Supplementary Information (SI) for Dalton Transactions.

Supporting Information

Unprecedented C−F bond cleavage from perfluoronaphthalene during cobaltocene reduction

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S1. General experimental information

All manipulations were carried out in an inert atmosphere of argon using standard Schlenk techniques and in argon filled glove box. The solvents, especially benzene, tetrahydrofuran, dichloromethane and hexane were purified by MBRAUN solvent purification system MB SPS-800. Benzene was dried and distilled over Na/benzophenone mixture prior to use. Other chemicals were purchased from Sigma Aldrich and TCI Chemicals and were used without further purification. The starting material, SIDipp was synthesized by using literature procedure.[S1] ^{1}H, ^{13}C, ^{19}F, ^{31}P and ^{11}B NMR spectra were recorded in DMSO-d_6, CD_3CN and $CDCl_3$ using a Bruker Avance DPX 200, Bruker Avance DPX 400 or a Bruker Avance DPX 500 spectrometer referenced to external $SiMe_4$. High resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific. Cyclic voltammetry (CV) experiments were carried out using a PGSTAT 101 electrochemical workstation (METROHM).

S2. Synthetic procedure and characterization of 3·2HF$_2$, 3·2B$_2$F$_7$, 3·2PF$_6$ and **5**

3·2HF$_2$. To a 10 ml hexane solution of 5-SIDipp (0.4 g, 0.104 mmol), 10 ml hexane solution of octafluoro naphthalene (0.170 g, 0.052 mmol) was added at room temperature. The resulting solution color was changed from colourless to red immediately with concomitant formation of a red precipitate. After stirring the reaction mixture for 1 h at room temperature, the precipitate was filtered through cannula and was collected and dried in vacuum. The precipitate was further washed with 10 ml diethyl ether 2-3 times for purification. Red colored crystals were obtained after keeping the concentrated dichloromethane solution of the red powder at -36 °C. **3·2HF$_2$** was further utilized for the characterization. Yield 0.4 g (70 %).

Note: *We were unable to do the characterization due to the low solubility in any deuterated solvents*.

3·2B_2F_7. To a 10 ml hexane solution of 5-SIDipp (0.4 g, 0.104 mmol), 10 ml hexane solution of octafluoronaphthalene (0.170 g, 0.052 mmol) was added at room temperature. After 1 h BF_3·ether (0.065 mL, 0.051 mmol) was added at 0 °C. The resulting solution color was changed from red to colorless immediately with concomitant formation of a white precipitate. After stirring the reaction mixture for another 1 h at room temperature, the precipitate was filtered through cannula and was collected and dried in vacuum. The precipitate was further washed with 10 ml diethyl ether 2-3 times for purification. Colourless product, **3·2B_2F_7** was further utilized for the characterization. Yield 0.456 g (70 %).

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ 1.23 (d, *J* = 6.50 Hz, 12 H*2, CH(CH_3)$_2$), 1.37 (d, *J* = 6.63 Hz, 12*2 H, CH(CH_3)$_2$), 3.10 (sept, *J* = 6.88 Hz, 4 H*2, C*H*(CH_3)$_2$), 4.84 (s, 4 H*2, N-CH_2CH_2-N), 7.19 (d, *J* = 7.88, 8 H, Ar-*H*), 7.39 (t, *J* = 7.88 Hz, 4 H, Ar-*H*) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, CD_3CN): δ 22.8, 27.1 (HC*Me$_2$*), 29.7 (H*C*Me$_2$), 55.7 (N-*CH$_2$CH$_2$*-N), 118.4, 132.2, 132.8 (Ar-*C$_6$*H$_3$), 147.5 (*ipso* Ar-*C$_6$*H$_3$) ppm.

^{19}F{^{1}H} NMR (377 MHz, 298 K, $CDCl_3$): δ –107.2 (2 F, *ortho*-Ar-$C_{10}F_6$), –131.9 (2 F, *ortho*-Ar-C_6F_4), -146.2 (2 F, *ortho*-Ar-C_6F_4), –148.3 (2* 7 F, 2BF_7^-) ppm.

^{11}B{^{1}H} NMR (128 MHz, 298 K, $CDCl_3$): δ -1.5 ppm.

UV-Vis (λ_{max}/nm (ε/ $M^{-1}cm^{-1}$)): 482 (1650), 362 (6200).

HRMS (CH_3CN): *m/z* calcd for $[C_{64}H_{72}F_6N_4]^{++}$ 507.2982 found 507.2983.

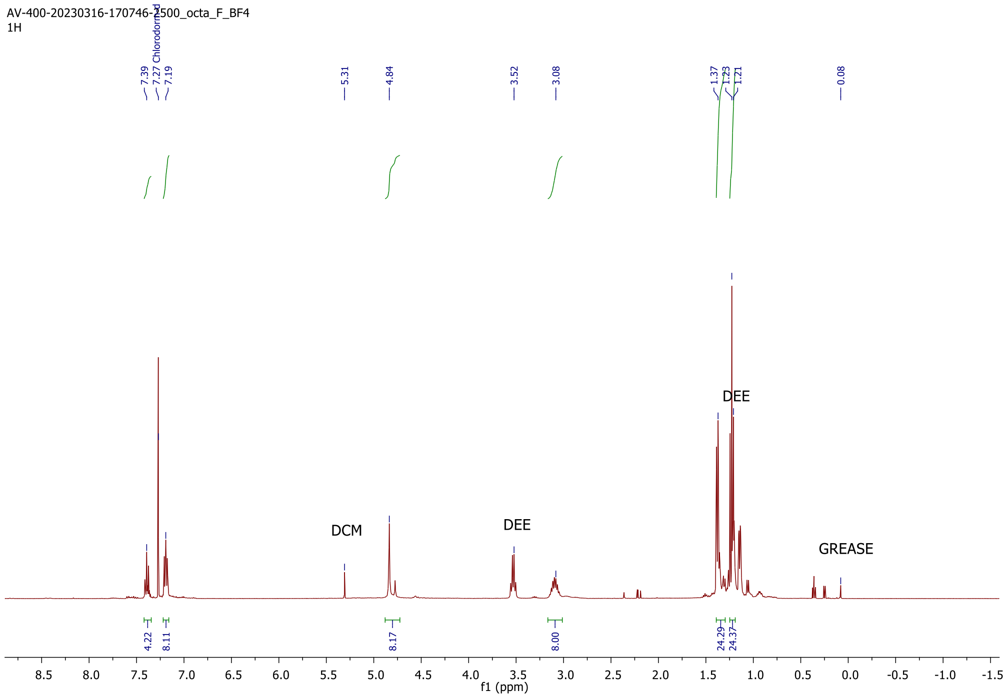

Figure S1: ^{1}H NMR of **3·2B$_2$F$_7$**.

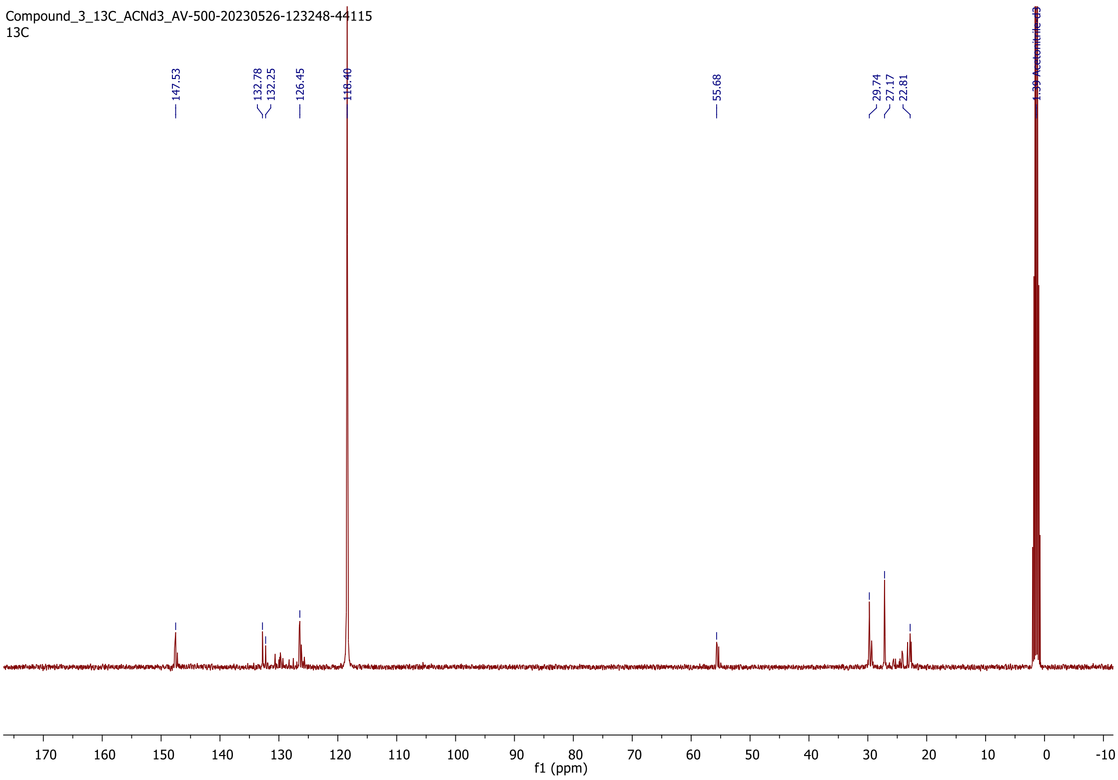

Figure S2: ^{13}C NMR of **3·2B$_2$F$_7$**.

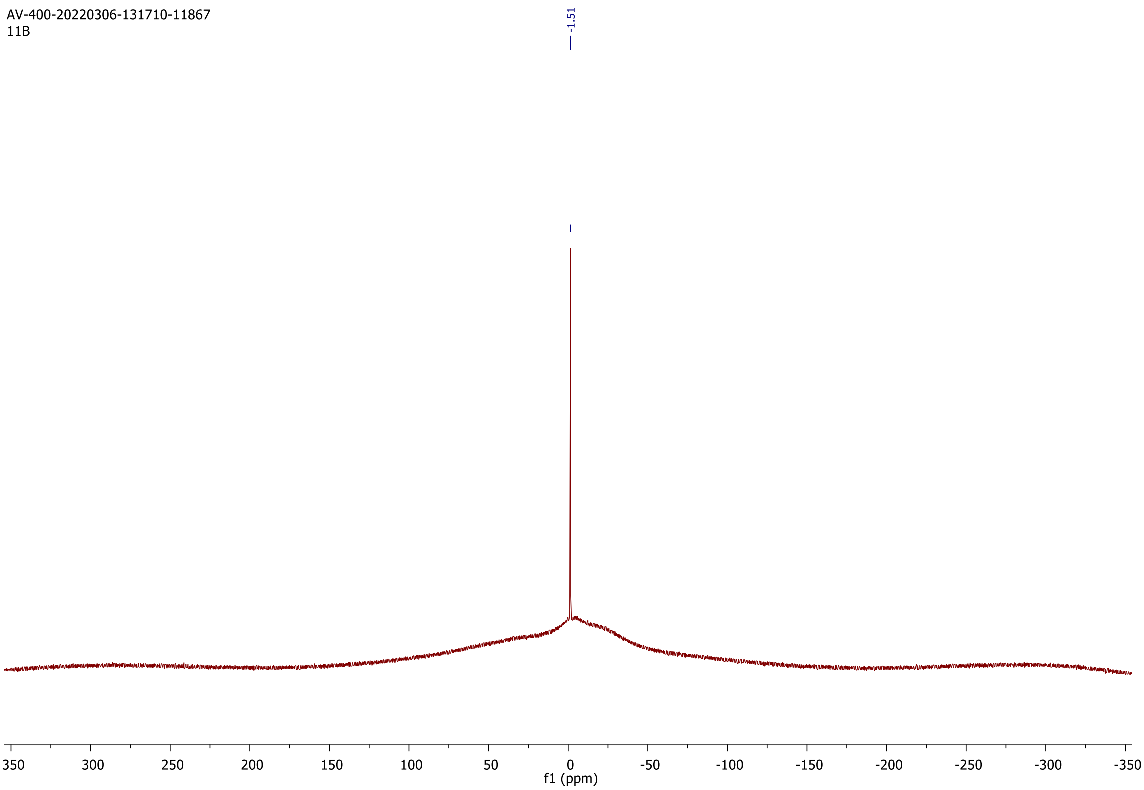

Figure S3: ^{11}B NMR of **3·2B$_2$F$_7$**.

