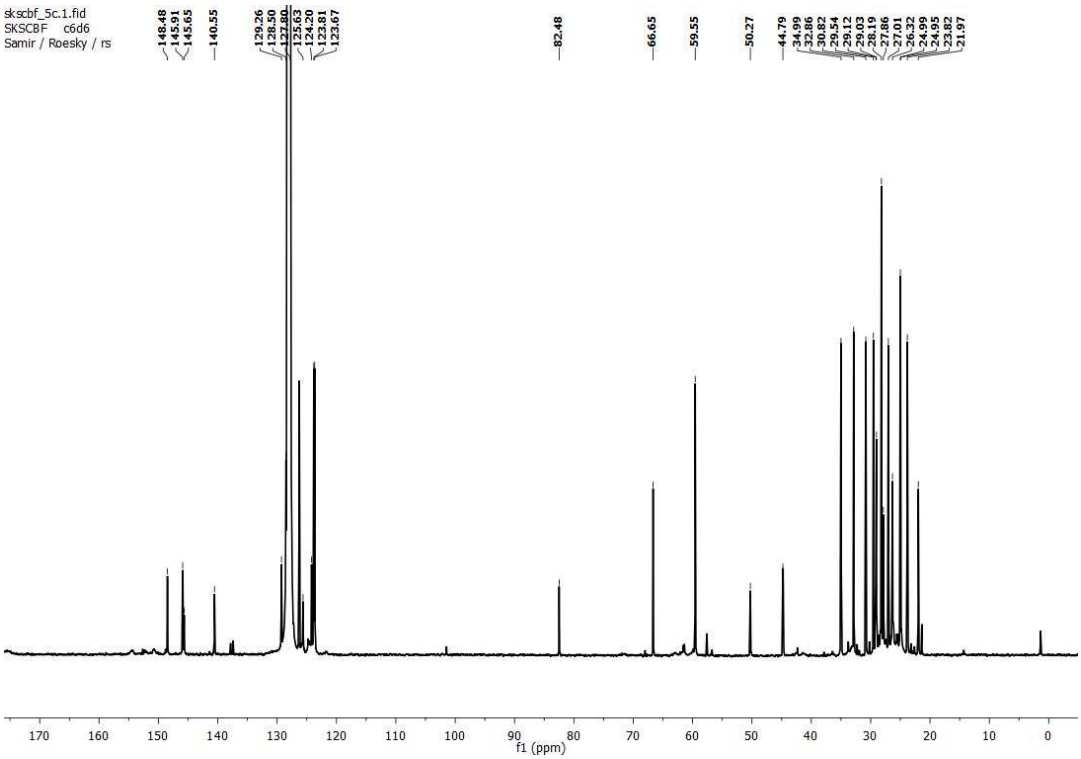


Figure S7. ^{13}C-NMR spectrum of **1**.

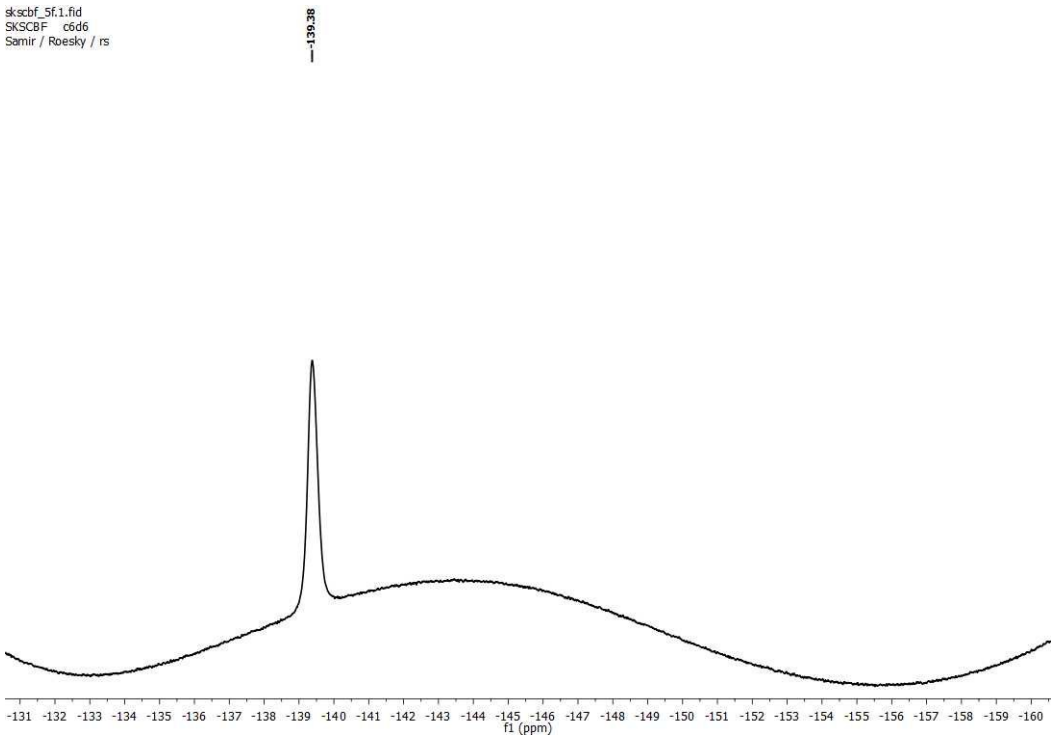


Figure S8. ^{19}F-NMR spectrum of **1**.

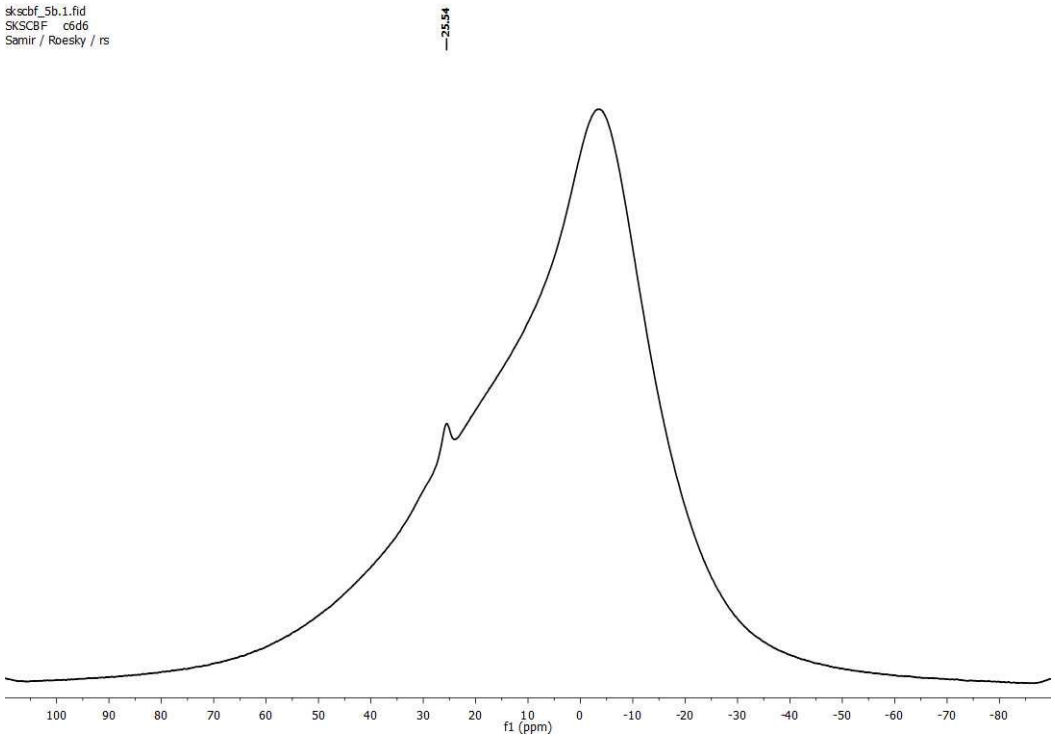


Figure S9. ^{11}B-NMR spectrum of **1**.

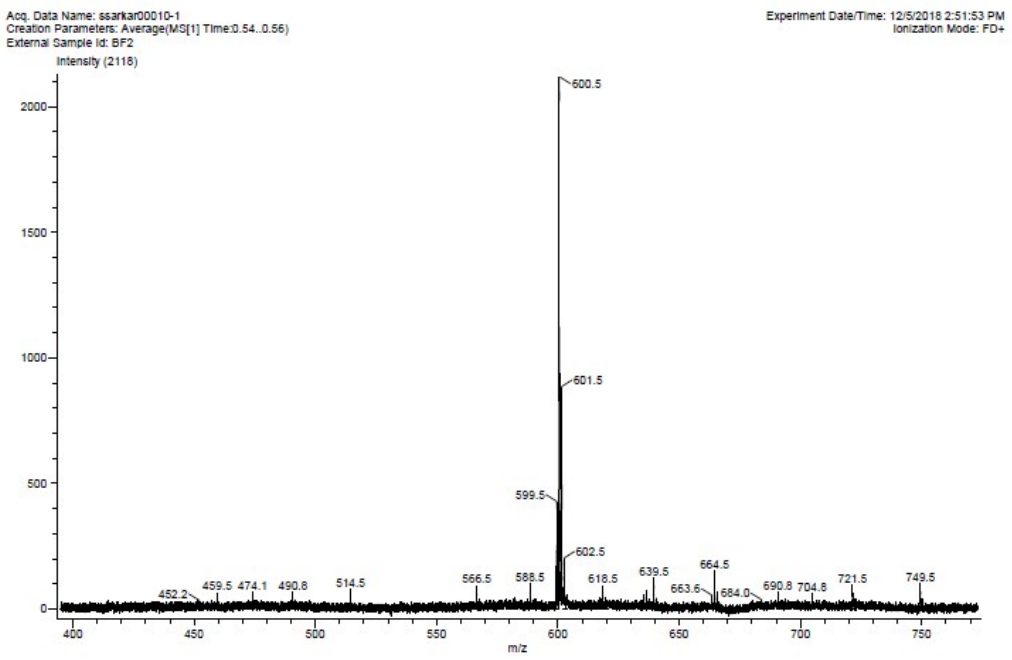


Figure S10. LIFDI-Mass spectrum of **1**.

