Trifluoromethylation for affecting the structural, electronic and redox properties of cobalt corroles.

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Supporting information

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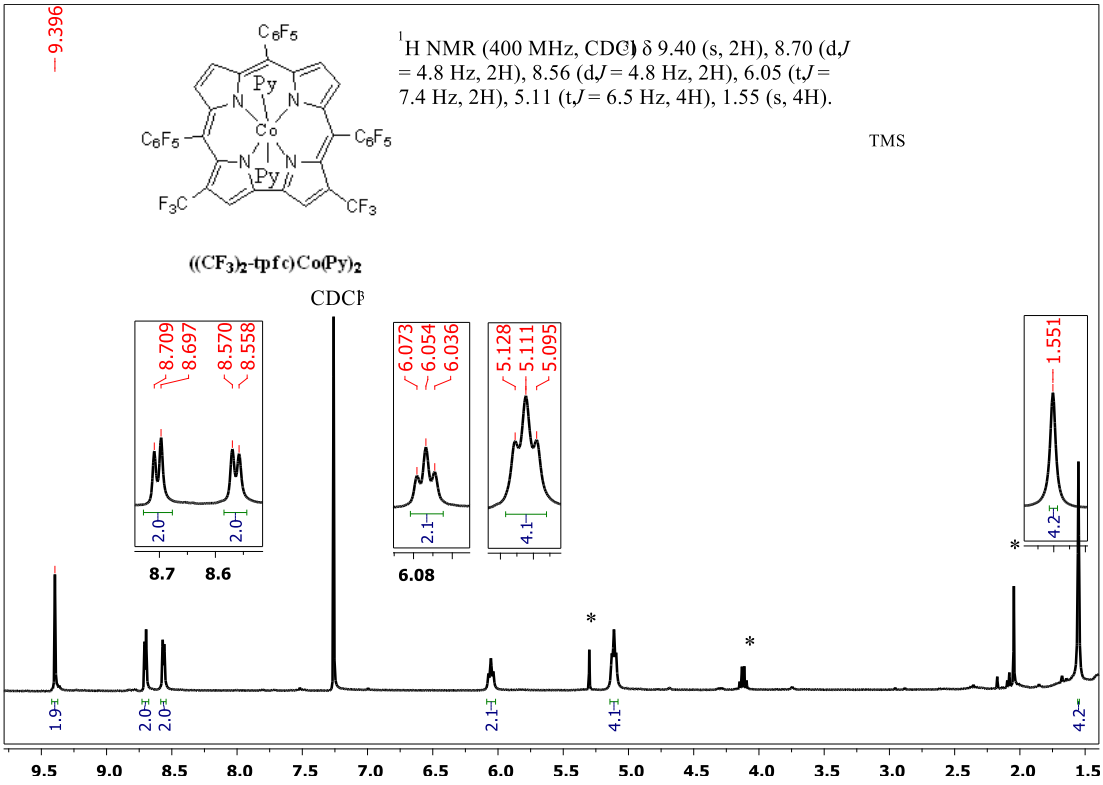


Fig. S1: ^{1}H NMR spectra of **((CF$_3$)$_2$-tpfc)Co(py)$_2$** recorded at 400 MHz in $CDCl_3$ and '*'indicates solvent impurities.