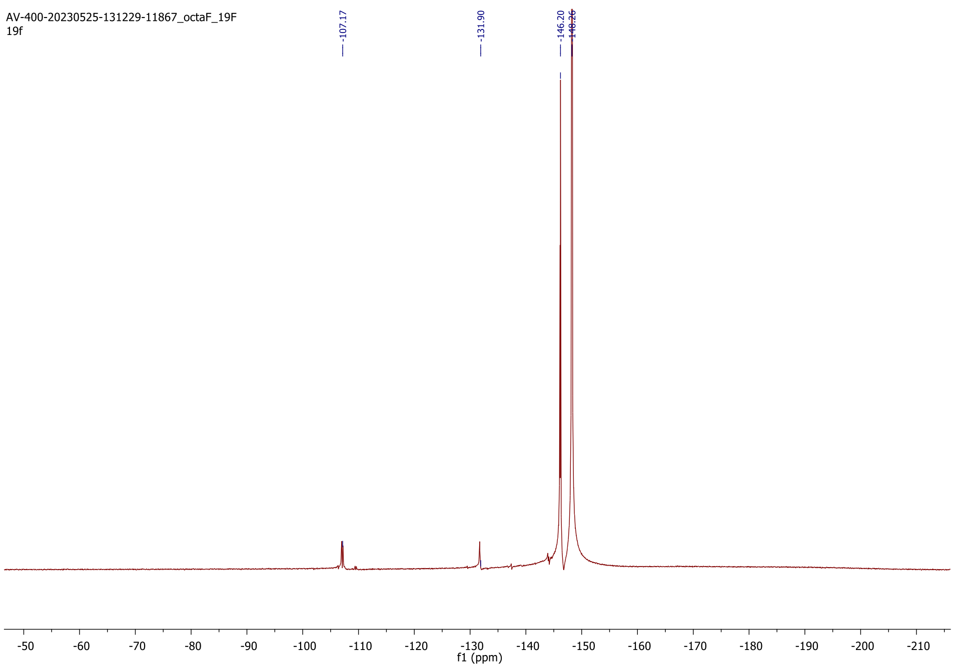

Figure S4: ^{19}F NMR of **3·2B$_2$F$_7$**.

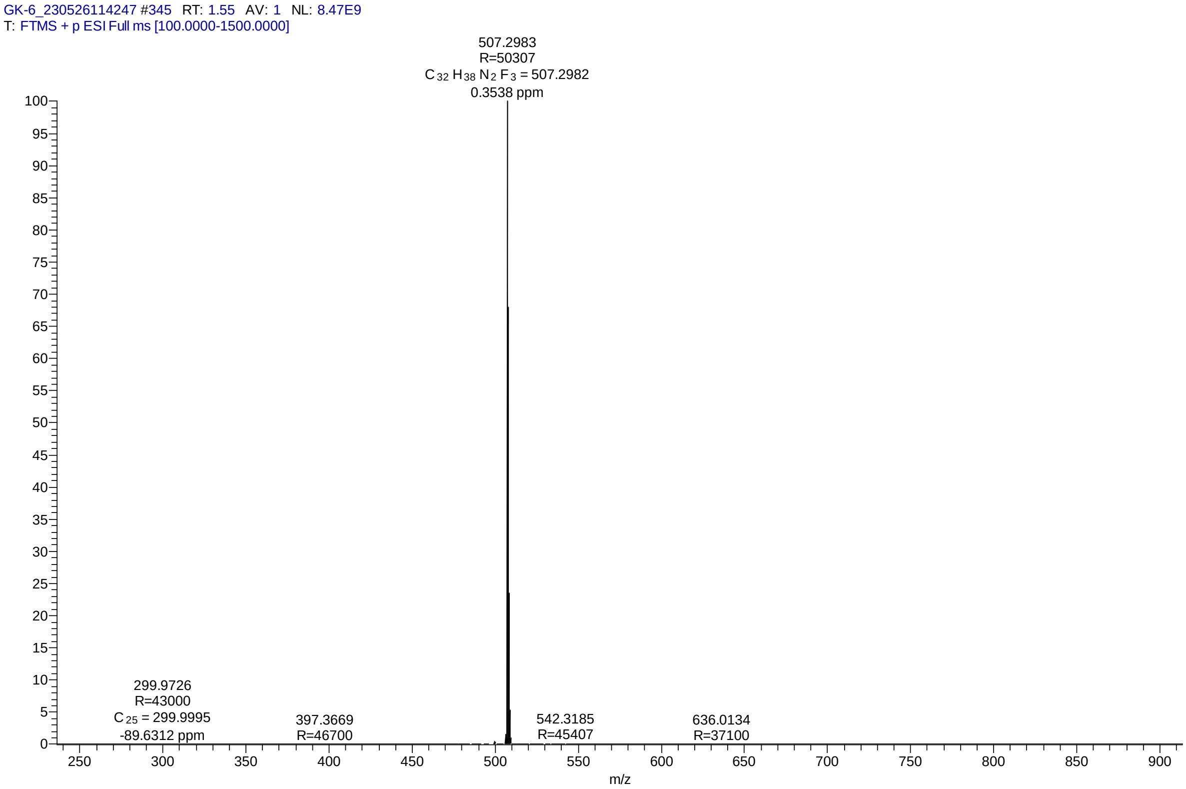

Figure S5: HRMS spectrum of **3·2B$_2$F$_7$**.

3·2PF$_6$. To a 10 ml of acetonitrile solution of **3·2B$_2$F$_7$** (0.2 g, 0.19 mmol), 10 ml of acetonitrile solution of Bu_4NPF_6 (0.073 g, 0.19 mmol) was added at room temperature. After stirring the reaction mixture for another 12 h, the resulting solution color was changed from colorless to red with concomitant formation of **3·2PF$_6$**. The reaction mixture was dried in vacuum and washed with diethyl ether 2-3 times for purification. Red colored crystals of **3·2PF$_6$** came after keeping the concentrated acetonitrile solution at room temperature. Red product, **3·2PF$_6$** was further utilized for the characterization. Yield 0.18 g (85 %).

^{19}F{^{1}H} NMR (377 MHz, 298 K, CDCl$_3$): δ –72.0 (PF_6), –73.9 (PF_6), -151.9 (Ar-C$_6F_4$) ppm.

^{31}P{^{1}H} NMR (128 MHz, 298 K, CD$_3$CN): δ -144.4 ppm.

UV-Vis (λ_{max}/nm (ε/ M^{-1}cm^{-1})): 370 (14780), 485 (7200).

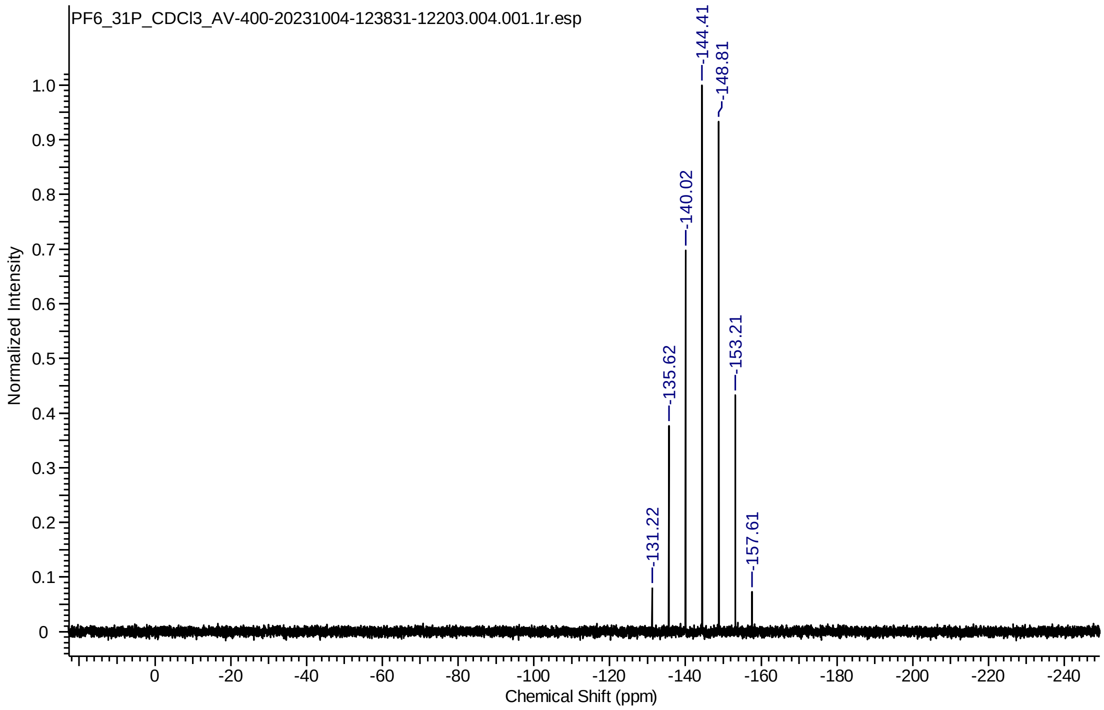

Figure S6: ^{31}P NMR of **3·2PF₆.**

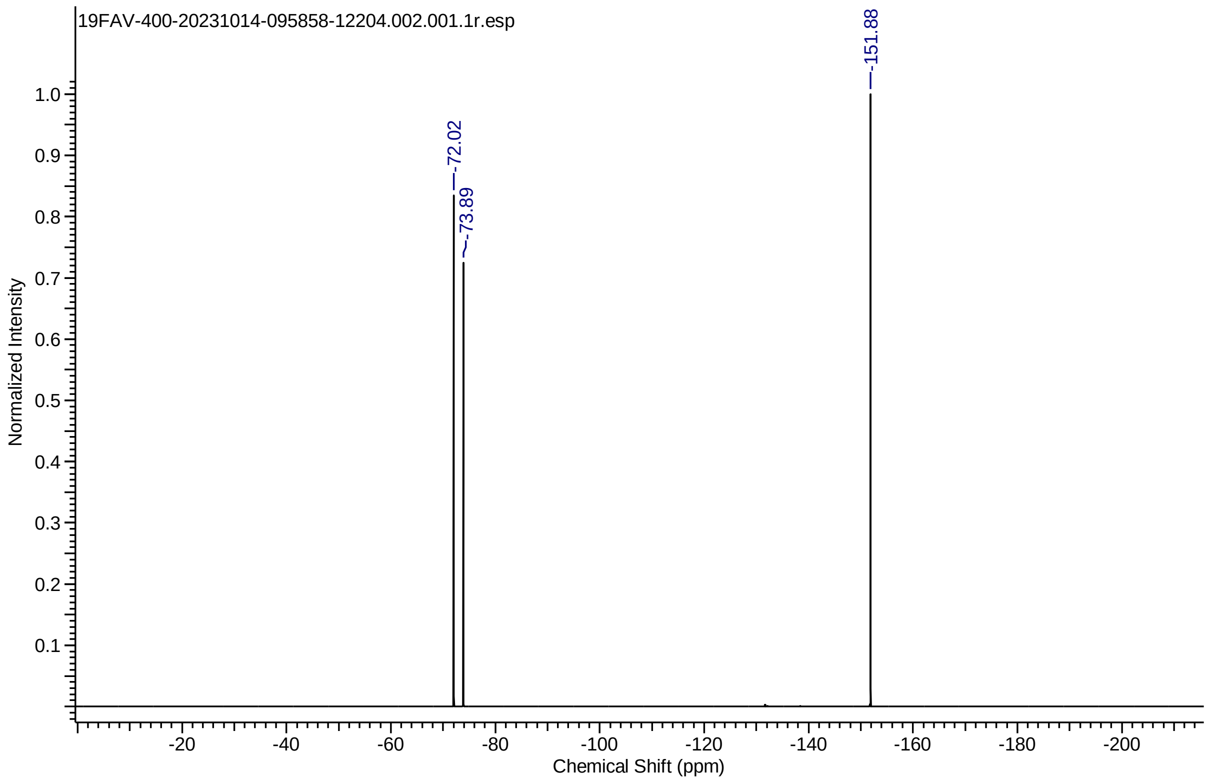

Figure S7: ^{19}F NMR of **3·2PF₆.**

5. In a 100 mL Schelnk flask, 5-SIDipp (0.4 g, 1.02 mmol), octafluoro toluene (0.14 g, 0.5 mmol), and cobaltocene (0.6 g, 3 mmol) were mixed and 15 ml THF solution was added drop by drop at -78 °C over 15 min. The reaction mixture was slowly allowed to come to room temperature and was stirred for another 3 hours at room temperature. The solvent was removed in vacuo, and the residue was extracted with hexane (10 mL). Purple colored crystals of **5** were obtained after keeping the concentrated hexane solution at room temperature for two days. Yield 0.04 g (19 %).