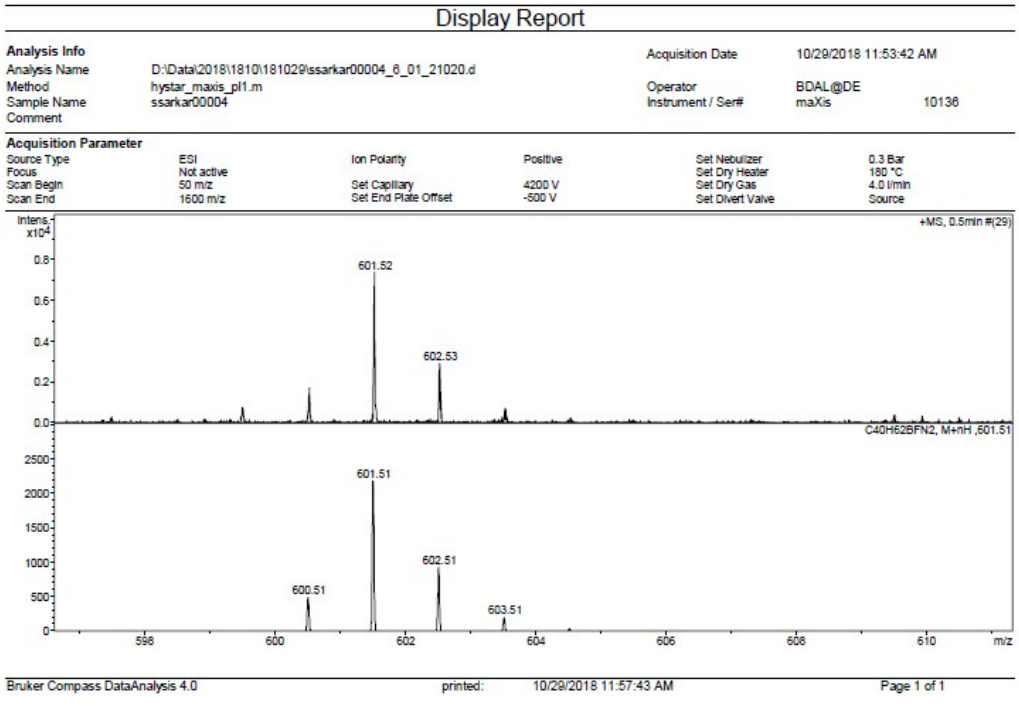


Figure S11. Isotopic mass distribution spectrum of **1**.

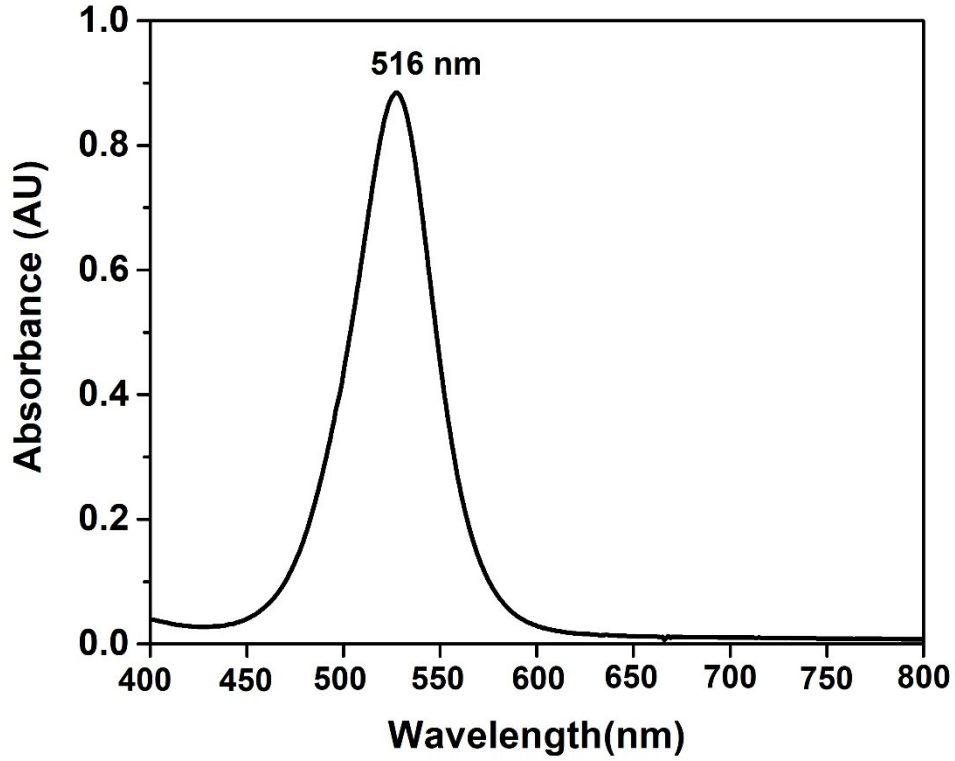


Figure S12. UV-Vis spectrum of **1** in Hexane.

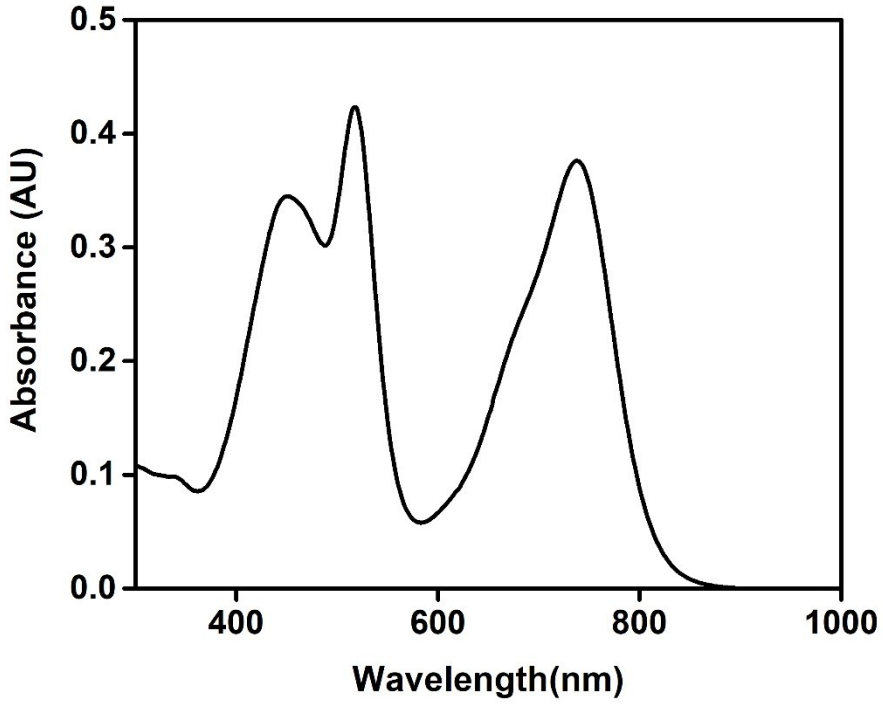


Figure S13. UV-Vis spectrum of **2** in THF. (λ_{max} = 738 nm, 518 nm, 451 nm)

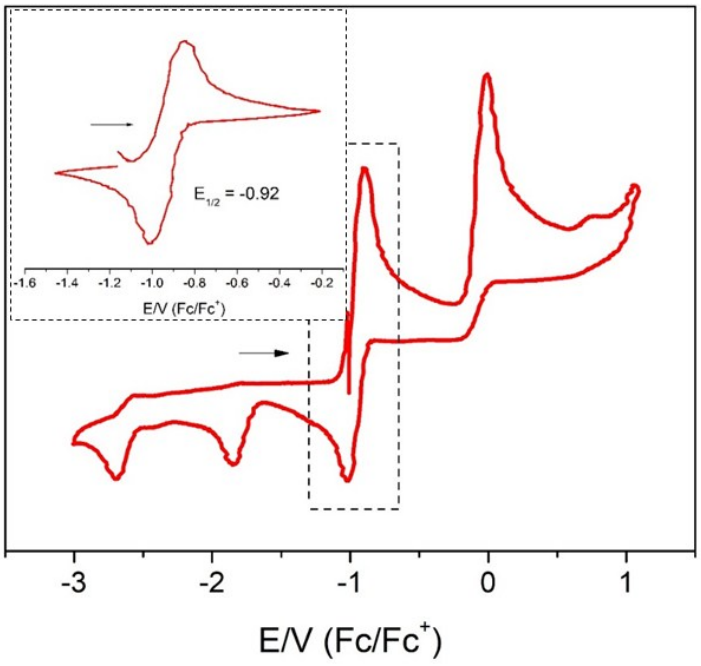


Figure S14. Cyclic Voltammogram of THF solution of **1** at 50mV/s scan rate in presence of 0.2 M $[n\text{-}Bu_4N]PF_6$ as an electrolyte. The dotted line in Fig X has been shown in large (left).

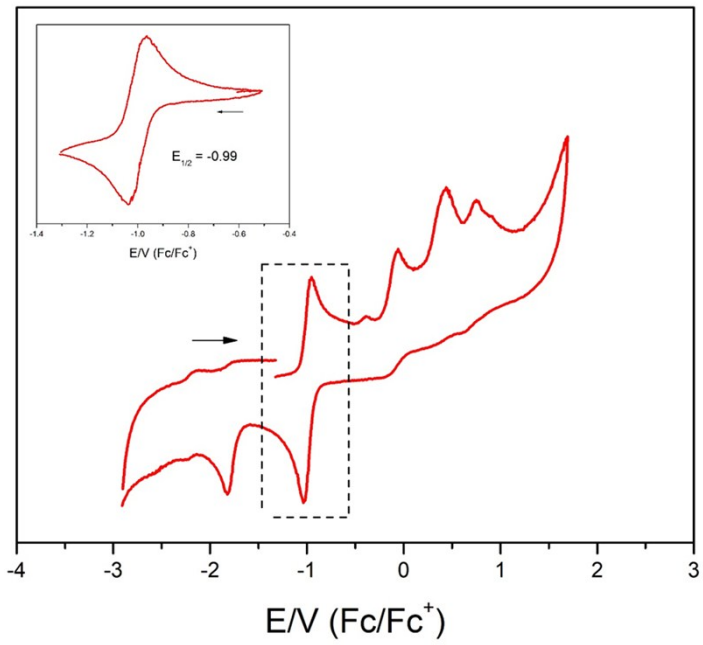


Figure S15. Cyclic Voltammogram of CH_3CN solution of **1** at 100 mV/s scan rate in presence of 0.1 M $[n\text{-}Bu_4N]PF_6$ as an electrolyte. The dotted line in Fig X has been shown in inset.

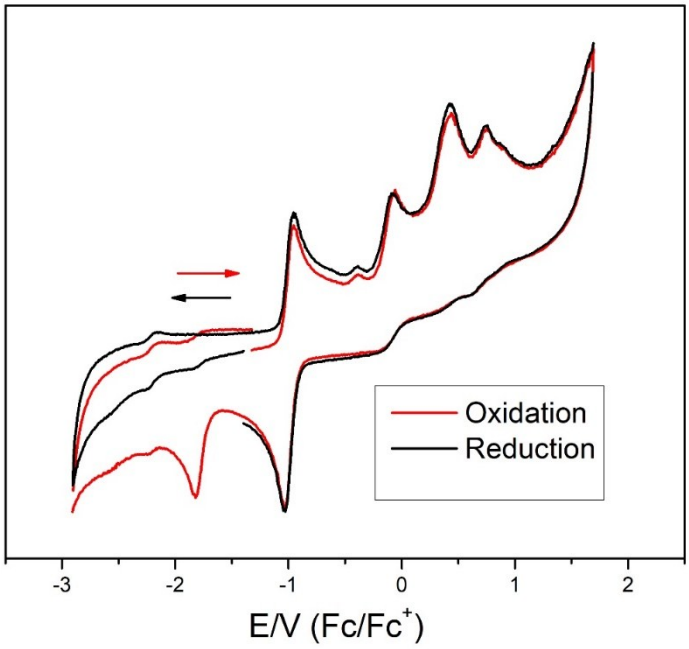


Figure S16. Cyclic Voltammogram of CH_3CN solution of **1** at 100 mV/s scan rate in presence of 0.1 M [n-Bu_4N]PF_6 as an electrolyte.