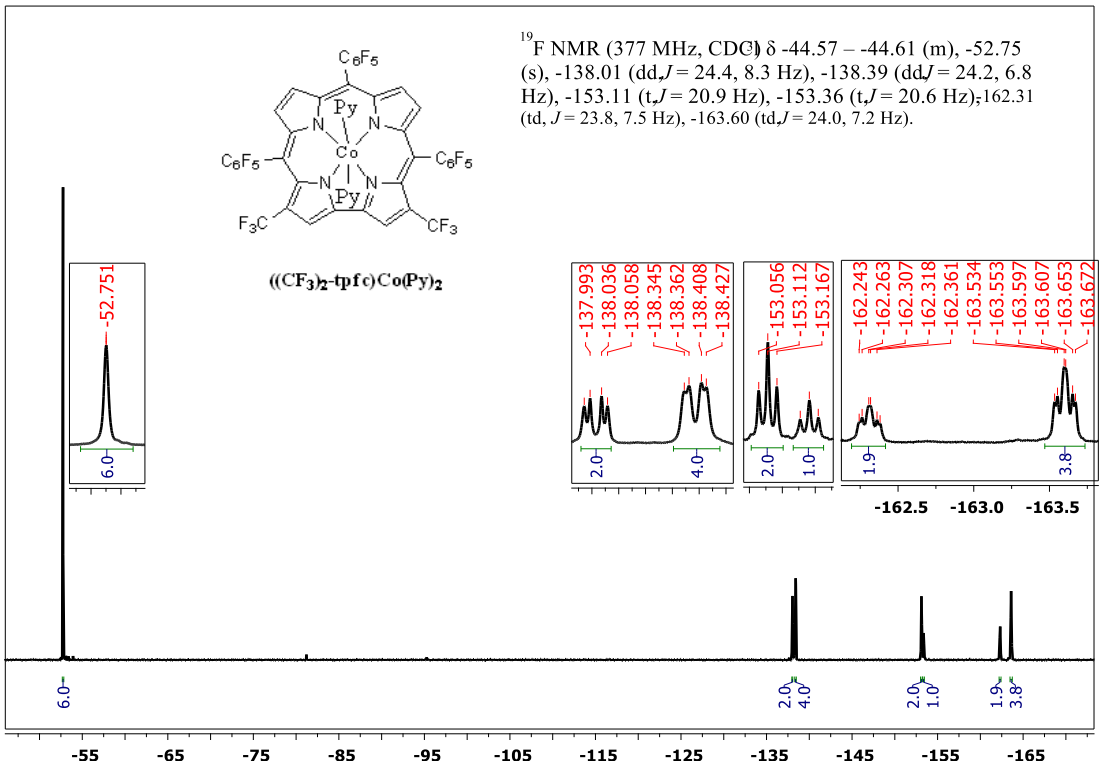


Fig. S2: ^{19}F NMR spectra of **((CF$_3$)$_3$-tpfc)Co(py)$_2$** recorded at 377 MHz in $CDCl_3$