^{1}H NMR (400 MHz, 298 K, toluene-d_8): *δ* 1.12-1.32 (m, 12 H*4, CH(C*H*$_3$)$_2$), 3.36 (bs, 4 H*2, C*H*(CH$_3$)$_2$), 4.67 (bs, 4 H*2, N-C*H*$_2$C*H*$_2$-N), 6.98-7.10 (m, 12 H, Ar-*H*) ppm.

^{19}F{^{1}H} NMR (377 MHz, 298 K, C_6D_6): *δ* –127.6 (2 F, *ortho*-Ar-C$_{10}$*F*$_6$), –142.3 (2 F, *ortho*-Ar-C$_6$*F*$_4$) ppm.

UV-Vis (λ_{max}/nm (ε/M^{-1}cm^{-1})): 461 (24993), 573 (18709).

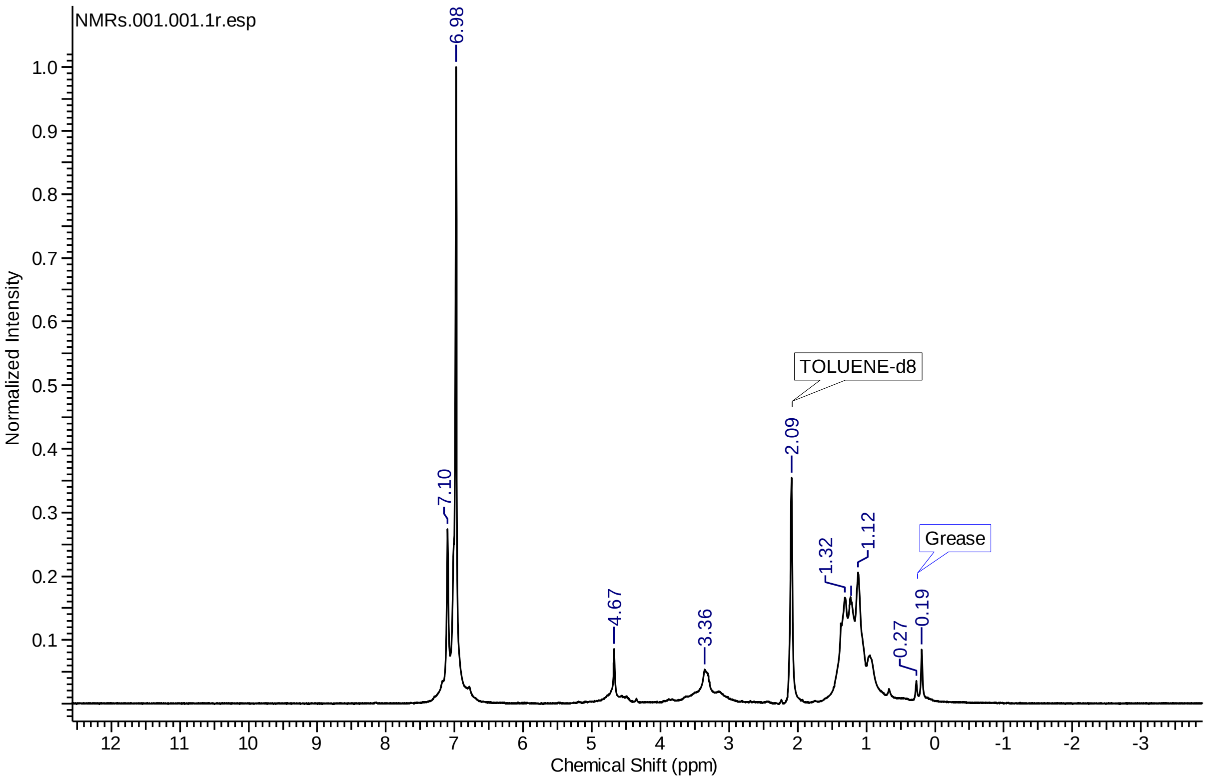

Figure S8: Room temperature ^{1}H NMR spectrum of **5**.

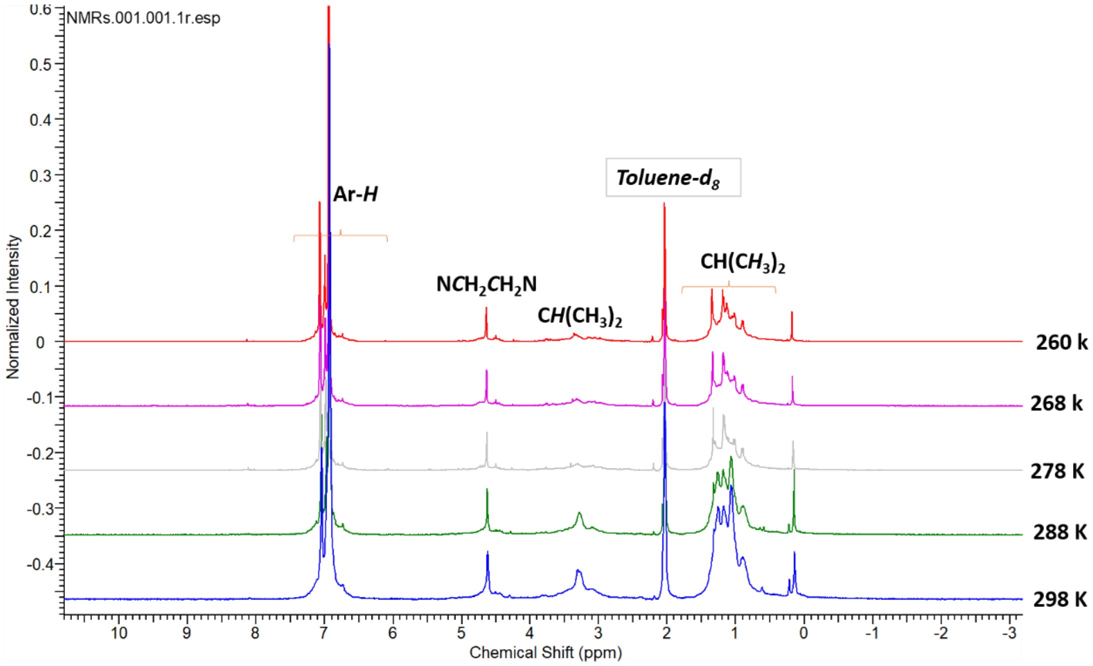

Figure S9: Variable temperature ^{1}H NMR spectrum of **5**.

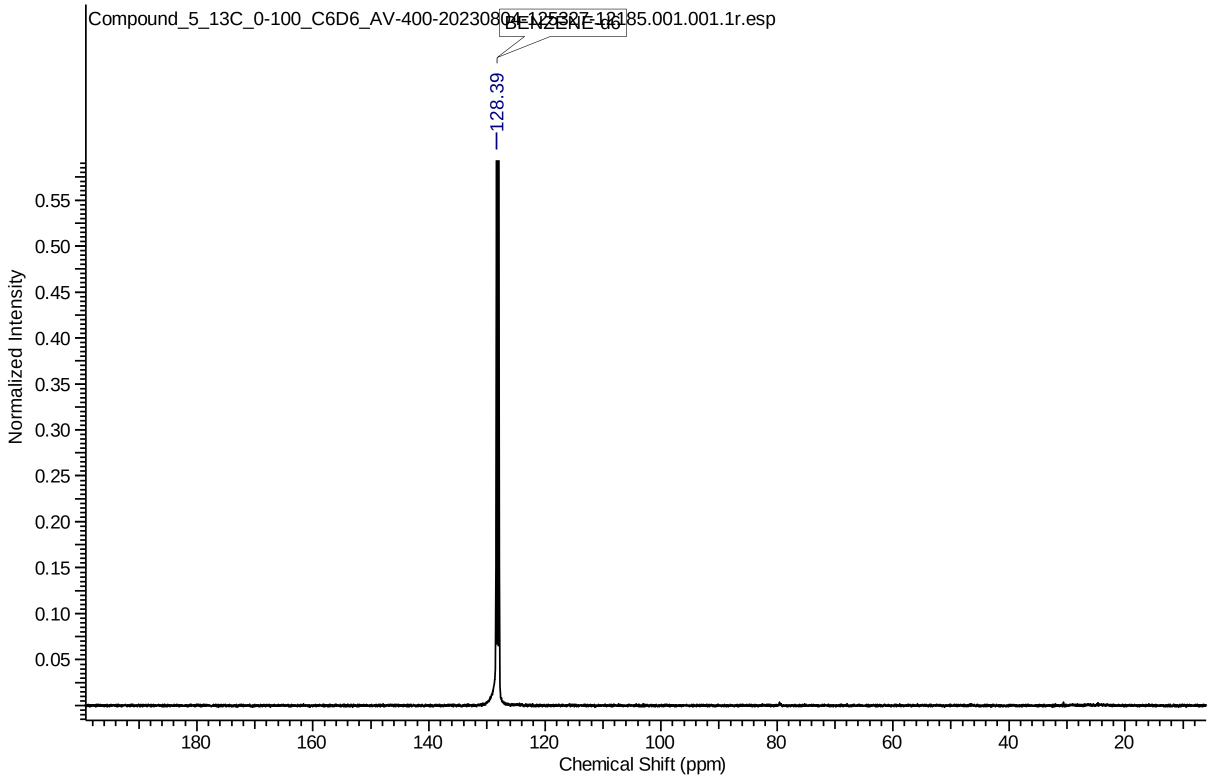

Figure S10: ^{13}C NMR spectrum of **5**.