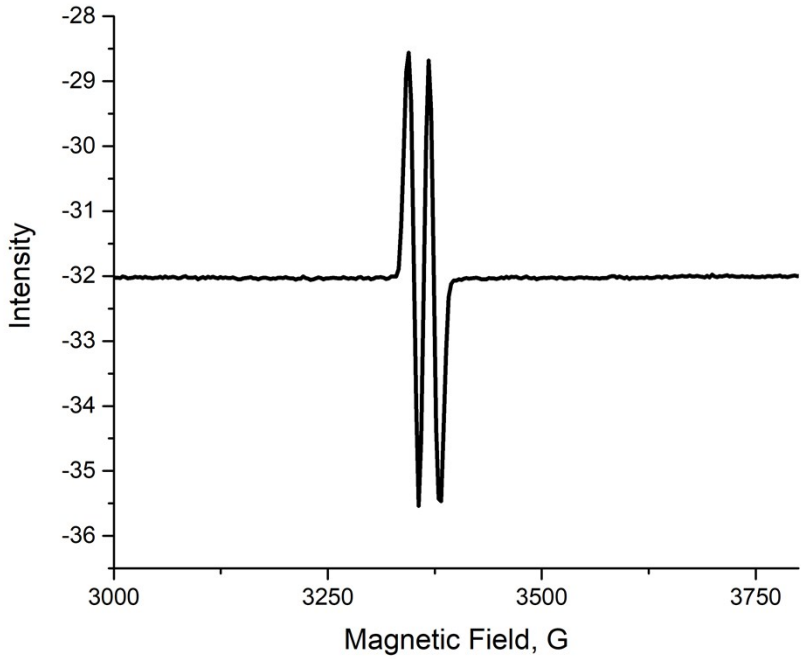


Figure S17: EPR spectrum of compound **2** in THF at room temperature

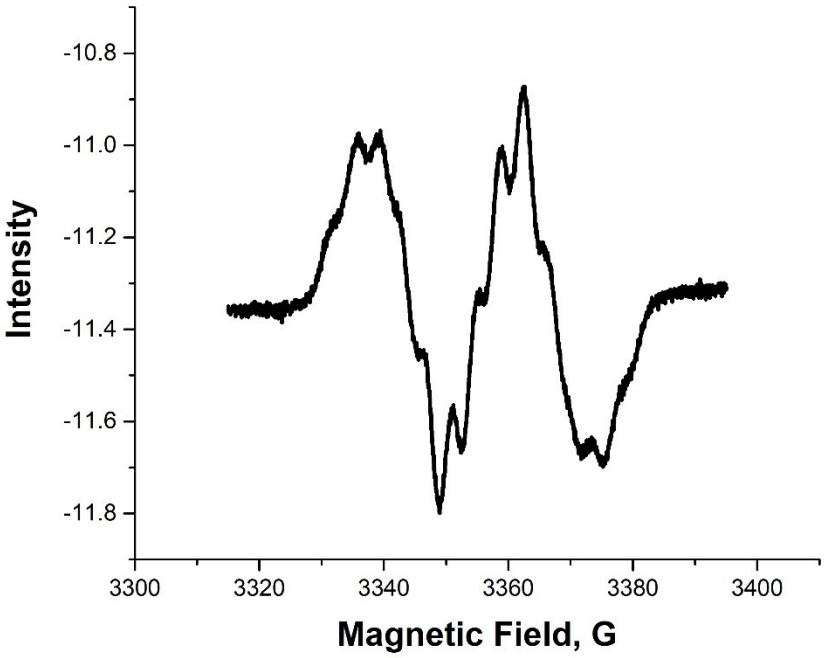


Figure S18: EPR spectrum of compound **2** in THF (High resolution).

(S2) X-Ray Crystallographic Analysis of 1 and 2

All experiments for crystal data acquisition were performed on Bruker Smart Apex II systems either on a Bruker D8 three circle diffractometer equipped with a Smart Apex II Quazar detector and an Incoatec Mo or Ag microsource with mirror optics, or a Bruker TXS-Mo rotating anode with mirror optics and a Smart Apex II Ultra detector.[S1] Crystal handling and selection of **1** and **2** were performed at low temperatures in an inert oil while under an argon atmosphere by application of the X-Temp2 device.[S2] Suitable crystals were mounted to the tip of a MiTeGen©MicroMount using a polarizer microscope and transferred to the diffractometer. Data collection has been performed at 100 K crystal temperature with a suitable 0.5° omega scan data collection strategy. Subsequent data reduction and integration has been carried out with Saint v8.38A[S3] and a multi-scan absorption correction and a 3λ correction[S4] was applied using Sadabs (v2016/2)[S5]. Structure solution was performed by Shelxt (v2018/2)[S6] and refined by full-matrix least-squares against F^2 using Shelxl (v2018/3)[S7] with the help of the Shelxle[S8] graphical user interface. All non-hydrogen-atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 U_{eq} of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. The disorder in **2** was refined using distance restraints and restraints for the anisotropic displacement parameter.[S9]

Table T1. Crystal data and structure refinement of **1** and **2**.

Compound	**1**	**2**
CCDC no.	1900360	1900361
Formula	C_{40} H_{62} B F N_2	
Molecular weight., [g·mol^{-1}]	600.72	1325.84
Wavelength, [Å]	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	C2/c
a, [Å]	10.679(2)	27.121(4)
b, [Å]	19.037(3)	28.125(4)
c, [Å]	20.054(3)	21.074(3)
α, [°]	104.98(2)	90
β, [°]	102.80(2)	128.85(2)
γ, [°]	102.62(2)	90
V, [Å^3]	3672.3(12)	12519(4)
z	4	8
Refl. measured	157775	124907
Refl. unique	15692	11510
R_{int}	0.0547	0.0793
Data/restraints/parameters	15692 / 0 / 826	11510 / 1646 / 1037
Final R indices [I>2σ(I)][a,b]	R1=0.0413 / wR2=0.0915	R1=0.0729 / wR2=0.1444
R indices (all ata)[a,b]	R1=0.0609 / wR2=0.1020	R1=0.0967 / wR2=0.1538
$\Delta\rho_{fin}$, [e·Å^{-3}]	0.282 and -0.202	1.364 and -0.328

a: $$R1 = \frac{\sum ||F_o| - |F_C||}{\sum |F_o|}$$

b: $$wR2 = \sqrt{\frac{\sum w\left(F_o^2 - F_c^2\right)^2}{w\left(F_o^2\right)^2}} \qquad w = \frac{1}{\sigma^2\left(F_o^2\right) + \left(g_1 P\right)^2 + g_2 P} \; P = \frac{\left(F_o^2 + 2F_c^2\right)}{3}$$

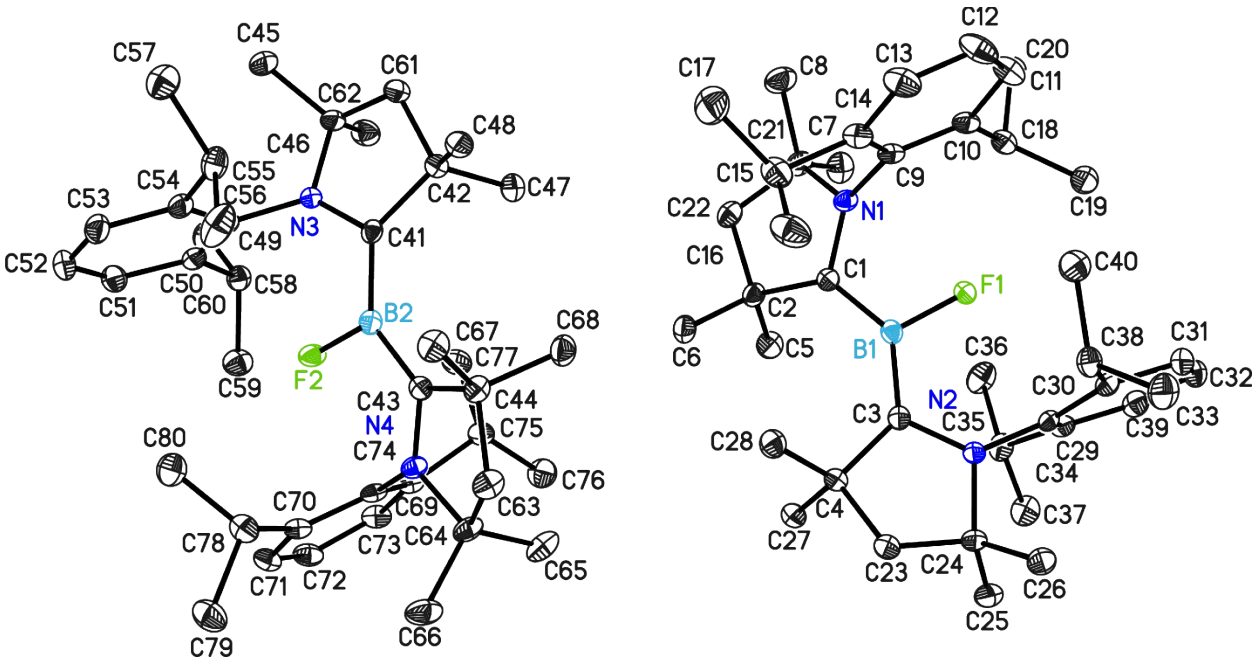


Figure S19. Crystal structure of **1**. The anisotropic displacement parameters are depicted at the 50% probability level. The hydrogen atoms are omitted for clarity.