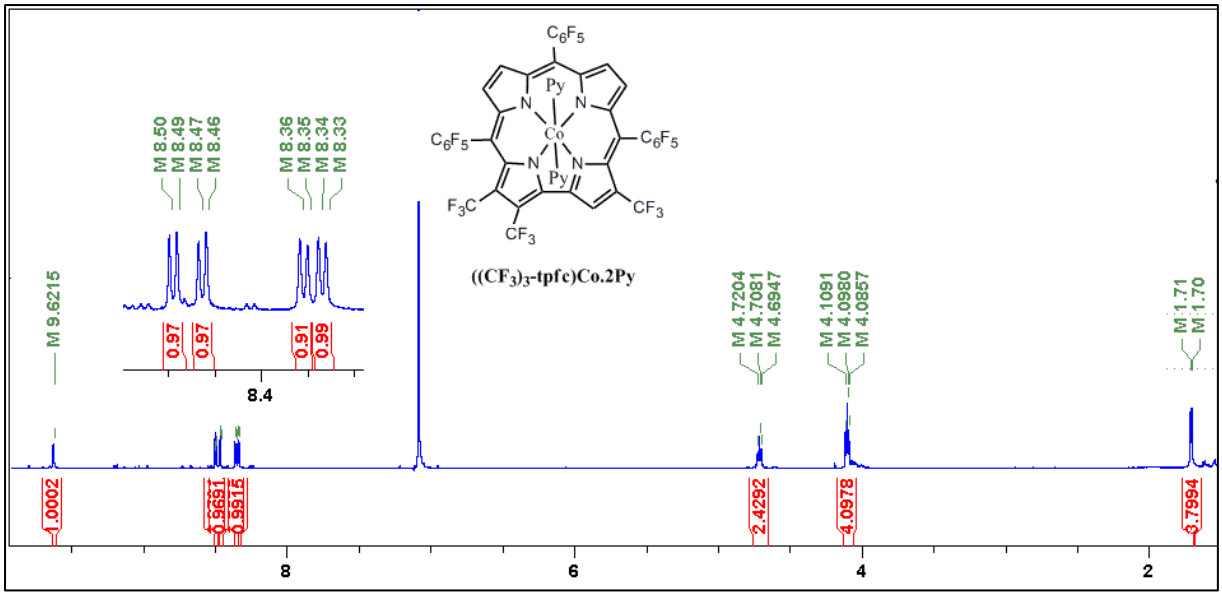
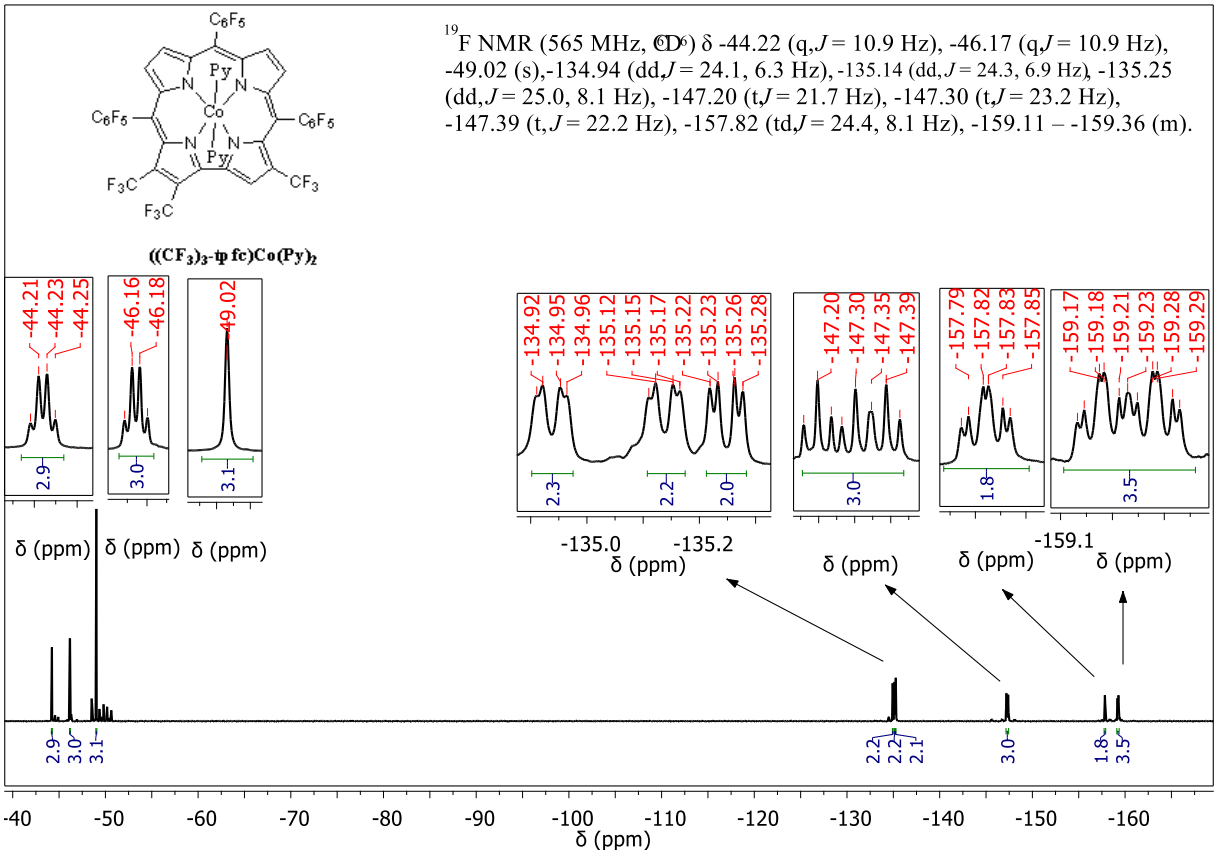


Fig. S3: ^{1}H NMR spectra of **((CF$_3$)$_3$-tpfc)Co(py)$_2$** recorded at 601MHz in C_6D_6 and '*'indicates solvent impurities.



^{19}F NMR (565 MHz, C_6D_6) δ -44.22 (q, J = 10.9 Hz), -46.17 (q, J = 10.9 Hz), -49.02 (s), -134.94 (dd, J = 24.1, 6.3 Hz), -135.14 (dd, J = 24.3, 6.9 Hz), -135.25 (dd, J = 25.0, 8.1 Hz), -147.20 (t, J = 21.7 Hz), -147.30 (t, J = 23.2 Hz), -147.39 (t, J = 22.2 Hz), -157.82 (td, J = 24.4, 8.1 Hz), -159.11 – -159.36 (m).