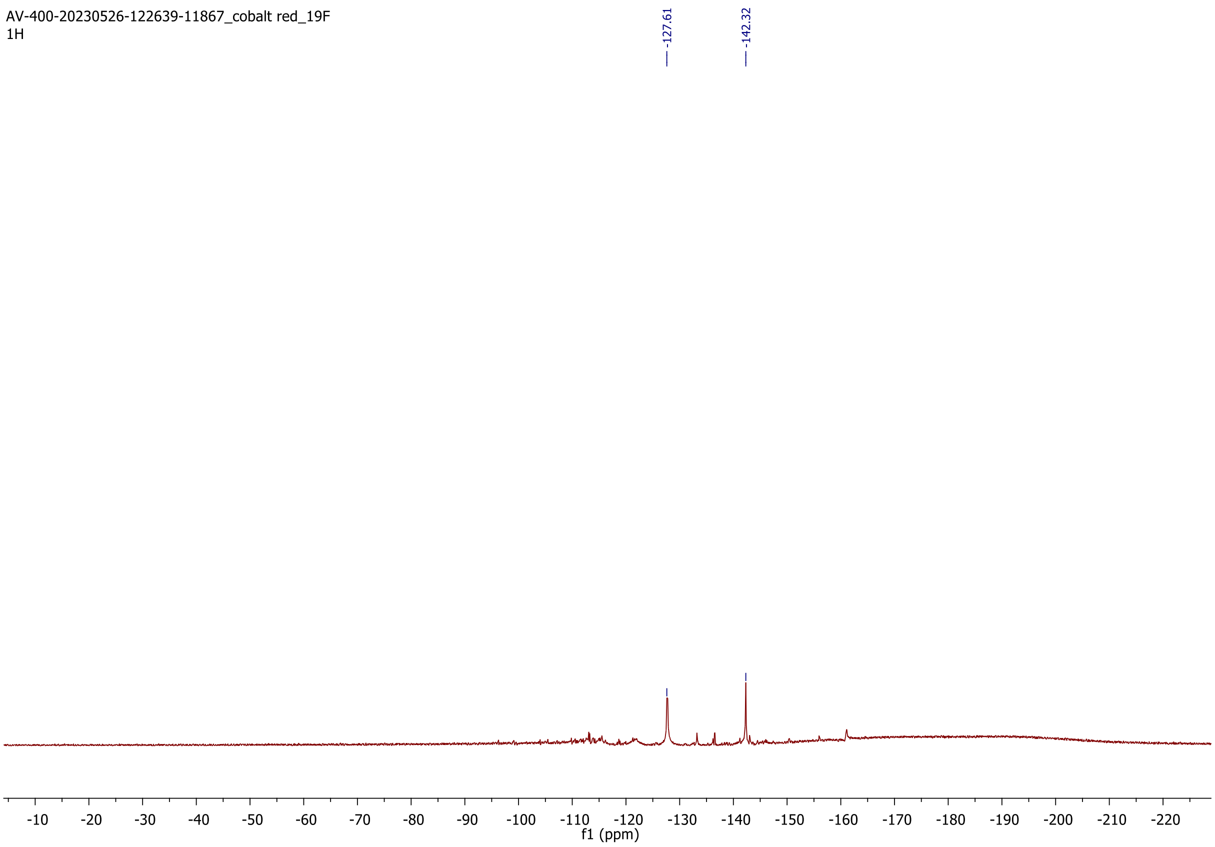

Figure S11: ^{19}F NMR spectrum of **5**.

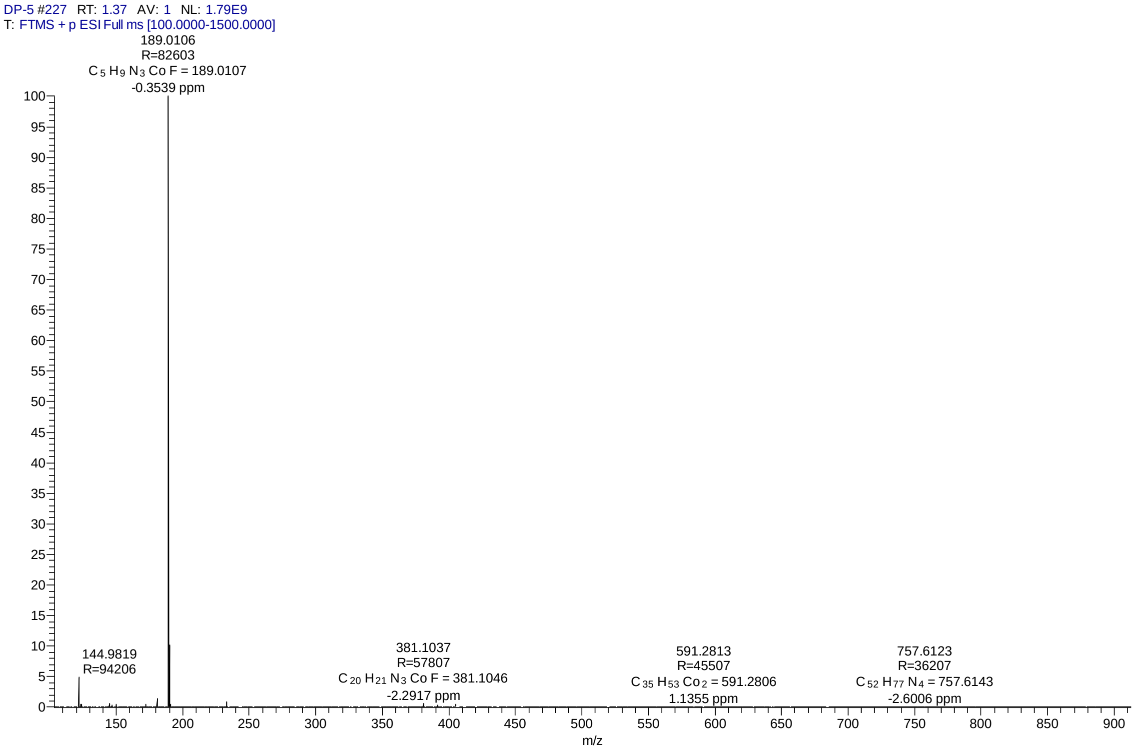

Figure S12: HRMS spectrum of **5**.

S3. Liquid state UV-Vis spectra of 3·2HF$_2$ and 3·2BF$_4$ at room temperature

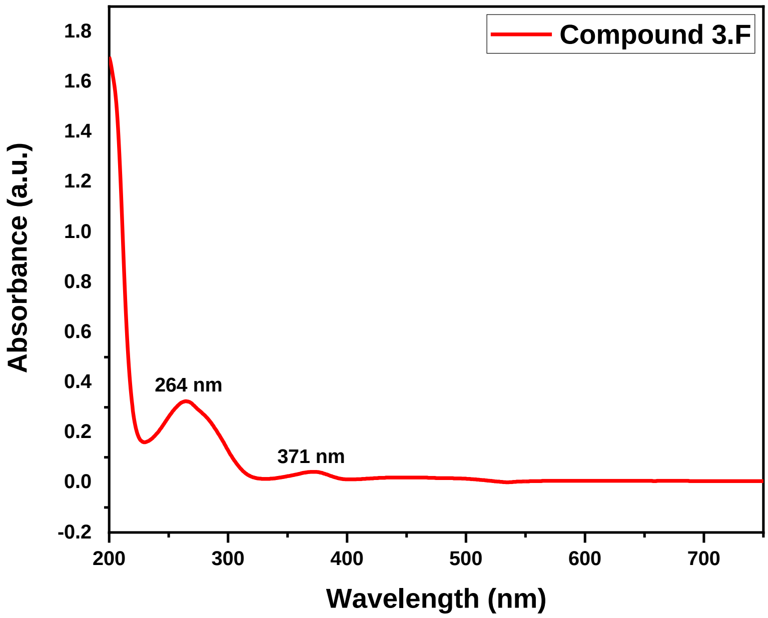

Figure S13: The absorption spectrum of **3·2HF$_2$** in acetonotrile (c = 1×10^{-5} M).

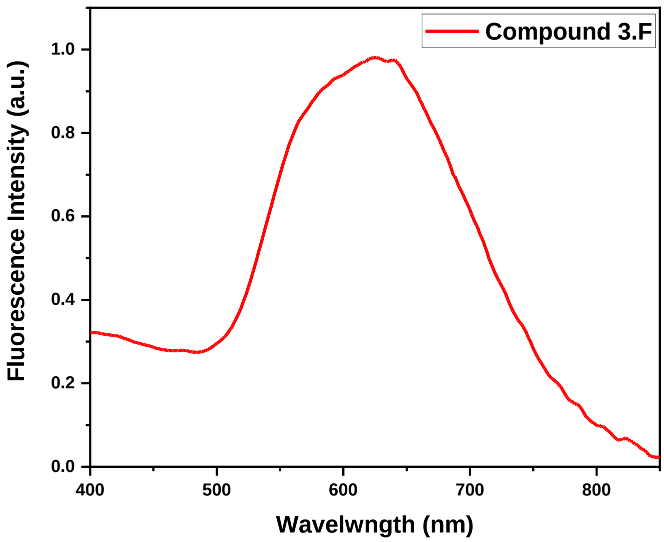

Figure S14**:** The emission spectrum of **3·2HF$_2$** at room temperature in acetonitrile (c = 1×10^{-5} M)

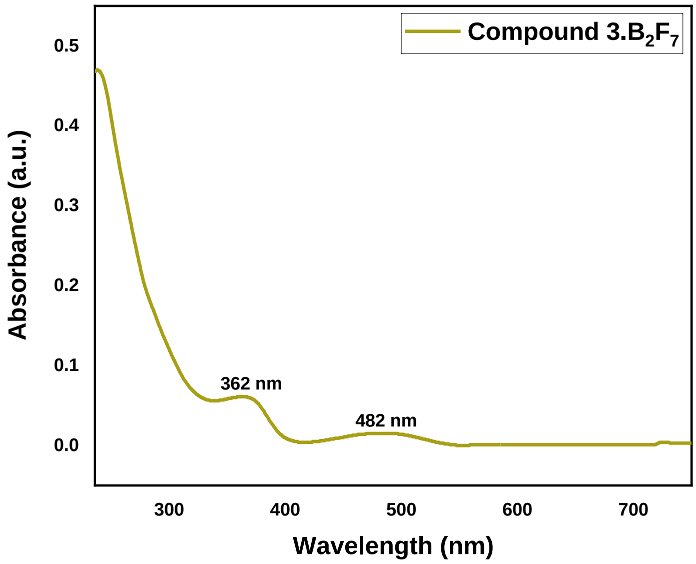

Figure S15: The absorption spectrum of **3·2B$_2$F$_7$** in acetonitrile (c = 1×10^{-5} M).

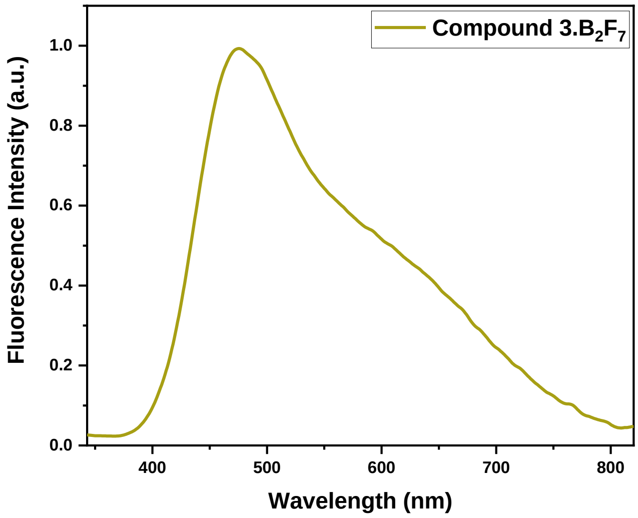

Figure S16**:** The emission spectrum of **3. 2B$_2$F$_7$** at room temperature in acetonitrile (c = 1×10^{-5} M)

S4. Liquid state UV-Vis spectrum, emission spectra of 3·2PF₆

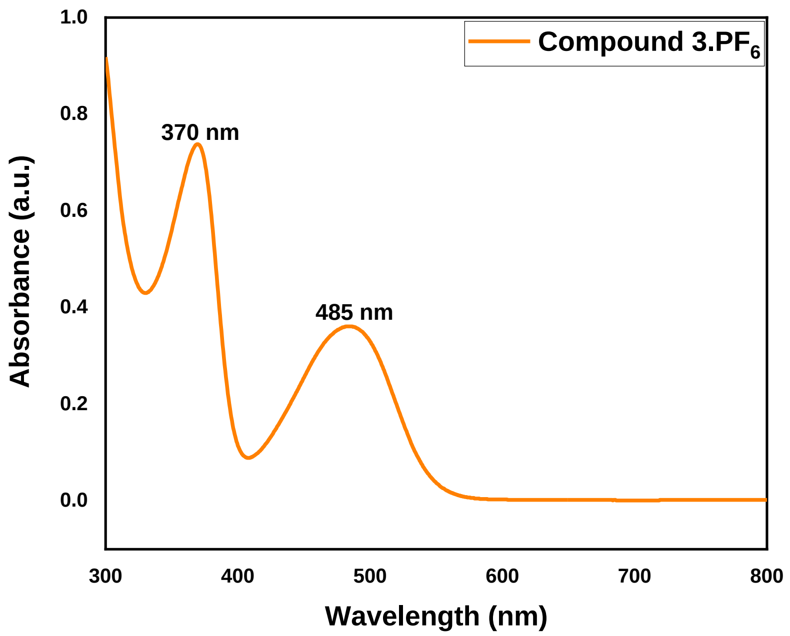

Figure S17: The absorption spectrum of **3·2PF$_6$** (c = 5×10^{-5} M) at room temperature in acetonitrile.