Table T2. Bond lengths [Å] and angles [°] for **1**.

bond lengths [Å]		angles [°]	
C(1)-N(1)	1.3955(16)	N(1)-C(1)-B(1)	116.91(11)
C(1)-B(1)	1.5137(19)	N(1)-C(1)-C(2)	107.27(10)
C(1)-C(2)	1.5462(17)	B(1)-C(1)-C(2)	134.41(11)
C(2)-C(6)	1.5377(18)	C(6)-C(2)-C(5)	108.50(11)
C(2)-C(5)	1.5403(18)	C(6)-C(2)-C(22)	106.28(10)
C(2)-C(22)	1.5447(18)	C(5)-C(2)-C(22)	111.59(11)
C(3)-N(2)	1.3787(16)	C(6)-C(2)-C(1)	115.74(11)
C(3)-B(1)	1.5270(19)	C(5)-C(2)-C(1)	111.63(10)
C(3)-C(4)	1.5360(17)	C(22)-C(2)-C(1)	102.90(10)
C(4)-C(28)	1.5353(18)	N(2)-C(3)-B(1)	120.48(11)
C(4)-C(27)	1.5405(18)	N(2)-C(3)-C(4)	107.18(10)
C(4)-C(23)	1.5433(18)	B(1)-C(3)-C(4)	132.11(11)
C(7)-C(21)	1.5473(19)	C(28)-C(4)-C(3)	112.16(10)
C(8)-C(21)	1.5198(19)	C(28)-C(4)-C(27)	110.34(11)
C(9)-C(10)	1.4103(18)	C(3)-C(4)-C(27)	112.01(11)
C(9)-C(14)	1.4137(18)	C(28)-C(4)-C(23)	108.59(11)
C(9)-N(1)	1.4474(16)	C(3)-C(4)-C(23)	103.39(10)
C(10)-C(11)	1.3959(19)	C(27)-C(4)-C(23)	110.08(11)
C(10)-C(18)	1.5205(18)	C(10)-C(9)-C(14)	120.10(12)
C(11)-C(12)	1.381(2)	C(10)-C(9)-N(1)	121.21(11)
C(12)-C(13)	1.382(2)	C(14)-C(9)-N(1)	118.67(11)

C(13)-C(14)	1.3959(19)	C(11)-C(10)-C(9)	118.81(12)
C(14)-C(15)	1.5219(19)	C(11)-C(10)-C(18)	117.55(12)
C(15)-C(16)	1.531(2)	C(9)-C(10)-C(18)	123.63(11)
C(15)-C(17)	1.536(2)	C(12)-C(11)-C(10)	121.48(13)
C(18)-C(19)	1.5339(19)	C(11)-C(12)-C(13)	119.36(13)
C(18)-C(20)	1.5403(18)	C(12)-C(13)-C(14)	121.70(13)
C(21)-N(1)	1.4978(17)	C(13)-C(14)-C(9)	118.49(12)
C(21)-C(22)	1.5213(19)	C(13)-C(14)-C(15)	117.48(12)
C(23)-C(24)	1.5257(18)	C(9)-C(14)-C(15)	124.01(12)
C(24)-N(2)	1.5038(16)	C(14)-C(15)-C(16)	110.07(12)
C(24)-C(26)	1.5273(19)	C(14)-C(15)-C(17)	112.85(12)
C(24)-C(25)	1.5338(19)	C(16)-C(15)-C(17)	109.88(12)
C(29)-C(34)	1.4076(18)	C(10)-C(18)-C(19)	112.44(11)
C(29)-C(30)	1.4111(18)	C(10)-C(18)-C(20)	110.33(11)
C(29)-N(2)	1.4489(15)	C(19)-C(18)-C(20)	109.89(11)
C(30)-C(31)	1.3973(18)	N(1)-C(21)-C(8)	112.46(11)
C(30)-C(38)	1.5245(18)	N(1)-C(21)-C(22)	100.30(10)
C(31)-C(32)	1.387(2)	C(8)-C(21)-C(22)	112.51(11)
C(32)-C(33)	1.3824(19)	N(1)-C(21)-C(7)	111.68(11)
C(33)-C(34)	1.3960(18)	C(8)-C(21)-C(7)	108.88(11)
C(34)-C(35)	1.5241(18)	C(22)-C(21)-C(7)	110.84(11)
C(35)-C(36)	1.5364(19)	C(21)-C(22)-C(2)	107.66(10)
C(35)-C(37)	1.5374(19)	C(24)-C(23)-C(4)	107.45(10)
C(38)-C(39)	1.5347(19)	N(2)-C(24)-C(23)	100.41(10)
C(38)-C(40)	1.5373(19)	N(2)-C(24)-C(26)	112.85(11)
C(41)-N(3)	1.3971(16)	C(23)-C(24)-C(26)	111.32(11)
C(41)-B(2)	1.5169(19)	N(2)-C(24)-C(25)	111.34(11)
C(41)-C(42)	1.5445(17)	C(23)-C(24)-C(25)	113.59(11)
C(42)-C(48)	1.5403(19)	C(26)-C(24)-C(25)	107.37(11)
C(42)-C(47)	1.5427(18)	C(34)-C(29)-C(30)	121.00(11)
C(42)-C(61)	1.5457(19)	C(34)-C(29)-N(2)	119.80(11)
C(43)-N(4)	1.3836(16)	C(30)-C(29)-N(2)	119.20(11)
C(43)-B(2)	1.5249(19)	C(31)-C(30)-C(29)	118.31(12)
C(43)-C(44)	1.5400(17)	C(31)-C(30)-C(38)	118.86(11)
C(44)-C(67)	1.5348(18)	C(29)-C(30)-C(38)	122.66(11)
C(44)-C(68)	1.5373(18)	C(32)-C(31)-C(30)	121.24(12)
C(44)-C(63)	1.5444(18)	C(33)-C(32)-C(31)	119.30(12)
C(45)-C(62)	1.5255(18)	C(32)-C(33)-C(34)	121.99(13)
C(46)-C(62)	1.5395(19)	C(33)-C(34)-C(29)	117.82(12)
C(49)-C(50)	1.4097(18)	C(33)-C(34)-C(35)	118.23(12)
C(49)-C(54)	1.4119(18)	C(29)-C(34)-C(35)	123.69(11)
C(49)-N(3)	1.4486(15)	C(34)-C(35)-C(36)	109.37(11)
C(50)-C(51)	1.3987(18)	C(34)-C(35)-C(37)	113.56(11)
C(50)-C(58)	1.5178(18)	C(36)-C(35)-C(37)	109.90(11)
C(51)-C(52)	1.381(2)	C(30)-C(38)-C(39)	112.29(11)
C(52)-C(53)	1.379(2)	C(30)-C(38)-C(40)	110.81(11)

C(53)-C(54)	1.3955(18)
C(54)-C(55)	1.5197(19)
C(55)-C(56)	1.532(2)
C(55)-C(57)	1.5372(19)
C(58)-C(59)	1.5362(18)
C(58)-C(60)	1.5374(19)
C(61)-C(62)	1.5253(18)
C(62)-N(3)	1.4996(16)
C(63)-C(64)	1.5217(18)
C(64)-N(4)	1.5013(16)
C(64)-C(66)	1.5281(19)
C(64)-C(65)	1.5323(19)
C(69)-C(74)	1.4057(18)
C(69)-C(70)	1.4117(18)
C(69)-N(4)	1.4457(16)
C(70)-C(71)	1.3923(18)
C(70)-C(78)	1.5255(18)
C(71)-C(72)	1.3857(19)
C(72)-C(73)	1.3833(19)
C(73)-C(74)	1.3952(18)
C(74)-C(75)	1.5268(18)
C(75)-C(76)	1.5371(18)
C(75)-C(77)	1.5382(19)
C(78)-C(80)	1.539(2)
C(78)-C(79)	1.5401(19)
B(1)-F(1)	1.3999(15)
B(2)-F(2)	1.3977(16)

C(39)-C(38)-C(40)	109.77(11)
N(3)-C(41)-B(2)	117.46(11)
N(3)-C(41)-C(42)	107.38(10)
B(2)-C(41)-C(42)	133.89(11)
C(48)-C(42)-C(47)	109.14(11)
C(48)-C(42)-C(41)	115.03(11)
C(47)-C(42)-C(41)	111.25(10)
C(48)-C(42)-C(61)	107.34(11)
C(47)-C(42)-C(61)	110.53(11)
C(41)-C(42)-C(61)	103.32(10)
N(4)-C(43)-B(2)	120.18(11)
N(4)-C(43)-C(44)	106.66(10)
B(2)-C(43)-C(44)	132.75(11)
C(67)-C(44)-C(68)	110.56(11)
C(67)-C(44)-C(43)	111.20(10)
C(68)-C(44)-C(43)	113.52(11)
C(67)-C(44)-C(63)	108.63(11)
C(68)-C(44)-C(63)	108.75(11)
C(43)-C(44)-C(63)	103.84(10)
C(50)-C(49)-C(54)	120.31(11)
C(50)-C(49)-N(3)	121.47(11)
C(54)-C(49)-N(3)	118.20(11)
C(51)-C(50)-C(49)	118.36(12)
C(51)-C(50)-C(58)	117.97(12)
C(49)-C(50)-C(58)	123.65(11)
C(52)-C(51)-C(50)	121.89(13)
C(53)-C(52)-C(51)	119.05(12)
C(52)-C(53)-C(54)	121.86(13)
C(53)-C(54)-C(49)	118.53(12)
C(53)-C(54)-C(55)	117.94(12)
C(49)-C(54)-C(55)	123.53(11)
C(54)-C(55)-C(56)	110.97(12)
C(54)-C(55)-C(57)	112.54(11)
C(56)-C(55)-C(57)	110.20(12)
C(50)-C(58)-C(59)	111.75(11)
C(50)-C(58)-C(60)	110.94(11)
C(59)-C(58)-C(60)	109.43(11)
C(62)-C(61)-C(42)	107.53(10)
N(3)-C(62)-C(61)	100.70(10)
N(3)-C(62)-C(45)	112.61(10)
C(61)-C(62)-C(45)	111.95(11)
N(3)-C(62)-C(46)	111.41(10)
C(61)-C(62)-C(46)	111.52(11)
C(45)-C(62)-C(46)	108.56(11)
C(64)-C(63)-C(44)	107.83(10)
N(4)-C(64)-C(63)	100.40(10)

N(4)-C(64)-C(66)	112.94(11)
C(63)-C(64)-C(66)	110.77(11)
N(4)-C(64)-C(65)	111.68(11)
C(63)-C(64)-C(65)	113.17(11)
C(66)-C(64)-C(65)	107.86(11)
C(74)-C(69)-C(70)	121.36(11)
C(74)-C(69)-N(4)	120.01(11)
C(70)-C(69)-N(4)	118.60(11)
C(71)-C(70)-C(69)	117.93(12)
C(71)-C(70)-C(78)	118.83(12)
C(69)-C(70)-C(78)	123.08(11)
C(72)-C(71)-C(70)	121.31(12)
C(73)-C(72)-C(71)	119.74(12)
C(72)-C(73)-C(74)	121.41(12)
C(73)-C(74)-C(69)	117.88(12)
C(73)-C(74)-C(75)	118.66(11)
C(69)-C(74)-C(75)	123.19(11)
C(74)-C(75)-C(76)	113.60(11)
C(74)-C(75)-C(77)	109.23(11)
C(76)-C(75)-C(77)	109.48(11)
C(70)-C(78)-C(80)	110.62(11)
C(70)-C(78)-C(79)	112.78(11)
C(80)-C(78)-C(79)	109.19(12)
F(1)-B(1)-C(1)	111.06(11)
F(1)-B(1)-C(3)	111.51(11)
C(1)-B(1)-C(3)	137.39(12)
F(2)-B(2)-C(41)	110.88(11)
F(2)-B(2)-C(43)	111.27(11)
C(41)-B(2)-C(43)	137.65(12)
C(1)-N(1)-C(9)	123.59(10)
C(1)-N(1)-C(21)	113.61(10)
C(9)-N(1)-C(21)	121.14(10)
C(3)-N(2)-C(29)	125.82(10)
C(3)-N(2)-C(24)	115.09(10)
C(29)-N(2)-C(24)	117.79(10)
C(41)-N(3)-C(49)	123.37(10)
C(41)-N(3)-C(62)	113.56(10)
C(49)-N(3)-C(62)	120.74(10)
C(43)-N(4)-C(69)	126.66(10)
C(43)-N(4)-C(64)	115.39(10)
C(69)-N(4)-C(64)	117.14(10)