Fig. S4: ^{19}F NMR spectra of **((CF$_3$)$_3$-tpfc)Co(py)$_2$** recorded at 565 MHz in C_6D_6

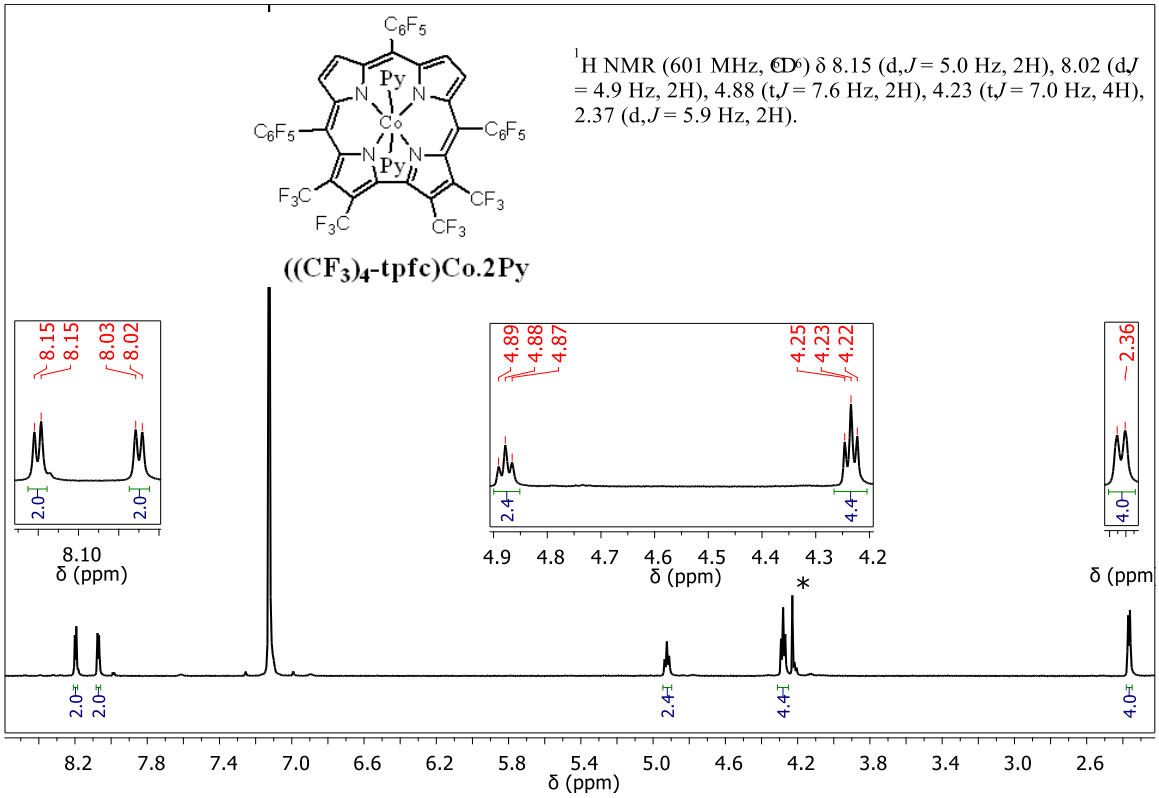


Fig. S5: ^{1}H NMR spectra of **((CF$_3$)$_4$-tpfc)Co(py)$_2$** recorded at 601 MHz in C_6D_6 and '*'indicates solvent impurities