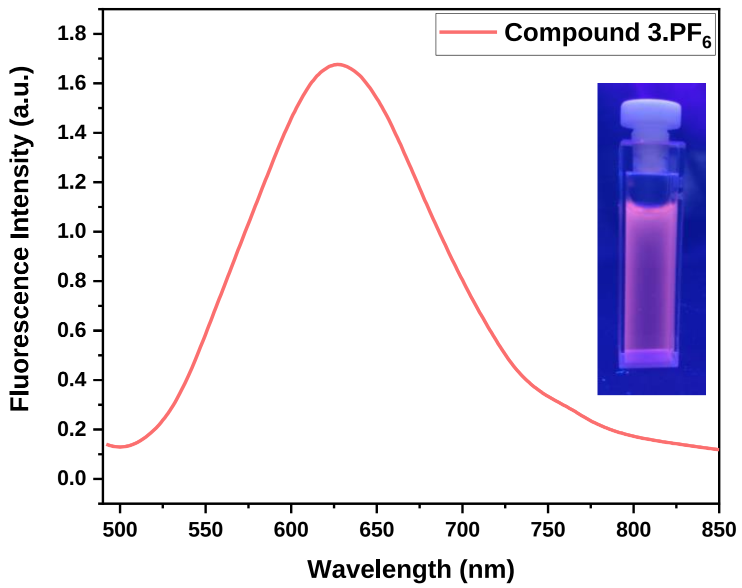

Figure S18**:** The emission spectrum of **3·2PF$_6$** (c = 5×10^{-5} M) at room temperature in acetonitrile

S5. Life time spectrum of 3·2PF6

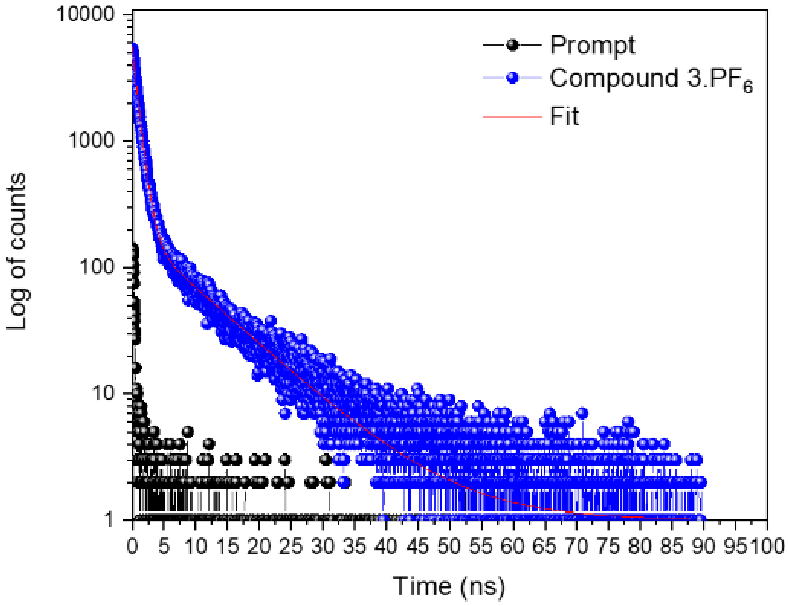

Figure S19: Lifetime measurement of compound **3. 2PF6** in acetonitrile (c =5×10^{-5} M).

S6. Liquid state UV-Vis spectrum spectra of 5 at room temperature

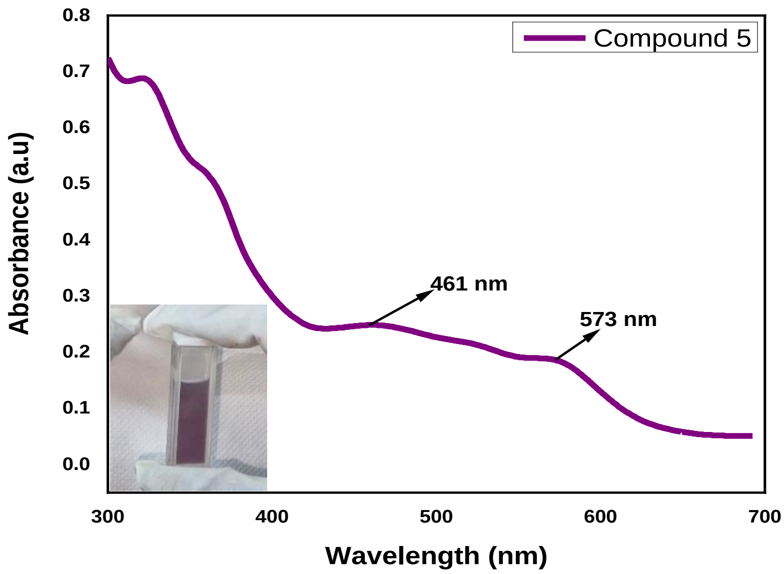

Figure S20: The absorption spectrum of **5** in THF (c =1×10^{-5} M).

S7. Cyclic voltammetry of compound 5

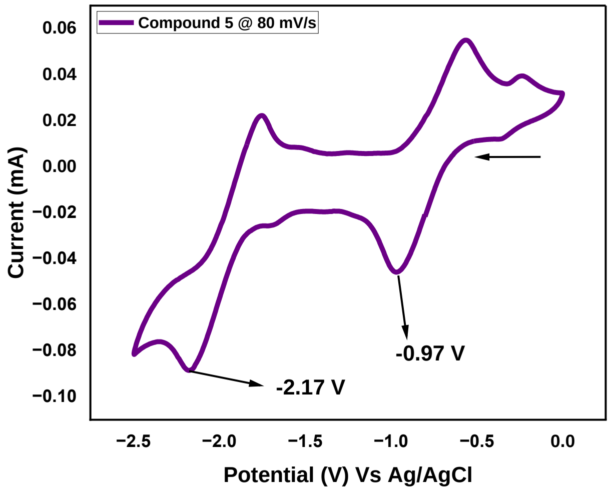

Figure S21: Cyclic voltammogram of **5** in THF with 0.1 M Bu_4NPF_6 as the supporting electrolyte, Ag/AgCl as the reference electrode, and a Pt wire as the counter electrode.

S8. EPR spectra of 5 at room temperature

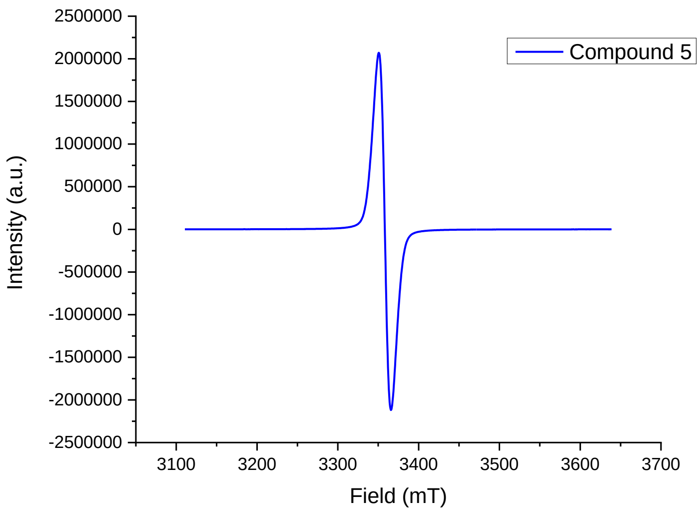

Figure S22: Solid state X-band EPR spectrum of **5**, recorded at 298 K.

S9. Magnetic studies of 5

Magnetic measurements of the samples were carried out using a Quantum Design make Magnetic Property Measurement System (MPMS). The following complex magnetic measurements were carried out on the samples using the SQUID and VSM modes of the instrument.

1. Magnetization versus magnetic field at two different temperatures (5 K and 300 K) up to a maximum magnetic field of 6 Tesla (60 kOe). [kOe= kilo oersted]

2. The Magnetization of the samples was recorded as a function of temperature in the range 5-

300 K, under:

a) Magnetic field of 100 Oe.

b) Zero field cooled (ZFC) and field cooled (FC) conditions

The samples were cooled in zero field to 5 K for ZFC measurements, and magnetization was measured while warming in a field of 100 Oe. For FC measurement, the samples were cooled from 300 K to 5 K in a magnetic field of 100 Oe, and the magnetization was measured while warming in a field of 100 Oe. Before the measurement, instrument was calibrated using a standard sample of high purity Palladium metal.

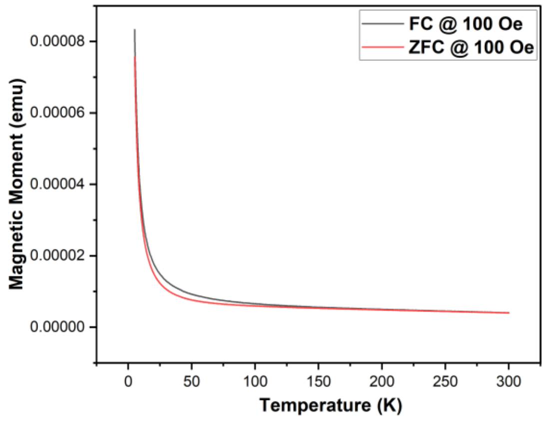

Figure S23: ZFC and FC magnetization curves as a function of temperature for **5** measured with an applied field of 100 Oe between 5 K (above) and 300 K (down).

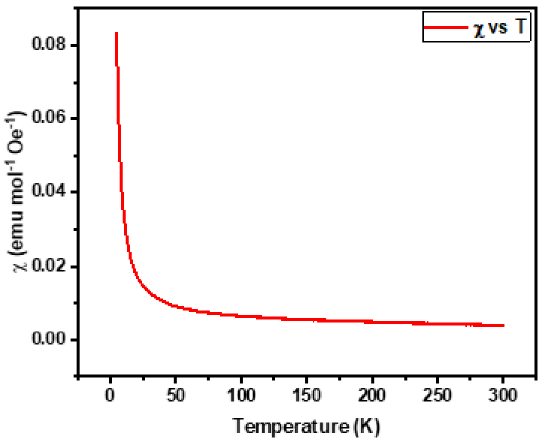

Figure S24: Susceptibility vs Temperature graph of **5**.

S10. Crystallographic data for the structural analysis of 3·2HF$_2$, 3·2B$_2$F$_7$ and 5, and molecular structure of 3·2PF$_6$

Single crystals of **3·2HF$_2$, 3·2B$_2$F$_7$** and **5** were mounted on a Bruker SMART APEX II single crystal X-ray CCD diffractometer having graphite monochromatised (Mo-Kα = 0.71073 Å) radiation at low temperature 100 K. The X-ray generator was operated at 50 kV and 30 mA. The X-ray data acquisition was monitored by APEX2 program suit. The data were corrected for Lorentz-polarization and absorption effects using SAINT and SADABS programs which are an integral part of APEX2 package.[S2] The structures were solved by direct methods and refined by full matrix least squares, based on F^2, using SHELXL Crystal structures were refined using Olex2-1.0 software. Anisotropic refinement was performed for all non-H atom. The C-H hydrogen atoms were calculated using the riding model.[S3,S4] The structures were examined using the ADSYM subroutine of PLATON to assure that no additional symmetry could be applied to the models. The molecular weight of each structure mentioned herein has been calculated considering the solvent molecules trapped in the crystal. Mercury software was used to understand packing diagrams and molecular interactions.[S5]