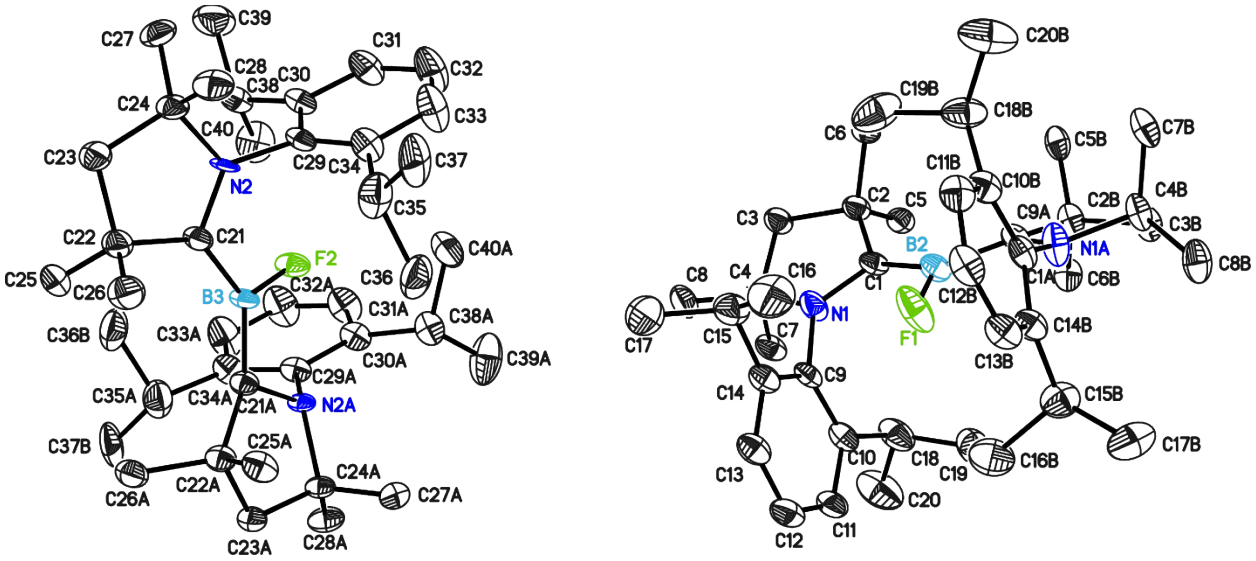


Figure S20. Crystal structure of **2**. The anisotropic displacement parameters are depicted at the 50% probability level. The hydrogen atoms, a toluene solvent molecule and the $[B(C_6F_5)_4]^-$ anion are omitted for clarity.

Table T3. Bond lengths [Å] and angles [°] for **2**.

bond lengths [Å]		angles [°]	
B(1)-C(1S)	1.654(5)	C(1S)-B(1)-C(19S)	102.8(3)
B(1)-C(19S)	1.654(5)	C(1S)-B(1)-C(13S)	113.4(3)
B(1)-C(13S)	1.655(5)	C(19S)-B(1)-C(13S)	113.5(3)
B(1)-C(7S)	1.664(5)	C(1S)-B(1)-C(7S)	113.3(3)
C(1S)-C(6S)	1.389(5)	C(19S)-B(1)-C(7S)	113.3(3)
C(1S)-C(2S)	1.389(5)	C(13S)-B(1)-C(7S)	101.0(3)
C(2S)-F(7)	1.351(4)	C(6S)-C(1S)-C(2S)	113.2(3)
C(2S)-C(3S)	1.381(5)	C(6S)-C(1S)-B(1)	119.2(3)
F(3)-C(6S)	1.355(4)	C(2S)-C(1S)-B(1)	127.4(3)
C(3S)-F(6)	1.345(4)	F(7)-C(2S)-C(3S)	114.9(3)
C(3S)-C(4S)	1.383(6)	F(7)-C(2S)-C(1S)	121.1(3)
F(4)-C(5S)	1.350(4)	C(3S)-C(2S)-C(1S)	123.9(3)
C(4S)-F(5)	1.350(4)	F(6)-C(3S)-C(2S)	120.7(4)
C(4S)-C(5S)	1.369(6)	F(6)-C(3S)-C(4S)	119.7(4)
C(5S)-C(6S)	1.375(5)	C(2S)-C(3S)-C(4S)	119.6(4)
C(7S)-C(12S)	1.389(5)	F(5)-C(4S)-C(5S)	120.8(4)
C(7S)-C(8S)	1.397(5)	F(5)-C(4S)-C(3S)	120.2(4)
F(8)-C(8S)	1.367(4)	C(5S)-C(4S)-C(3S)	119.0(4)
C(8S)-C(9S)	1.365(5)	F(4)-C(5S)-C(4S)	119.9(4)
F(9)-C(9S)	1.346(4)	F(4)-C(5S)-C(6S)	120.9(4)
C(9S)-C(10S)	1.391(5)	C(4S)-C(5S)-C(6S)	119.2(4)
F(10)-C(10S)	1.343(4)	F(3)-C(6S)-C(5S)	116.3(3)

C(10S)-C(11S)	1.370(5)	F(3)-C(6S)-C(1S)	118.7(3)
F(11)-C(11S)	1.353(4)	C(5S)-C(6S)-C(1S)	125.0(4)
C(11S)-C(12S)	1.379(5)	C(12S)-C(7S)-C(8S)	112.2(3)
F(12)-C(12S)	1.356(4)	C(12S)-C(7S)-B(1)	127.7(3)
F(13)-C(14S)	1.356(5)	C(8S)-C(7S)-B(1)	119.4(3)
C(13S)-C(14S)	1.380(5)	C(9S)-C(8S)-F(8)	115.6(3)
C(13S)-C(18S)	1.400(5)	C(9S)-C(8S)-C(7S)	125.7(3)
F(14)-C(15S)	1.354(5)	F(8)-C(8S)-C(7S)	118.6(3)
C(14S)-C(15S)	1.386(6)	F(9)-C(9S)-C(8S)	121.3(3)
F(15)-C(16S)	1.347(4)	F(9)-C(9S)-C(10S)	119.7(3)
C(15S)-C(16S)	1.363(6)	C(8S)-C(9S)-C(10S)	118.9(3)
F(16)-C(17S)	1.349(5)	F(10)-C(10S)-C(11S)	121.1(3)
C(16S)-C(17S)	1.375(6)	F(10)-C(10S)-C(9S)	120.4(3)
F(17)-C(18S)	1.357(4)	C(11S)-C(10S)-C(9S)	118.4(3)
C(17S)-C(18S)	1.380(5)	F(11)-C(11S)-C(10S)	119.5(3)
F(18)-C(24S)	1.363(4)	F(11)-C(11S)-C(12S)	120.3(3)
F(19)-C(23S)	1.348(4)	C(10S)-C(11S)-C(12S)	120.2(3)
C(19S)-C(24S)	1.381(5)	F(12)-C(12S)-C(11S)	114.6(3)
C(19S)-C(20S)	1.396(5)	F(12)-C(12S)-C(7S)	120.9(3)
F(20)-C(22S)	1.343(4)	C(11S)-C(12S)-C(7S)	124.5(3)
C(20S)-F(22)	1.356(4)	C(14S)-C(13S)-C(18S)	113.0(3)
C(20S)-C(21S)	1.373(5)	C(14S)-C(13S)-B(1)	127.9(3)
F(21)-C(21S)	1.348(4)	C(18S)-C(13S)-B(1)	118.6(3)
C(21S)-C(22S)	1.382(5)	F(13)-C(14S)-C(13S)	121.1(3)
C(22S)-C(23S)	1.375(5)	F(13)-C(14S)-C(15S)	114.6(3)
C(23S)-C(24S)	1.376(5)	C(13S)-C(14S)-C(15S)	124.2(4)
F(1)-B(2)	1.369(6)	F(14)-C(15S)-C(16S)	119.9(4)
B(2)-C(1)	1.541(4)	F(14)-C(15S)-C(14S)	120.1(4)
B(2)-C(1)#1	1.541(4)	C(16S)-C(15S)-C(14S)	119.9(4)
C(1)-N(1)	1.376(4)	F(15)-C(16S)-C(15S)	120.8(4)
C(1)-C(2)	1.526(6)	F(15)-C(16S)-C(17S)	120.1(4)
C(1)-C(2A)	1.551(12)	C(15S)-C(16S)-C(17S)	119.1(4)
N(1)-C(9)	1.473(4)	F(16)-C(17S)-C(16S)	120.3(4)
N(1)-C(4)	1.550(6)	F(16)-C(17S)-C(18S)	120.5(4)
N(1)-C(4A)	1.557(12)	C(16S)-C(17S)-C(18S)	119.2(4)
C(2)-C(6)	1.533(7)	F(17)-C(18S)-C(17S)	116.1(3)
C(2)-C(3)	1.544(6)	F(17)-C(18S)-C(13S)	119.5(3)
C(2)-C(5)	1.546(7)	C(17S)-C(18S)-C(13S)	124.4(4)
C(3)-C(4)	1.525(7)	C(24S)-C(19S)-	112.9(3)

		C(20S)	
C(4)-C(8)	1.517(7)	C(24S)-C(19S)-B(1)	127.0(3)
C(4)-C(7)	1.529(7)	C(20S)-C(19S)-B(1)	119.9(3)
C(9)-C(14)	1.398(5)	F(22)-C(20S)-C(21S)	116.1(3)
C(9)-C(10)	1.410(5)	F(22)-C(20S)-C(19S)	118.9(3)
C(10)-C(11)	1.390(5)	C(21S)-C(20S)-C(19S)	124.9(3)
C(10)-C(18)	1.522(5)	F(21)-C(21S)-C(20S)	121.2(3)
C(11)-C(12)	1.381(5)	F(21)-C(21S)-C(22S)	120.0(3)
C(12)-C(13)	1.384(5)	C(20S)-C(21S)-C(22S)	118.9(3)
C(13)-C(14)	1.386(5)	F(20)-C(22S)-C(23S)	120.4(3)
C(14)-C(15)	1.533(5)	F(20)-C(22S)-C(21S)	120.7(3)
C(15)-C(16)	1.534(6)	C(23S)-C(22S)-C(21S)	118.9(3)
C(15)-C(17)	1.538(6)	F(19)-C(23S)-C(22S)	119.3(3)
C(18)-C(20)	1.538(5)	F(19)-C(23S)-C(24S)	121.0(3)
C(18)-C(19)	1.540(6)	C(22S)-C(23S)-C(24S)	119.7(3)
C(2A)-C(5A)	1.542(12)	F(18)-C(24S)-C(23S)	114.8(3)
C(2A)-C(6A)	1.543(12)	F(18)-C(24S)-C(19S)	120.7(3)
C(2A)-C(3A)	1.551(13)	C(23S)-C(24S)-C(19S)	124.5(3)
C(3A)-C(4A)	1.515(14)	F(1)-B(2)-C(1)	112.1(2)
C(4A)-C(7A)	1.513(12)	F(1)-B(2)-C(1)#1	112.1(2)
C(4A)-C(8A)	1.525(12)	C(1)-B(2)-C(1)#1	135.8(5)
C(1T)-C(2T)	1.445(16)	N(1)-C(1)-C(2)	107.3(3)
C(2T)-C(3T)	1.369(11)	N(1)-C(1)-B(2)	118.5(3)
C(2T)-C(7T)	1.387(11)	C(2)-C(1)-B(2)	132.1(3)
C(3T)-C(4T)	1.383(11)	N(1)-C(1)-C(2A)	107.2(6)
C(4T)-C(5T)	1.380(12)	B(2)-C(1)-C(2A)	134.2(6)
C(5T)-C(6T)	1.425(12)	C(1)-N(1)-C(9)	126.5(3)
C(6T)-C(7T)	1.390(11)	C(1)-N(1)-C(4)	114.0(3)
F(2)-B(3)	1.382(7)	C(9)-N(1)-C(4)	115.6(3)
N(2)-C(21)	1.348(8)	C(1)-N(1)-C(4A)	112.4(5)
N(2)-C(29)	1.454(8)	C(9)-N(1)-C(4A)	120.8(5)
N(2)-C(24)	1.538(9)	C(1)-C(2)-C(6)	111.6(4)
B(3)-C(21A)	1.502(8)	C(1)-C(2)-C(3)	103.8(4)
B(3)-C(21)	1.550(8)	C(6)-C(2)-C(3)	109.0(4)
C(21)-C(22)	1.534(8)	C(1)-C(2)-C(5)	110.7(4)
C(22)-C(25)	1.535(9)	C(6)-C(2)-C(5)	111.1(4)
C(22)-C(26)	1.539(9)	C(3)-C(2)-C(5)	110.4(5)
C(22)-C(23)	1.541(8)	C(4)-C(3)-C(2)	108.3(4)
C(23)-C(24)	1.529(10)	C(8)-C(4)-C(3)	111.5(5)
C(24)-C(28)	1.515(9)	C(8)-C(4)-C(7)	109.6(4)
C(24)-C(27)	1.518(9)	C(3)-C(4)-C(7)	114.3(5)

N(2A)-C(21A)	1.511(9)
N(2A)-C(29)#2	1.527(8)
N(2A)-C(24A)	1.563(9)
C(21A)-C(22A)	1.538(8)
C(22A)-C(26A)	1.540(8)
C(22A)-C(23A)	1.543(8)
C(22A)-C(25A)	1.549(8)
C(23A)-C(24A)	1.529(9)
C(24A)-C(28A)	1.515(8)
C(24A)-C(27A)	1.525(9)
C(29)-C(34)	1.392(5)
C(29)-C(30)	1.409(5)
C(30)-C(31)	1.395(5)
C(30)-C(38)	1.522(5)
C(31)-C(32)	1.380(6)
C(32)-C(33)	1.377(6)
C(33)-C(34)	1.392(5)
C(34)-C(35)	1.529(5)
C(35)-C(37)	1.478(9)
C(35)-C(36A)	1.502(8)
C(35)-C(37A)	1.611(10)
C(35)-C(36)	1.613(9)
C(38)-C(40)	1.538(5)
C(38)-C(39)	1.540(5)

C(8)-C(4)-N(1)	110.7(4)
C(3)-C(4)-N(1)	97.7(4)
C(7)-C(4)-N(1)	112.7(4)
C(14)-C(9)-C(10)	121.8(3)
C(14)-C(9)-N(1)	118.9(3)
C(10)-C(9)-N(1)	119.3(3)
C(11)-C(10)-C(9)	117.4(3)
C(11)-C(10)-C(18)	117.3(3)
C(9)-C(10)-C(18)	125.1(3)
C(12)-C(11)-C(10)	122.1(4)
C(11)-C(12)-C(13)	118.9(3)
C(12)-C(13)-C(14)	121.9(4)
C(13)-C(14)-C(9)	117.9(3)
C(13)-C(14)-C(15)	117.4(3)
C(9)-C(14)-C(15)	124.5(3)
C(14)-C(15)-C(16)	109.8(3)
C(14)-C(15)-C(17)	112.2(3)
C(16)-C(15)-C(17)	110.2(4)
C(10)-C(18)-C(20)	112.2(3)
C(10)-C(18)-C(19)	109.3(4)
C(20)-C(18)-C(19)	109.4(4)
C(5A)-C(2A)-C(6A)	108.8(11)
C(5A)-C(2A)-C(3A)	104.1(11)
C(6A)-C(2A)-C(3A)	109.9(11)
C(5A)-C(2A)-C(1)	118.9(11)
C(6A)-C(2A)-C(1)	111.8(10)
C(3A)-C(2A)-C(1)	102.6(8)
C(4A)-C(3A)-C(2A)	108.0(9)
C(7A)-C(4A)-C(3A)	113.0(11)
C(7A)-C(4A)-C(8A)	108.6(11)
C(3A)-C(4A)-C(8A)	112.2(11)
C(7A)-C(4A)-N(1)	108.1(10)
C(3A)-C(4A)-N(1)	97.3(8)
C(8A)-C(4A)-N(1)	117.3(10)
C(3T)-C(2T)-C(7T)	119.1(9)
C(3T)-C(2T)-C(1T)	117.2(8)
C(7T)-C(2T)-C(1T)	123.7(9)
C(2T)-C(3T)-C(4T)	122.0(10)
C(5T)-C(4T)-C(3T)	121.0(10)
C(4T)-C(5T)-C(6T)	116.8(10)
C(7T)-C(6T)-C(5T)	121.7(9)
C(2T)-C(7T)-C(6T)	119.3(9)
C(21)-N(2)-C(29)	126.4(6)
C(21)-N(2)-C(24)	114.9(6)
C(29)-N(2)-C(24)	117.8(6)
F(2)-B(3)-C(21A)	110.4(5)

F(2)-B(3)-C(21)	112.1(5)
C(21A)-B(3)-C(21)	137.2(6)
N(2)-C(21)-C(22)	108.7(6)
N(2)-C(21)-B(3)	119.7(6)
C(22)-C(21)-B(3)	131.5(6)
C(21)-C(22)-C(25)	110.9(6)
C(21)-C(22)-C(26)	109.5(6)
C(25)-C(22)-C(26)	111.6(6)
C(21)-C(22)-C(23)	103.9(5)
C(25)-C(22)-C(23)	110.3(6)
C(26)-C(22)-C(23)	110.5(6)
C(24)-C(23)-C(22)	108.3(6)
C(28)-C(24)-C(27)	109.6(7)
C(28)-C(24)-C(23)	114.0(6)
C(27)-C(24)-C(23)	111.6(7)
C(28)-C(24)-N(2)	109.9(7)
C(27)-C(24)-N(2)	110.9(6)
C(23)-C(24)-N(2)	100.5(6)
C(21A)-N(2A)-C(29)#2	120.6(6)
C(21A)-N(2A)-C(24A)	110.1(6)
C(29)#2-N(2A)-C(24A)	115.9(6)
B(3)-C(21A)-N(2A)	110.3(6)
B(3)-C(21A)-C(22A)	139.5(6)
N(2A)-C(21A)-C(22A)	107.4(5)
C(21A)-C(22A)-C(26A)	116.3(6)
C(21A)-C(22A)-C(23A)	103.6(5)
C(26A)-C(22A)-C(23A)	107.5(5)
C(21A)-C(22A)-C(25A)	111.0(5)
C(26A)-C(22A)-C(25A)	108.2(6)
C(23A)-C(22A)-C(25A)	110.0(6)
C(24A)-C(23A)-C(22A)	109.6(5)
C(28A)-C(24A)-C(27A)	109.8(7)
C(28A)-C(24A)-C(23A)	111.9(6)

C(27A)-C(24A)-C(23A)	113.3(6)
C(28A)-C(24A)-N(2A)	113.8(6)
C(27A)-C(24A)-N(2A)	107.0(6)
C(23A)-C(24A)-N(2A)	100.8(6)
C(34)-C(29)-C(30)	122.8(3)
C(34)-C(29)-N(2)	121.7(5)
C(30)-C(29)-N(2)	115.0(5)
C(31)-C(30)-C(29)	116.8(3)
C(31)-C(30)-C(38)	117.5(3)
C(29)-C(30)-C(38)	125.6(3)
C(32)-C(31)-C(30)	121.7(4)
C(33)-C(32)-C(31)	119.6(4)
C(32)-C(33)-C(34)	121.9(4)
C(29)-C(34)-C(33)	117.2(3)
C(29)-C(34)-C(35)	124.8(3)
C(33)-C(34)-C(35)	117.8(3)
C(37)-C(35)-C(34)	119.0(6)
C(36A)-C(35)-C(34)	111.9(5)
C(36A)-C(35)-C(37A)	105.4(6)
C(34)-C(35)-C(37A)	106.7(6)
C(37)-C(35)-C(36)	112.6(6)
C(34)-C(35)-C(36)	106.3(5)
C(30)-C(38)-C(40)	111.5(3)
C(30)-C(38)-C(39)	111.9(3)
C(40)-C(38)-C(39)	109.8(4)

(S3) DFT caculations

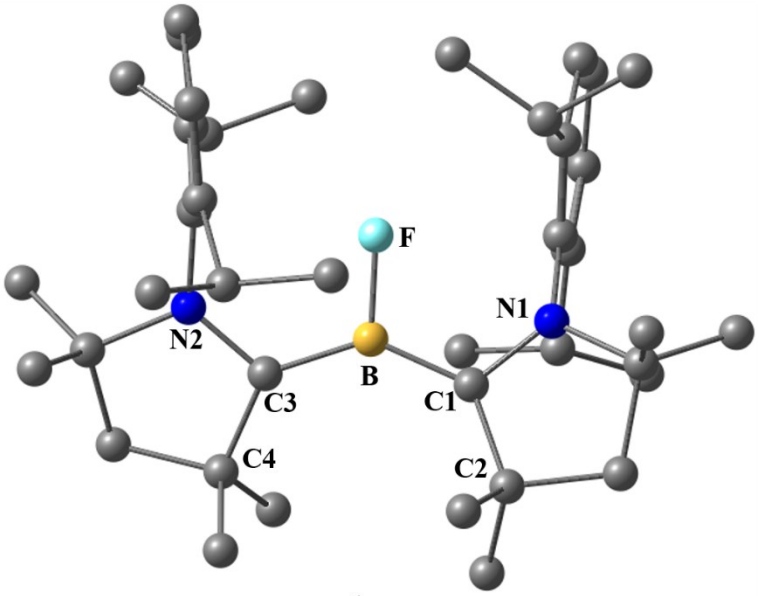
Table T4. Comparison of selected structural parameters (bond lenght, Å) of 1 and 2 from X-Ray Structure analysis and DFT (BP86-GD3(BJ)/def2-tzvp.