Identification code	**3·2HF$_2$**	**3·2B$_2$F$_7$**	**5**
Empirical formula	$C_{68}H_{88}Cl_8F_{12}N_4$	$C_{68}H_{84}B_4Cl_8F_{20}N_4$	$C_{93}H_{117}Co_2F_4N_4$
Formula weight	1473.02	1664.23	1484.76
Temperature/K	100.0	100.0	100.0
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/n$	*P*-1
a/Å	14.6927(8)	10.5204(8)	14.0847(15)
b/Å	18.5978(11)	18.2379(15)	14.5294(16)
c/Å	14.5593(8)	21.2226(15)	21.074(2)
α/°	90	90	92.130(4)
β/°	112.463(2)	102.566(2)	99.925(3)
γ/°	90	90	107.864(3)
Volume/Å^3	3676.5(4)	3974.4(5)	4024.6(8)
Z	2	2	2
ρ_{calc}g/cm^3	1.331	1.391	1.225
μ/mm^{-1}	0.378	0.372	0.469
F(000)	1536.0	1712.0	1586.0
Crystal size/mm^3	0.16 × 0.12 × 0.1	0.15 × 0.12 × 0.1	0.27 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.002 to 56.68	3.932 to 49.992	3.894 to 74.646
Index ranges	-19 ≤ h ≤ 19, -24 ≤ k ≤ 24, -19 ≤ l ≤ 19	-12 ≤ h ≤ 12, -21 ≤ k ≤ 21, -25 ≤ l ≤ 25	-23 ≤ h ≤ 23, -24 ≤ k ≤ 24, -35 ≤ l ≤ 35
Reflections collected	61641	172534	252002
Independent reflections	9146 [R_{int} = 0.0438, R_{sigma} = 0.0266]	6971 [R_{int} = 0.0714, R_{sigma} = 0.0225]	38853 [R_{int} = 0.0520, R_{sigma} = 0.0334]
Data/restraints/parameters	9146/0/441	6971/0/477	38853/0/958

Goodness-of-fit on F^2	1.073	1.121	1.105
Final R indexes [I>=2σ (I)]	R_1 = 0.0652, wR_2 = 0.1714	R_1 = 0.1070, wR_2 = 0.2566	R_1 = 0.0509, wR_2 = 0.1530
Final R indexes [all data]	R_1 = 0.0759, wR_2 = 0.1818	R_1 = 0.1121, wR_2 = 0.2660	R_1 = 0.0673, wR_2 = 0.1714
Largest diff. peak/hole / e $Å^{-3}$	1.49/-0.72	2.64/-1.24	1.21/-2.22
CCDC No:	2270083	2270084	2270085

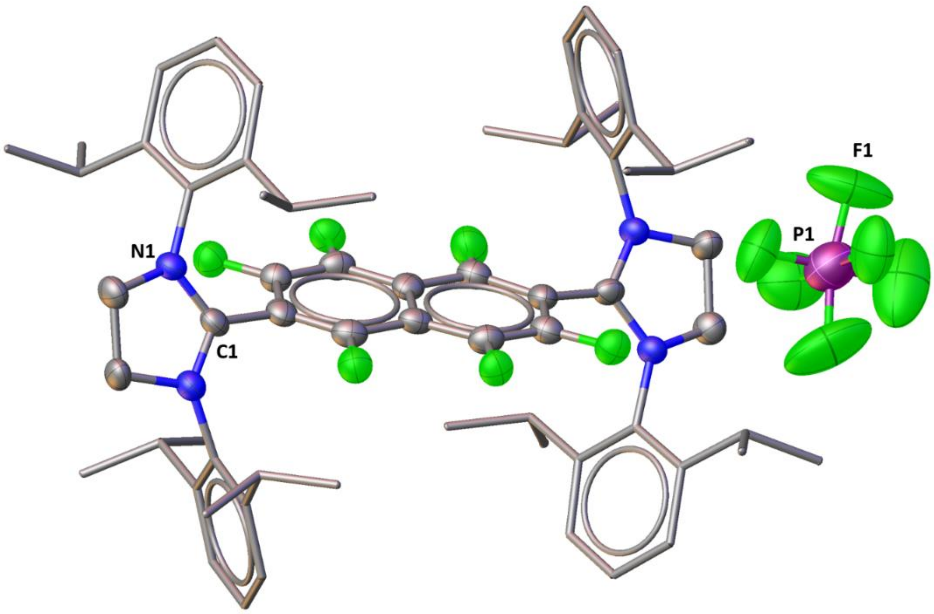

Figure S25: The molecular structure of **3·2PF$_6$**. Hydrogen atoms have been omitted for clarity. While the X-ray analysis unequivocally confirms the constitution of **3·2PF$_6$**, one of the PF_6 moiety is highly disordered, and hence masked during the refinement. Despite several attempts the data quality is very poor R_{int} is >25. Hence, we refrain from discussing the crystal structure and provide the molecular structure only in the supporting information.

S11. Details of the theoretical computational for 5

Computational Methods:

All the density functional theory (DFT) calculations were performed by using Gaussian 09 program package.[S6] R/U-B3LYP/def2-SVP[S7,S8] level of thoery was employed for geometry optimization. Restricted methods were used for calculations involving the singlet state and unrestricted methods were used for calculations involving the triplet states and the diradical character. Harmonic frequency calculations were carried out to confirm the optimizied geometries as local minima and to obtain the zero point correction energies. Single point calculations were performed by using the def2-TZVPP[S9] basis set along with the B3LYP, PBE0[S10] and M06-2X[S11] functionals to improve the electronic energies and refine the singlet-triplet gap (Table 1 and SA). The B3LYP/def2-SVP geoemtries were further used to carry out the TDDFT calculations by employing CAM-B3LYP[S12] functional along with def2-SVP basis set.

Table S1. Singlet-triplet gap (ΔE_{S-T} in kcal/mol) of **5** with and without the Zero-point energy (ZPE) correction.

Methods	**5 (no ZPE)**	**5 (with ZPE)**
B3LYP/def2-SVP	18.9	17.4
B3LYP/def2-TZVPP	20.4	18.9
PBE0/def2-TZVPP	19.5	18.0
M06-2X/def2-TZVPP	24.3	22.8

Table S2. CASSCF(2,2) + CASPT2 energies (in Hartree) using def2-SVP basis set for the calculation of singlet-triplet gap (in kcal/mol) and diradical character for the methyl analogue of 5.

Molecules	**5^{Me}**
CASSCF(2,2) Energy (in Hartree)	-4913.795807 (S) -4913.724973 (T)
ΔE_{S-T} at **CASSCF (2,2)** (in kcal/mol)	44.4
CASSCF(2,2) + **CASPT2** Energy (in Hartree)	-4921.405046 (S) -4921.354111 (T)
ΔE_{S-T} at CASSCF(2,2)+ **CASPT2** (in kcal/mol)	32.0
Occ(HOMO) Occ(LUMO)	1.94122 0.058784

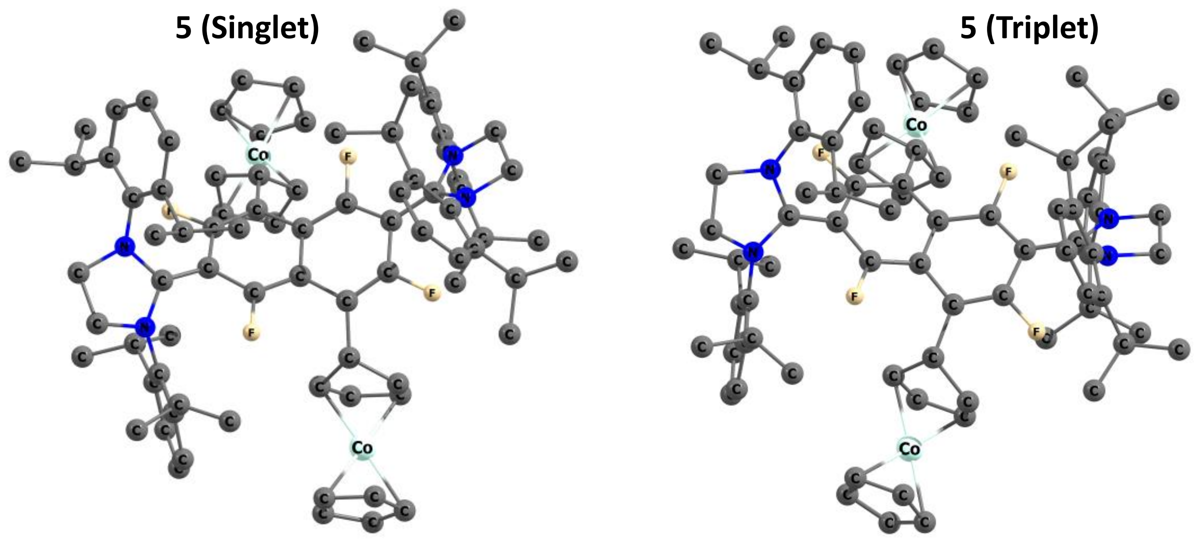

Figure S26: Optimized geometries of **5** for both singlet and triplet electronic state. Hydrogen atoms have been omitted for clarity.

Table S3. TDDFT results of **5** at the CAM-B3LYP/def2-SVP (CPCM = THF) level of theory. Wavelength (λ), oscillator strength (f).

Compound	Singlet			Triplet		
	λ_{max} (nm)	*f*	Assignment	λ_{max} (nm)	*f*	Assignment
5 (Gas)	511.23	0.9575	HOMO-LUMO (c=0.70)	878.34	0.1364	SOMO(α)-LUMO (c=0.93)
5 (THF)	522.27	1.2091	HOMO-LUMO (c=0.70)	959.50	1.2922	SOMO(α)-LUMO (c=0.95)

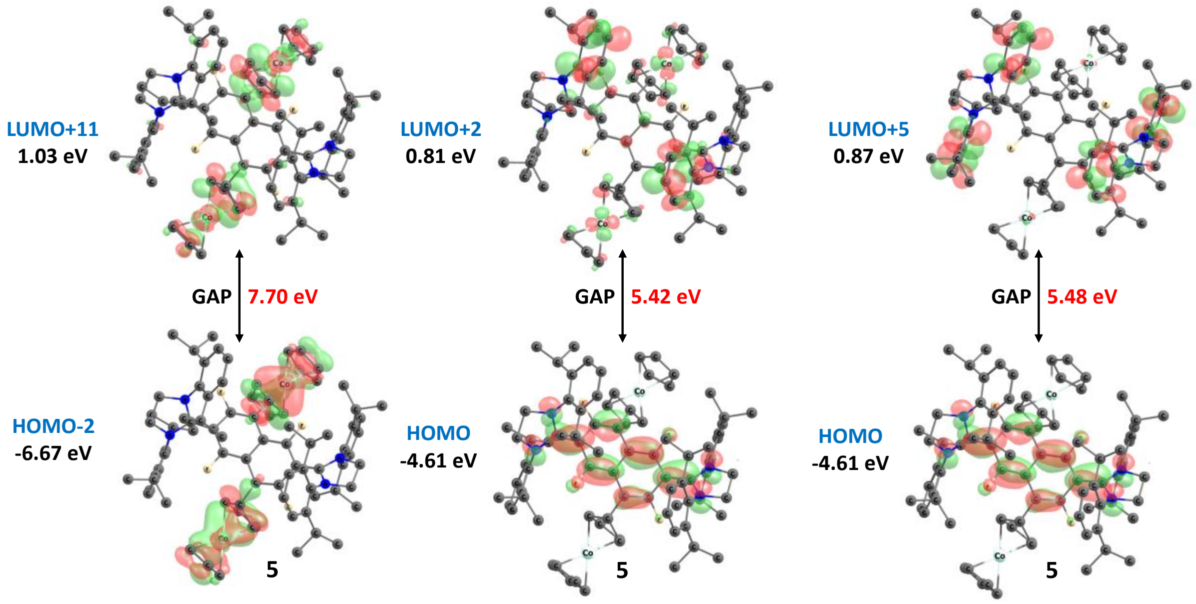

Figure S27: Frontier molecular orbitals of **5** involved in the UV-Vis transition with their respective energies, evaluated at the CAM-B3LYP/def2-SVP (CPCM =THF) level of theory. Hydrogen atoms have been omitted for clarity.