Parameter	Structure 1		Structure 2	
	X-Ray	DFT	X-Ray	DFT
B1-F1	1.399	1.415	1.369	1.369
B1-C1	1.513	1.521	1.541	1.563
B1-C3	1.527	1.526	1.541	1.567
C1-C2	1.546	1.533	1.526	1.534
C3-C4	1.536	1.541	1.526	1.528
N1-C1	1.395	1.380	1.376	1.348
C3-N2	1.378	1.393	1.376	1.339

Table T5. EDA-NOCV results of **1** and **2** in their most favorable electronic state at the BP86-D3(BJ)/TZ2P level of theory.

	1	**2**
	BF (Singlet) $[cAAC]_2$ (Singlet)	BF^+ (Doublet) $[cAAC]_2$ (Singlet)
ΔE_{int}	-398.8	-434.6
ΔE_{disp}	-12.9	-12.9
ΔE_{Pauli}	264.5	297.4
ΔE_{elstat}	-241.2	-274.8
ΔE_{orb}	-409.2	-444.3
$\Delta E(1)$	-176.9	-124.9
$\Delta E(2)$	-104.6	-117.1
$\Delta E(3)$	-91.6	-112.2

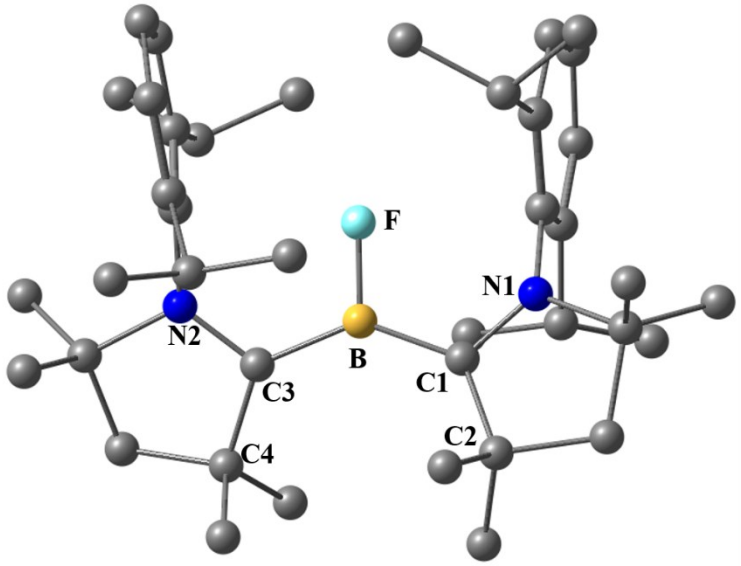
a.



B-F : 1.415 (1.398)
B-C1 : 1.521 (1.525)
B-C3 : 1.526 (1.540)
C1-N1: 1.380 (1.384)
C1-C2 : 1.533 (1.517)
C3-N2 : 1.393 (1.397)
C3-C4: 1.541 (1.545)
C1-B-C3 : 138.0 (137.7)

1

b.



B-F : 1.369 (1.353)
B-C1 : 1.563 (1.542)
B-C3 : 1.567 (1.542)
C1-N1: 1.348 (1.374)
C1-C2 : 1.534 (1.523)
C3-N2 : 1.339 (1.374)
C3-C4: 1.528 (1.523)
C1-B-C3 : 137.9 (135.6)

2

Figure S21: Optimized structures of (a**) 1** and (b) **2** at the BP86-D3(BJ)/def2-tzvp level of theory. Bond distances are given in Å. Hydrogen atoms have been omitted for clarity. Values given in parenthesis are obtained from crystal structure data.

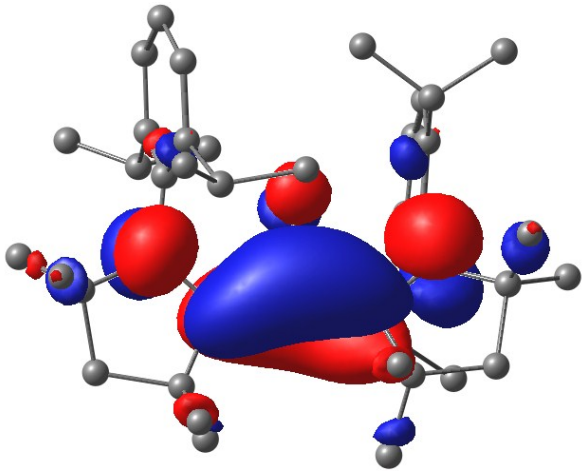


Figure S22: HOMO of **1**.

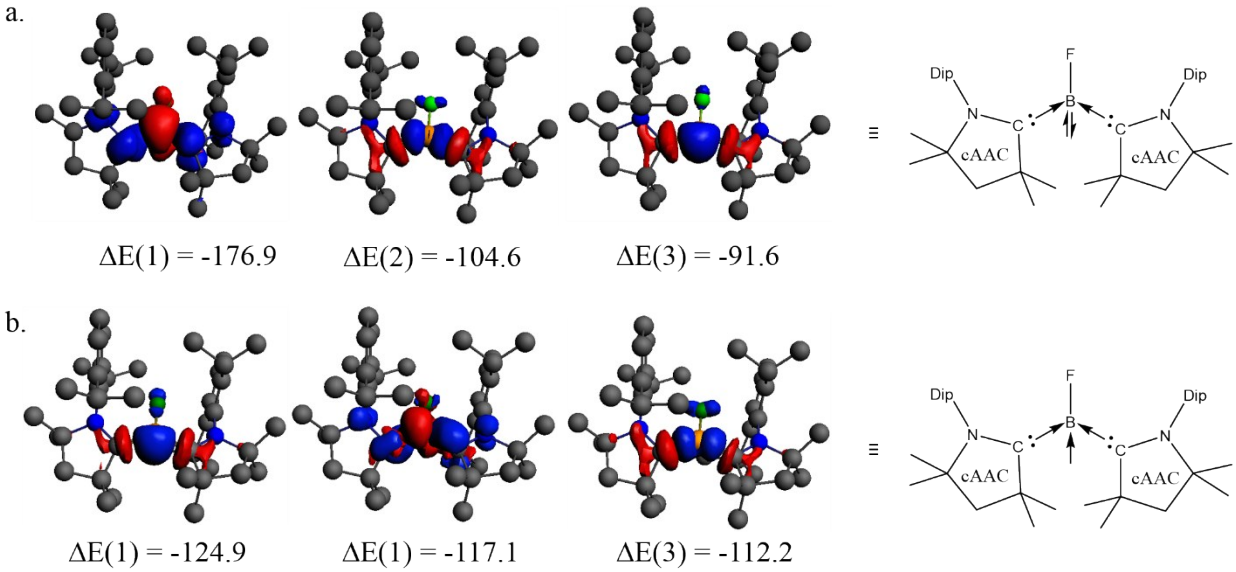


Figure S23: Plot of the deformation densities of the interactions for the pairwise orbital interactions of three strongest orbital interactions with associated interaction energies between (a) BF and $[cAAC]_2$ in **1** and (b) BF^+ and $[cAAC]_2$ in **2**. The direction of the charge flow is red→blue. Best description of **1** and **2**.

Computational details:

All the calculations are carried out using Gaussian 09 (version D) program package.[S10] Geometry optimization were carried out using dispersion corrected BP86 functional with Becke-Johnson damping (BP86-D3(BJ))[S11] and def2-tzvp basis set. Natural populaton analyses were performed at the same level of theory as implemented in the Gaussian 09 suite of programs.

Energy decomposition analysis (EDA) studies[S12] have been carried out with the ADF18 program package[S13] using BP86-D3(BJ) functional on the Gaussian optimized structures. TZ2P basis set has been employed for all the atoms. Fragment interactions have been analyzed with the energy decomposition scheme ETS. For the energy partitioning analysis, the interaction energy ΔE is calculated and decomposed for the bonding between different fragments. The interaction energy is composed of four components:

$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{pauli} + \Delta E_{orb} + \Delta E_{dis}$

ΔE_{elstat} is the electrostatic interaction energy between the fragments calculated with a frozen electron density distribution in the given input geometry. ΔE_{pauli} is the repulsive four-electron interactions between occupied orbitals. ΔE_{orb} is an estimate of the covalent contributions to the bonding. ΔE_{dis} is the dispersion energy. The EDA-NOCV calculations provide pairwise energy contributions for each pair of interacting orbital to the total bond energy.[S14] The contours of deformation densities are plotted using ADF-GUI interface. The color code of the charge flow red to blue visualizes the area of depletion and concentration of charge associated with the donor-acceptor interactions.

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Cartesian coordinates of the optimized geometries of **1** and **2** using G09 program package.

1 (Spin multiplicity = 1)

Total energy: -1796.6676 a. u.

9	-0.045199000	-0.593914000	0.000149000
7	2.374008000	0.389241000	-0.540498000
6	1.358223000	1.332202000	-0.398126000
5	-0.005499000	0.820160000	0.021707000
7	-2.475558000	0.574218000	0.401945000
6	1.876562000	2.664830000	-0.972015000
6	3.376910000	2.375151000	-1.231072000
1	3.756726000	2.924902000	-2.104044000
1	3.960659000	2.697184000	-0.353781000
6	3.524047000	0.856621000	-1.383105000
6	1.140284000	3.023729000	-2.281698000
1	1.506392000	3.985269000	-2.677569000
1	0.059752000	3.101336000	-2.112726000
1	1.288331000	2.258116000	-3.052912000
6	1.814157000	3.871608000	-0.017418000
1	2.233309000	3.619769000	0.967571000
1	0.800177000	4.254517000	0.127732000
1	2.415830000	4.692783000	-0.439863000
6	3.373316000	0.425698000	-2.855986000
1	4.069898000	1.004695000	-3.481081000
1	2.354427000	0.601387000	-3.222390000
1	3.607396000	-0.636061000	-2.990258000
6	4.865138000	0.353663000	-0.847407000
1	5.678341000	0.763092000	-1.464541000
1	4.925918000	-0.742937000	-0.881398000
1	5.024784000	0.672773000	0.190986000
6	2.513477000	-0.768533000	0.300944000
6	2.397182000	-2.075341000	-0.228023000
6	2.647431000	-3.167282000	0.611614000
1	2.556892000	-4.177206000	0.206396000
6	2.973731000	-2.993133000	1.953534000
1	3.160134000	-3.857494000	2.593712000
6	3.034575000	-1.704705000	2.475843000
1	3.265522000	-1.562958000	3.533794000
6	2.809422000	-0.578485000	1.673112000

6	2.854823000	0.790433000	2.332469000
1	2.726343000	1.547494000	1.548030000
6	1.673166000	0.938265000	3.306012000
1	1.750360000	0.211003000	4.128843000
1	0.723883000	0.766527000	2.779500000
1	1.650124000	1.948414000	3.743411000
6	4.190815000	1.063205000	3.041182000
1	5.043088000	0.951969000	2.354850000
1	4.349799000	0.372295000	3.882722000
1	4.207607000	2.087222000	3.445083000
6	1.930230000	-2.351878000	-1.646382000
1	1.732800000	-1.382071000	-2.121639000
6	0.606067000	-3.135536000	-1.652384000
1	0.728496000	-4.130156000	-1.196487000
1	0.256883000	-3.282642000	-2.686034000
1	-0.172023000	-2.597833000	-1.100604000
6	2.997239000	-3.102689000	-2.460990000
1	3.970801000	-2.590796000	-2.441248000
1	2.682839000	-3.206516000	-3.510957000
1	3.154598000	-4.115368000	-2.058452000
6	-1.366179000	1.395113000	0.383307000
6	-1.800419000	2.773285000	0.896119000
6	-3.225458000	2.522814000	1.455839000
1	-3.162350000	2.346180000	2.540172000
1	-3.889221000	3.384569000	1.298556000
6	-3.761325000	1.257644000	0.780736000
6	-4.620209000	1.549706000	-0.461113000
1	-5.536095000	2.077345000	-0.157253000
1	-4.914949000	0.611344000	-0.950695000
1	-4.092891000	2.171201000	-1.194092000
6	-4.602426000	0.424169000	1.749648000
1	-4.052703000	0.212730000	2.674355000
1	-4.914865000	-0.526286000	1.295162000
1	-5.508509000	0.990126000	2.011680000
6	-1.869549000	3.825997000	-0.229197000
1	-2.270956000	4.772528000	0.166806000
1	-2.524329000	3.495174000	-1.046623000
1	-0.887380000	4.032285000	-0.664454000
6	-0.901010000	3.254775000	2.046797000
1	0.148867000	3.319940000	1.751018000
1	-0.961712000	2.549924000	2.887503000
1	-1.230815000	4.244721000	2.403083000

6	-2.568160000	-0.753662000	-0.152652000
6	-2.584175000	-1.869345000	0.717870000
6	-2.851760000	-3.132018000	0.175084000
1	-2.868369000	-4.001976000	0.834232000
6	-3.065342000	-3.301810000	-1.191258000
1	-3.279501000	-4.293131000	-1.595170000
6	-2.949222000	-2.208159000	-2.044594000
1	-3.045852000	-2.354921000	-3.122192000
6	-2.681921000	-0.923415000	-1.551460000
6	-2.396032000	0.196663000	-2.541613000
1	-2.317080000	1.135936000	-1.977573000
6	-1.025249000	-0.043255000	-3.205017000
1	-0.782352000	0.784355000	-3.889076000
1	-1.031260000	-0.978047000	-3.786568000
1	-0.233349000	-0.113417000	-2.448167000
6	-3.485642000	0.358589000	-3.611948000
1	-3.257756000	1.220601000	-4.257249000
1	-4.477722000	0.516265000	-3.166925000
1	-3.545799000	-0.528630000	-4.259990000
6	-2.189991000	-1.766879000	2.185378000
1	-2.124824000	-0.698150000	2.437351000
6	-3.202950000	-2.435813000	3.128688000
1	-2.920739000	-2.257495000	4.177528000
1	-3.222900000	-3.525845000	2.978624000
1	-4.224172000	-2.060326000	2.977981000
6	-0.789400000	-2.375530000	2.405123000
1	-0.036879000	-1.892274000	1.772720000
1	-0.791722000	-3.451081000	2.169304000
1	-0.489019000	-2.262277000	3.458246000

1 (Spin multiplicity = 3)

Total energy: -1796.6336 a. u.

9	-0.037375000	-0.584275000	0.072948000
7	2.414537000	0.364146000	-0.552215000
6	1.388364000	1.308366000	-0.417201000
5	-0.004428000	0.800791000	0.049755000
7	-2.507098000	0.564513000	0.439552000
6	1.860864000	2.629888000	-1.028001000
6	3.352050000	2.351011000	-1.353140000
1	3.677886000	2.866869000	-2.267535000
1	3.974986000	2.721937000	-0.523838000

6	3.522012000	0.828253000	-1.452271000
6	1.049934000	2.982998000	-2.293742000
1	1.348154000	3.968605000	-2.686549000
1	-0.025162000	3.012367000	-2.069538000
1	1.196128000	2.239218000	-3.086859000
6	1.829244000	3.833783000	-0.064616000
1	2.307932000	3.583053000	0.893233000
1	0.814031000	4.184819000	0.142412000
1	2.383186000	4.675818000	-0.512031000
6	3.319186000	0.354633000	-2.905625000
1	3.990670000	0.918804000	-3.570463000
1	2.286673000	0.524379000	-3.236695000
1	3.549430000	-0.709934000	-3.023991000
6	4.889233000	0.364776000	-0.949769000
1	5.673676000	0.758314000	-1.612616000
1	4.963423000	-0.731825000	-0.942505000
1	5.082909000	0.728793000	0.068252000
6	2.574090000	-0.781234000	0.297655000
6	2.390318000	-2.092296000	-0.204297000
6	2.615420000	-3.177059000	0.651834000
1	2.471613000	-4.189943000	0.270034000
6	2.980870000	-2.991110000	1.982131000
1	3.142463000	-3.850734000	2.635245000
6	3.119432000	-1.696601000	2.476517000
1	3.393432000	-1.546605000	3.522816000
6	2.927384000	-0.579159000	1.654215000
6	3.077375000	0.806219000	2.258900000
1	3.046951000	1.532727000	1.435923000
6	1.885791000	1.107062000	3.181919000
1	1.869371000	0.415116000	4.038399000
1	0.937178000	0.994822000	2.638198000
1	1.939627000	2.134715000	3.573260000
6	4.411774000	0.992482000	2.997135000
1	5.267770000	0.762033000	2.345813000
1	4.482421000	0.342100000	3.882008000
1	4.513222000	2.032450000	3.343382000
6	1.888073000	-2.374602000	-1.609557000
1	1.700791000	-1.405337000	-2.090074000
6	0.551297000	-3.135705000	-1.593447000
1	0.660469000	-4.130656000	-1.134845000
1	0.186789000	-3.281576000	-2.621888000
1	-0.213226000	-2.584298000	-1.036530000

6	2.930136000	-3.150471000	-2.433485000
1	3.912082000	-2.654824000	-2.431456000
1	2.599139000	-3.258984000	-3.477890000
1	3.075626000	-4.161458000	-2.022328000
6	-1.381292000	1.396632000	0.443298000
6	-1.795165000	2.752881000	1.009019000
6	-3.205997000	2.476671000	1.590132000
1	-3.113703000	2.227345000	2.658399000
1	-3.868759000	3.349965000	1.508728000
6	-3.771939000	1.257816000	0.849334000
6	-4.623881000	1.637179000	-0.375746000
1	-5.513916000	2.193656000	-0.046839000
1	-4.963614000	0.732400000	-0.898957000
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6	-4.639078000	0.400499000	1.773113000
1	-4.104112000	0.141137000	2.694058000
1	-4.961965000	-0.524556000	1.275274000
1	-5.538864000	0.969975000	2.048742000
6	-1.887764000	3.854479000	-0.071659000
1	-2.255962000	4.793682000	0.373401000
1	-2.575212000	3.570356000	-0.879181000
1	-0.916119000	4.059992000	-0.532821000
6	-0.865799000	3.209473000	2.146438000
1	0.176622000	3.283899000	1.819555000
1	-0.902832000	2.489274000	2.975632000
1	-1.177072000	4.194656000	2.530621000
6	-2.605402000	-0.737276000	-0.159600000
6	-2.627359000	-1.883119000	0.674755000
6	-2.893037000	-3.128043000	0.091008000
1	-2.919075000	-4.017535000	0.723588000
6	-3.093537000	-3.256498000	-1.281503000
1	-3.306267000	-4.234619000	-1.717090000
6	-2.968715000	-2.137078000	-2.100073000
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6	-2.707267000	-0.868262000	-1.564485000
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1	-2.363676000	1.206756000	-1.921473000
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1	-0.847809000	0.916269000	-3.879957000
1	-1.056650000	-0.851660000	-3.782401000
1	-0.256580000	0.022637000	-2.456256000
6	-3.531418000	0.473502000	-3.575324000

1	-3.318647000	1.361375000	-4.190009000
1	-4.521663000	0.603009000	-3.117302000
1	-3.585626000	-0.390631000	-4.254354000
6	-2.255538000	-1.829194000	2.150824000
1	-2.175150000	-0.768856000	2.432370000
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1	-3.328345000	-3.593388000	2.875285000
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6	-0.872419000	-2.472973000	2.382756000
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1	-0.597374000	-2.403263000	3.446609000

2 (Spin multiplicity = 2)

Total energy: -1796.4821 a. u.

9	-0.016076000	0.568535000	-0.079554000
7	2.405905000	-0.453699000	0.505673000
6	1.395969000	-1.340011000	0.403374000
5	0.002250000	-0.799878000	-0.054442000
7	-2.469081000	-0.571709000	-0.411866000
6	1.837936000	-2.679557000	1.005322000
6	3.354114000	-2.471742000	1.248394000
1	3.688941000	-2.969859000	2.167383000
1	3.918051000	-2.909709000	0.411546000
6	3.609822000	-0.963704000	1.289586000
6	1.074210000	-2.946115000	2.320045000
1	1.376082000	-3.918896000	2.735054000
1	-0.011084000	-2.961912000	2.157463000
1	1.282145000	-2.173543000	3.070727000
6	1.702646000	-3.887430000	0.060081000
1	2.153153000	-3.674857000	-0.920040000
1	0.673101000	-4.216904000	-0.092849000
1	2.253038000	-4.731054000	0.503450000
6	3.591706000	-0.426902000	2.727504000
1	4.366046000	-0.955165000	3.301596000
1	2.626216000	-0.595924000	3.221771000
1	3.821326000	0.641994000	2.763743000
6	4.919080000	-0.571463000	0.609477000
1	5.751887000	-1.017155000	1.171185000
1	5.060432000	0.517065000	0.592840000

1	4.963414000	-0.945361000	-0.420973000
6	2.534493000	0.773970000	-0.261181000
6	2.413329000	2.041016000	0.349854000
6	2.673293000	3.170816000	-0.435696000
1	2.580331000	4.159336000	0.016503000
6	3.018547000	3.061477000	-1.779671000
1	3.217602000	3.956808000	-2.370396000
6	3.084219000	1.804522000	-2.371095000
1	3.326755000	1.721683000	-3.431506000
6	2.844768000	0.636501000	-1.634926000
6	2.875712000	-0.695584000	-2.370668000
1	2.821273000	-1.509296000	-1.632660000
6	1.638439000	-0.809683000	-3.280005000
1	1.652162000	-0.024632000	-4.050211000
1	0.708695000	-0.692763000	-2.704082000
1	1.613801000	-1.785840000	-3.786379000
6	4.163501000	-0.901838000	-3.184313000
1	5.062684000	-0.779968000	-2.564111000
1	4.236195000	-0.187003000	-4.016449000
1	4.179994000	-1.912200000	-3.618254000
6	1.918226000	2.254782000	1.771442000
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6	0.560256000	2.981154000	1.777901000
1	0.651023000	3.990066000	1.349479000
1	0.196792000	3.090612000	2.810289000
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1	2.993465000	4.087983000	2.281077000
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1	-2.666912000	-3.524188000	0.885594000
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6	-0.885081000	-3.199016000	-2.119905000
1	0.160032000	-3.274961000	-1.807669000
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1	-2.397931000	-1.210349000	1.960728000
6	-1.097111000	-0.083514000	3.235582000
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