Optimized Cartesian Coordinates:

5 (Singlet)				5 (Triplet)			
Co	-1.57600200	-4.57726700	-2.69529400	Co	-1.99993100	-4.57686400	-2.46553500
F	2.01985400	-3.27477700	0.01115400	F	1.75425600	-3.41731700	-0.00006500
F	2.62633200	1.38029700	0.43523400	F	2.73954100	1.14552500	0.45400700
N	4.81857700	-0.48672300	0.59531500	N	4.83249200	-0.96882800	0.36462000
C	2.36230100	-0.97887500	0.43981200	C	2.28736300	-1.15753100	0.35228900
N	4.04540800	-2.30638600	1.67523300	N	3.88446500	-2.58913300	1.64338000
C	7.08688100	2.41839700	1.52606200	C	7.53540600	1.61917200	1.07215400
H	7.13469900	2.79852500	2.55990400	H	7.73045200	1.97146400	2.09862500
H	7.62992300	3.13193600	0.88441000	H	8.09058600	2.27775400	0.38372600
H	7.63442700	1.46395200	1.49034700	H	7.96083200	0.60861700	0.97328500
C	5.62330200	2.26619900	1.06769500	C	6.02621900	1.64393200	0.76306300
H	5.11907600	1.57015900	1.75299500	H	5.51657200	0.99786200	1.49100700
C	5.53312400	1.66049000	-0.33148400	C	5.72830600	1.07613600	-0.62347800
C	5.08466900	0.33197500	-0.55128000	C	5.10500200	-0.18864600	-0.79996400
C	3.67376000	-1.22959400	0.87330600	C	3.61577200	-1.54203200	0.75703900
C	1.78811400	0.32982700	0.23364100	C	1.83643800	0.16446100	0.21237100
C	0.45941400	0.57513000	-0.00563000	C	0.48638600	0.53231500	-0.00895600
C	3.24450000	-2.85951200	2.72987100	C	3.09738300	-2.92392800	2.79075500
C	2.75298600	-2.02567500	3.76923700	C	2.72597900	-1.93446100	3.74346100
C	3.11432000	-0.54623300	3.90177400	C	3.20641100	-0.48491700	3.67662300
H	3.66850800	-0.24221000	3.00619500	H	3.61458500	-0.30252800	2.67559100
C	4.05130800	-0.32149700	5.10508800	C	4.34796400	-0.24755500	4.68467700
H	3.55522900	-0.57182300	6.05694700	H	4.00268800	-0.38776400	5.72231000
H	4.36399800	0.73448200	5.15986500	H	4.73780100	0.78029600	4.59649400
H	4.95956000	-0.94171700	5.03451300	H	5.18592300	-0.94416700	4.52070200
C	4.85685900	-5.93434900	2.26612100	C	4.29632500	-6.23766200	2.55617800
H	5.62522000	-5.23918700	2.63783400	H	5.17781300	-5.62911200	2.81019300
H	5.31887300	-6.56395700	1.48751000	H	4.60959100	-6.99502300	1.81836100
H	4.57701300	-6.59298600	3.10507400	H	3.99082700	-6.77023200	3.47213200
C	3.62354000	-5.19544300	1.70933400	C	3.13986400	-5.38119700	2.00433800
H	3.94855700	-4.56802400	0.86798600	H	3.48668500	-4.88054100	1.09017000
C	2.60683700	-6.20533100	1.15255500	C	1.95747500	-6.27799800	1.60076100
H	1.70410300	-5.69607700	0.78885500	H	1.11164500	-5.67642400	1.23972000
H	2.30264200	-6.94569000	1.91013300	H	1.60235100	-6.89802700	2.43982100

H	3.04809100	-6.76542700	0.31200000	H	2.25827500	-6.96604300	0.79364800
C	3.02183500	-4.26039700	2.75511000	C	2.73567100	-4.28448400	2.98704600
C	4.88478600	3.61110600	1.18006500	C	5.46053800	3.05979900	0.96279200
H	3.84080300	3.52100200	0.84949000	H	4.38695600	3.09534800	0.72987200
H	5.37110500	4.39704100	0.57911700	H	5.97687400	3.80130900	0.33143500
H	4.88530700	3.95845300	2.22631300	H	5.59582700	3.37880100	2.00922300
C	5.91570700	2.42955800	-1.43760100	C	6.08905100	1.81191900	-1.75939100
H	6.27824600	3.44849900	-1.28286800	H	6.58179600	2.77971300	-1.63858300
C	5.83293600	1.92290300	-2.73329300	C	5.81896000	1.33810800	-3.04196500
H	6.13176700	2.53945600	-3.58503600	H	6.10316000	1.92750500	-3.91772700
C	5.37725900	0.62269900	-2.93569700	C	5.19625800	0.10203500	-3.20272300
H	5.32853700	0.22668400	-3.95271800	H	5.00607800	-0.27099900	-4.21142600
C	5.01529500	-0.20566800	-1.86165600	C	4.84632000	-0.69421000	-2.10148600
C	4.64691200	-1.65879800	-2.15634800	C	4.31178900	-2.10300500	-2.35253700
H	4.27692900	-2.11872500	-1.23216400	H	3.88177100	-2.48145800	-1.41686200
C	3.50712900	-1.78087100	-3.18083400	C	3.18518700	-2.14278600	-3.39666700
H	2.61335300	-1.23033700	-2.85171100	H	2.36061200	-1.46724700	-3.12333200
H	3.22100800	-2.83693300	-3.30544200	H	2.77251500	-3.16101800	-3.46803200
H	3.79943800	-1.39786400	-4.17248200	H	3.53828300	-1.86221600	-4.40254900
C	5.88510600	-2.46003400	-2.60209600	C	5.46056200	-3.05338300	-2.74367600
H	5.62539200	-3.52057600	-2.75512000	H	5.08684300	-4.08265300	-2.87305000
H	6.69087800	-2.41352400	-1.85156500	H	6.24946700	-3.07417700	-1.97463900
H	6.29647800	-2.07627700	-3.55015400	H	5.93170800	-2.74363000	-3.69121800
C	5.95434400	-1.00193800	1.37591400	C	5.93421400	-1.60588800	1.09891100
H	6.12163300	-0.40398000	2.29003200	H	6.26628100	-0.98984800	1.95484900
H	6.87288800	-0.97040300	0.77472000	H	6.79788000	-1.75998600	0.43636800
C	5.50771600	-2.42453700	1.71021400	C	5.30962400	-2.92202000	1.57202200
H	5.87125800	-3.15177500	0.96110400	H	5.49890600	-3.73616500	0.84729200
H	5.84323000	-2.75538000	2.70182300	H	5.68392900	-3.24058500	2.55370700
C	0.11679800	-1.92017100	-0.17019300	C	-0.04926100	-1.91121600	-0.14200600
C	1.43443500	-2.05527100	0.13727200	C	1.28367000	-2.15100800	0.08450900
C	-0.71469200	-3.06503000	-0.78990100	C	-1.00224200	-3.01528900	-0.66402000
H	-1.36160500	-3.49709500	-0.01016800	H	-1.69560300	-3.30140600	0.14042100
C	0.02623800	-4.17540400	-1.53917900	C	-0.38240800	-4.25966500	-1.30395700
H	0.61322300	-4.94946000	-1.04862500	H	0.10749600	-5.04938900	-0.73730700
C	-2.35492100	-5.83228400	-4.25143600	C	-2.87028700	-5.85749500	-3.94911400
H	-2.06802600	-5.78864600	-5.30121000	H	-2.55409200	-5.92413400	-4.98924800
C	-1.71887200	-6.60494500	-3.23937900	C	-2.34570600	-6.61383800	-2.86343200

H	-0.86967200	-7.27235700	-3.38096700	H	-1.57086000	-7.37671400	-2.92928700
C	-2.40138700	-6.36915300	-1.99718900	C	-3.02770300	-6.21333400	-1.66424100
H	-2.15988400	-6.82693400	-1.03918900	H	-2.85960500	-6.61984600	-0.66821200
C	-3.43254300	-5.42456000	-2.23914600	C	-3.94578700	-5.18701900	-2.00810600
H	-4.12009500	-5.01848500	-1.50098200	H	-4.60239600	-4.65529900	-1.32466100
C	-3.38742000	-5.07396300	-3.63178700	C	-3.83004500	-4.94986000	-3.42029600
H	-4.03905900	-4.35406100	-4.12447900	H	-4.38804400	-4.20406300	-3.98411400
C	0.22917100	-3.79397400	-2.90143200	C	-0.11750300	-4.01514500	-2.68723700
H	0.96170300	-4.20158600	-3.59841800	H	0.57365800	-4.55830500	-3.33183100
C	-0.78695900	-2.82686600	-3.20119600	C	-1.01571500	-2.97055800	-3.08706600
H	-0.97256300	-2.36092500	-4.16936300	H	-1.13400300	-2.56752400	-4.09315900
C	-1.55500200	-2.66549000	-2.00925900	C	-1.78019300	-2.63082800	-1.92981000
H	-2.44443900	-2.03936000	-1.94871500	H	-2.59516800	-1.90784500	-1.94064400
C	2.25766100	-4.79665300	3.80091000	C	1.99728900	-4.62673200	4.12825000
H	2.07521800	-5.87300100	3.83432300	H	1.71672200	-5.66986500	4.29184000
C	1.71730600	-3.98226200	4.79329300	C	1.59904100	-3.66165200	5.04985800
H	1.11075400	-4.41757300	5.59179200	H	1.01260400	-3.94635800	5.92732600
C	1.97075400	-2.61262000	4.77459700	C	1.96183400	-2.33112300	4.85024700
H	1.57308700	-1.98513500	5.57591300	H	1.66810600	-1.58237500	5.58946900
C	1.88347800	0.36912700	3.98018200	C	2.07661400	0.53856100	3.87315200
H	1.22594300	0.22758800	3.11094500	H	1.25029900	0.36354900	3.16876300
H	2.19267300	1.42647900	3.99946500	H	2.45274500	1.55952500	3.70103300
H	1.29113000	0.18206500	4.89022600	H	1.66176700	0.51093300	4.89374400
Co	1.57604400	4.57728600	-2.69525900	Co	1.99987300	4.57708200	-2.46524300
F	-2.01982700	3.27468200	0.01096200	F	-1.75433700	3.41738800	0.00019400
F	-2.62631100	-1.38037000	0.43522900	F	-2.73955400	-1.14549100	0.45396900
N	-4.81855600	0.48660400	0.59528200	N	-4.83249400	0.96867400	0.36467300
C	-2.36229100	0.97880300	0.43970900	C	-2.28740400	1.15757300	0.35240000
N	-4.04543600	2.30642400	1.67497300	N	-3.88465500	2.58912800	1.64338800
C	-7.08651900	-2.41852000	1.52643800	C	-7.53517200	-1.61996100	1.07202200
H	-7.13426900	-2.79851700	2.56033100	H	-7.73029200	-1.97217300	2.09850700
H	-7.62955800	-3.13216300	0.88489900	H	-8.08998000	-2.27884400	0.38358200
H	-7.63411100	-1.46410600	1.49063100	H	-7.96094300	-0.60957500	0.97292100
C	-5.62296900	-2.26632000	1.06797000	C	-6.02591500	-1.64422700	0.76322900
H	-5.11873000	-1.57017100	1.75315000	H	-5.51663400	-0.99788200	1.49118500
C	-5.53290700	-1.66077700	-0.33128400	C	-5.72793400	-1.07651200	-0.62333000
C	-5.08465100	-0.33221800	-0.55122700	C	-5.10483500	0.18836500	-0.79986400
C	-3.67375700	1.22954400	0.87317400	C	-3.61584400	1.54200400	0.75711200

C	-1.78809000	-0.32990700	0.23362200	C	-1.83646200	-0.16439800	0.21240500
C	-0.45938300	-0.57521800	-0.00560300	C	-0.48641700	-0.53222000	-0.00898800
C	-3.24454700	2.85973200	2.72952800	C	-3.09764300	2.92406100	2.79076900
C	-2.75298100	2.02605500	3.76899700	C	-2.72622400	1.93469200	3.74357100
C	-3.11421100	0.54660500	3.90170300	C	-3.20658900	0.48512100	3.67684300
H	-3.66844100	0.24246700	3.00618900	H	-3.61472700	0.30263000	2.67581400
C	-4.05110400	0.32191800	5.10510000	C	-4.34816100	0.24779400	4.68488300
H	-3.55497700	0.57235300	6.05690500	H	-4.00292100	0.38810500	5.72251500
H	-4.36373000	-0.73407400	5.15998700	H	-4.73795100	-0.78008100	4.59677500
H	-4.95939600	0.94208100	5.03453100	H	-5.18614500	0.94435700	4.52082600
C	-4.85705900	5.93444500	2.26538500	C	-4.29662700	6.23779600	2.55586500
H	-5.62539200	5.23930200	2.63719000	H	-5.17811900	5.62928600	2.80996100
H	-5.31909900	6.56393400	1.48669200	H	-4.60989200	6.99507100	1.81795900
H	-4.57723500	6.59320200	3.10425100	H	-3.99111600	6.77047400	3.47175200
C	-3.62371100	5.19551600	1.70869100	C	-3.14017700	5.38125400	2.00412000
H	-3.94870200	4.56797200	0.86742800	H	-3.48700500	4.88049500	1.09001000
C	-2.60705300	6.20537800	1.15177800	C	-1.95778200	6.27799600	1.60043100
H	-1.70427600	5.69612500	0.78818200	H	-1.11196300	5.67637000	1.23944900
H	-2.30292400	6.94587600	1.90924600	H	-1.60264200	6.89811600	2.43941600
H	-3.04832100	6.76531300	0.31112300	H	-2.25858300	6.96595200	0.79324300
C	-3.02195900	4.26063300	2.75458800	C	-2.73598900	4.28464900	2.98695000
C	-4.88440900	-3.61118400	1.18047300	C	-5.45977600	-3.05986800	0.96325500
H	-3.84048300	-3.52110500	0.84971400	H	-4.38612700	-3.09505900	0.73059000
H	-5.37081700	-4.39723000	0.57974200	H	-5.97570000	-3.80163800	0.33186600
H	-4.88476000	-3.95835000	2.22678000	H	-5.59519200	-3.37879300	2.00969300
C	-5.91543600	-2.43001300	-1.43730200	C	-6.08835700	-1.81249400	-1.75921700
H	-6.27770100	-3.44903900	-1.28248400	H	-6.58092500	-2.78037400	-1.63837600
C	-5.83293900	-1.92339900	-2.73302900	C	-5.81816000	-1.33877200	-3.04180200
H	-6.13185800	-2.54001600	-3.58469700	H	-6.10210500	-1.92832500	-3.91754200
C	-5.37748200	-0.62314000	-2.93558500	C	-5.19565700	-0.10260400	-3.20260300
H	-5.32896300	-0.22718400	-3.95263900	H	-5.00536900	0.27034100	-4.21131800
C	-5.01546500	0.20533600	-1.86164900	C	-4.84602700	0.69382300	-2.10140000
C	-4.64723100	1.65847300	-2.15649300	C	-4.31162000	2.10265700	-2.35250700
H	-4.27724900	2.11851900	-1.23236800	H	-3.88182600	2.48126000	-1.41678800
C	-3.50749800	1.78053800	-3.18103800	C	-3.18481800	2.14247100	-3.39642000
H	-2.61365800	1.23012200	-2.85189000	H	-2.36021500	1.46705900	-3.12285500
H	-3.22147700	2.83661200	-3.30577600	H	-2.77225600	3.16074700	-3.46780500
H	-3.79981400	1.39739000	-4.17263000	H	-3.53768100	1.86176000	-4.40234400

C	-5.88550600	2.45956500	-2.60226800
H	-5.62588300	3.52011400	-2.75540400
H	-6.69124500	2.41306200	-1.85170200
H	-6.29688600	2.07569100	-3.55027500
C	-5.95432900	1.00187400	1.37583500
H	-6.12158000	0.40402300	2.29003100
H	-6.87288200	0.97022900	0.77466100
C	-5.50774800	2.42453000	1.70994700
H	-5.87132000	3.15165700	0.96074200
H	-5.84326700	2.75549200	2.70151500
C	-0.11677000	1.92006900	-0.17030000
C	-1.43441500	2.05517800	0.13713400
C	0.71469200	3.06496500	-0.78998600
H	1.36142600	3.49719200	-0.01018800
C	-0.02629800	4.17516100	-1.53947600
H	-0.61350600	4.94916000	-1.04910400
C	2.35144300	5.83581500	-4.25031400
H	2.06155400	5.79513800	-5.29938200
C	1.71850900	6.60596600	-3.23434700
H	0.86911000	7.27400400	-3.37174700
C	2.40451400	6.36676000	-1.99471800
H	2.16599400	6.82214300	-1.03483400
C	3.43445100	5.42228100	-2.24220100
H	4.12381000	5.01378500	-1.50707500
C	3.38541300	5.07551600	-3.63566700
H	4.03547100	4.35677700	-4.13214300
C	-0.22890400	3.79362000	-2.90175500
H	-0.96137400	4.20105100	-3.59891400
C	0.78745500	2.82667400	-3.20125900
H	0.97337700	2.36072300	-4.16936100
C	1.55527800	2.66547600	-2.00917000
H	2.44480800	2.03950000	-1.94842100
C	-2.25781800	4.79706500	3.80032200
H	-2.07543800	5.87342800	3.83359800
C	-1.71741400	3.98283000	4.79280700
H	-1.11088700	4.41827700	5.59125100
C	-1.97077900	2.61317100	4.77428100
H	-1.57307100	1.98580700	5.57567200
C	-5.46043400	3.05285400	-2.74396300
H	-5.08681600	4.08215500	-2.87337300
H	-6.24948900	3.07363300	-1.97508000
H	-5.93136200	2.74294400	-3.69156300
C	-5.93430600	1.60569500	1.09886100
H	-6.26637400	0.98968000	1.95481600
H	-6.79794700	1.75968900	0.43626100
C	-5.30983700	2.92190000	1.57193900
H	-5.49914500	3.73599300	0.84715800
H	-5.68421800	3.24048600	2.55358900
C	0.04921000	1.91132400	-0.14184100
C	-1.28372900	2.15108000	0.08467900
C	1.00215700	3.01545700	-0.66378600
H	1.69543600	3.30162900	0.14070500
C	0.38228300	4.25978100	-1.30378200
H	-0.10772100	5.04947400	-0.73717500
C	2.87028100	5.85771400	-3.94879200
H	2.55419100	5.92427700	-4.98896300
C	2.34552600	6.61406900	-2.86320300
H	1.57062900	7.37688200	-2.92917800
C	3.02742600	6.21367500	-1.66392100
H	2.85918900	6.62022200	-0.66792800
C	3.94562600	5.18741400	-2.00763600
H	4.60220100	4.65577700	-1.32409500
C	3.83005200	4.95017800	-3.41982800
H	4.38816800	4.20439600	-3.98354900
C	0.11750000	4.01522600	-2.68707900
H	-0.57365500	4.55832800	-3.33172900
C	1.01581800	2.97070000	-3.08682900
H	1.13420900	2.56766300	-4.09290800
C	1.78023200	2.63103500	-1.92951100
H	2.59525600	1.90810500	-1.94027200
C	-1.99765200	4.62702700	4.12814500
H	-1.71712800	5.67018400	4.29165000
C	-1.59939500	3.66204400	5.04985200
H	-1.01299500	3.94685000	5.92731100
C	-1.96212900	2.33148200	4.85034600
H	-1.66839000	1.58281100	5.58964100

C	-1.88330200	-0.36866500	3.98011300	C	-2.07675300	-0.53829100	3.87349000
H	-1.22585100	-0.22718700	3.11080200	H	-1.25042800	-0.36330400	3.16910700
H	-2.19242400	-1.42603600	3.99954800	H	-2.45283500	-1.55928600	3.70144900
H	-1.29088600	-0.18145400	4.89008200	H	-1.66193300	-0.51055600	4.89409000

	5Me (Singlet)						
Co	-5.09678800	0.36047200	1.48318300	C	-0.71360300	-0.19298400	-0.81485100
F	-2.22063100	3.16479600	-0.81969600	C	-1.56796300	-5.89361900	-1.69719800
F	2.30466300	1.90050600	-1.17936400	H	-2.29452300	-5.88128600	-2.53345300
N	1.48147100	4.59796800	-1.03713800	H	-1.89191000	-6.66936300	-0.98595000
C	0.03655900	2.57802200	-1.14683200	C	-0.12989300	-6.11279600	-2.19640400
N	-0.38648700	4.75453000	-2.25082600	H	0.45516300	-6.75074000	-1.50348500
C	0.36150500	3.90756600	-1.45934300	C	1.73265400	-0.86846400	-0.68610100
C	1.00929900	1.51813700	-1.00059300	C	1.32613700	-2.14555700	-0.91511700
C	0.71360900	0.19295700	-0.81486000	C	3.14937100	-0.52399300	-0.18652200
C	1.56797500	5.89357800	-1.69724700	H	3.65320300	0.07169200	-0.96087400
H	2.29449800	5.88125300	-2.53353300	C	4.07435200	-1.64146800	0.29380000
H	1.89196300	6.66930500	-0.98599800	H	4.55055100	-2.35772400	-0.37540800
C	0.12988500	6.11277800	-2.19638700	C	6.76499400	-0.17017800	2.82458100
H	-0.45512900	6.75071800	-1.50343200	H	6.81976800	-0.58650600	3.82953100
H	0.09366600	6.58165100	-3.19232400	C	7.14161300	-0.83052900	1.62134200
C	-1.73264900	0.86843400	-0.68610000	H	7.55560400	-1.83523200	1.54459800
C	-1.32613900	2.14552700	-0.91511400	C	6.90695700	0.06494300	0.52212200
C	-3.14936200	0.52396400	-0.18652400	H	7.11058600	-0.14396600	-0.52694100
H	-3.65317300	-0.07176700	-0.96085000	C	6.34887000	1.25936500	1.04712400
C	-4.07436200	1.64145200	0.29372300	H	6.04643900	2.13442300	0.47392400
H	-4.55056800	2.35766200	-0.37553300	C	6.23920600	1.10390200	2.47191400
C	-6.76544000	0.17118800	2.82415200	H	5.83806600	1.84449900	3.16286800
H	-6.82062300	0.58841600	3.82870600	C	3.85769700	-1.89967900	1.68069100
C	-7.14165400	0.83044000	1.62017400	H	4.12679200	-2.80069900	2.23262500
H	-7.55569400	1.83504300	1.54238900	C	3.28756200	-0.70317900	2.22848000
C	-6.90654600	-0.06599400	0.52183300	H	3.03928600	-0.52528600	3.27534200
H	-7.10982400	0.14194300	-0.52749000	C	3.18871700	0.22655800	1.15013700
C	-6.34852500	-1.25987700	1.04813100	H	2.83211400	1.24901200	1.27068900
H	-6.04576700	-2.13541100	0.47582800	H	-0.09371100	-6.58165500	-3.19235000
C	-6.23943300	-1.10316300	2.47282700	C	2.23209000	4.32246200	0.16544100
H	-5.83849800	-1.84311800	3.16458600	H	1.72129800	3.54183700	0.74475700

C	-3.85772300	1.89974800	1.68060100	H	3.25784700	3.97616600	-0.04373600
H	-4.12682700	2.80079700	2.23248400	H	2.29138600	5.23249200	0.79035800
C	-3.28757500	0.70328800	2.22846300	C	-1.39145200	4.36209500	-3.20685200
H	-3.03930300	0.52545800	3.27533700	H	-1.32561900	3.27921200	-3.38246500
C	-3.18870800	-0.22651100	1.15017500	H	-2.41655600	4.58897600	-2.86706200
H	-2.83208200	-1.24895100	1.27078800	H	-1.21783300	4.88004600	-4.16698300
Co	5.09678100	-0.36042800	1.48319600	C	-2.23203800	-4.32252500	0.16552200
F	2.22061900	-3.16483800	-0.81972800	H	-1.72122500	-3.54191900	0.74484400
F	-2.30466800	-1.90053200	-1.17929100	H	-3.25779200	-3.97620900	-0.04363400
N	-1.48143900	-4.59802200	-1.03707000	H	-2.29133700	-5.23256700	0.79042000
C	-0.03656300	-2.57805000	-1.14681200	C	1.39141500	-4.36209500	-3.20688000
N	0.38645800	-4.75454000	-2.25084800	H	1.32557400	-3.27921200	-3.38248900
C	-0.36150900	-3.90759500	-1.45932600	H	2.41652200	-4.58897100	-2.86709800
C	-1.00929800	-1.51816400	-1.00056100	H	1.21779000	-4.88004300	-4.16701100

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