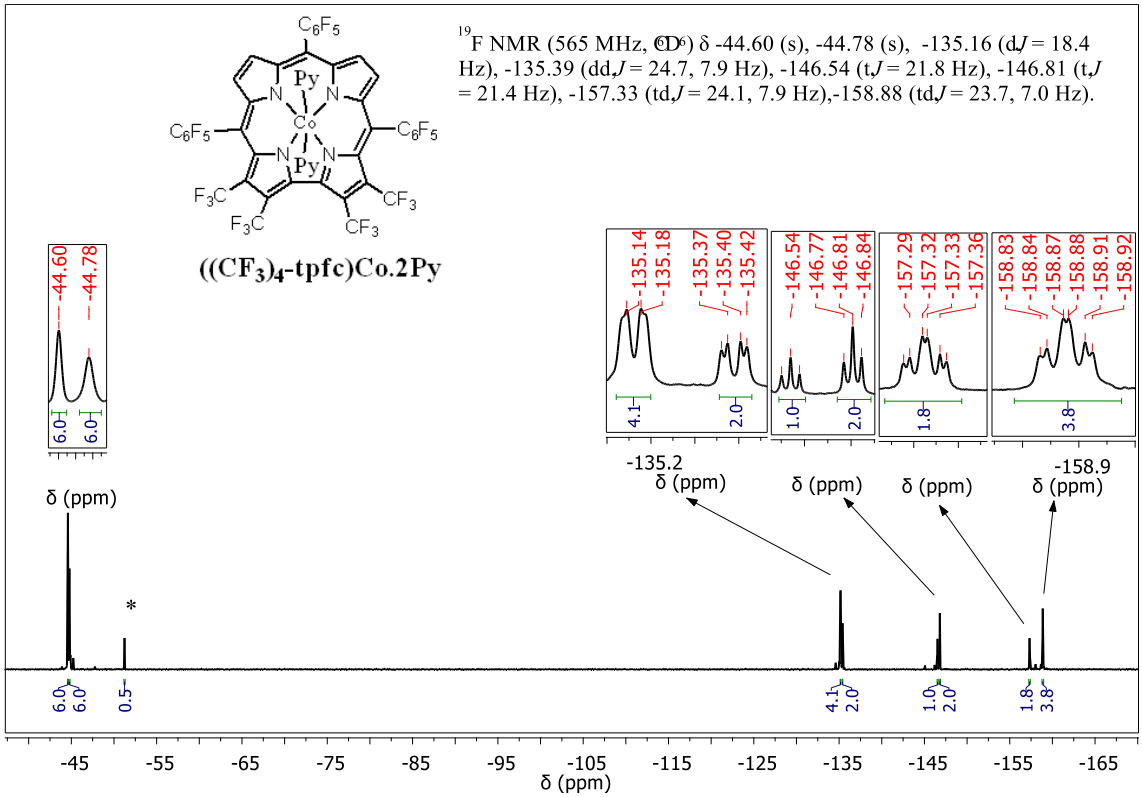


Fig. S6: ^{19}F NMR spectra of **((CF$_3$)$_4$-tpfc)Co(py)$_2$** recorded at 565 MHz in C_6D_6 and '*'indicates other compound impurities.

Compound Spectrum SmartFormula Report

Analysis Info

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Method	APCI_pos_SolidProbe.m	Operator	Larisa Panz
Sample Name	CoTPFC-2CF3 2py	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

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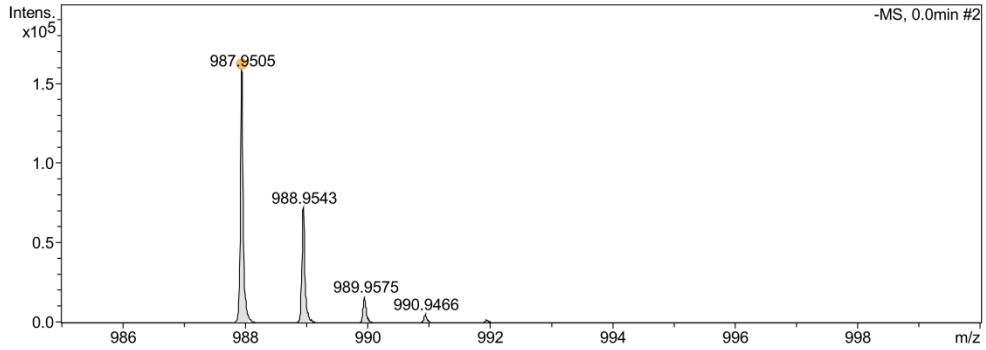
-MS, 0.0min #2



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968.9542	1	C35H3CoF21N4O2	968.9258	-29.3	29.3	1	100.00	26.0	odd		-	28.4	28.4
987.9505	1	C39H6CoF21N4	987.9595	9.1	16.6	1	100.00	28.5	even		-	9.0	9.0
	1	C35H6CoF21N4O3	987.9442	-6.4	35.4	1	100.00	24.5	even		-	6.3	6.3
	1	C35H6CoF21N4O3	987.9442	-6.4	35.4	1	100.00	24.5	even		-	6.3	6.3
1008.9344	1	C35H4CoF21N4NaO3	1008.9183	-15.9	422.5	1	100.00	25.0	odd		-	16.0	16.0
1022.9246	1	C35H6ClCoF21N4O3	1022.9131	-11.3	425.8	1	100.00	24.0	odd		-	11.6	11.6

Gr_4436n000001.d
Bruker Compass DataAnalysis 4.2 printed: 2/6/2017 5:59:48 PM by: Larisa Panz Page 1 of 1

Fig. S7: High resolution APCI mass spectra of **(((CF₃)₂-tpfc)Co(py)₂**.

Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Gross\Gr_4296p000002.d	Acquisition Date	1/12/2017 5:13:30 PM
Method	APCI_pos_SolidProbe.m	Operator	Larisa Panz
Sample Name	CoTPFC-3CF3	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

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Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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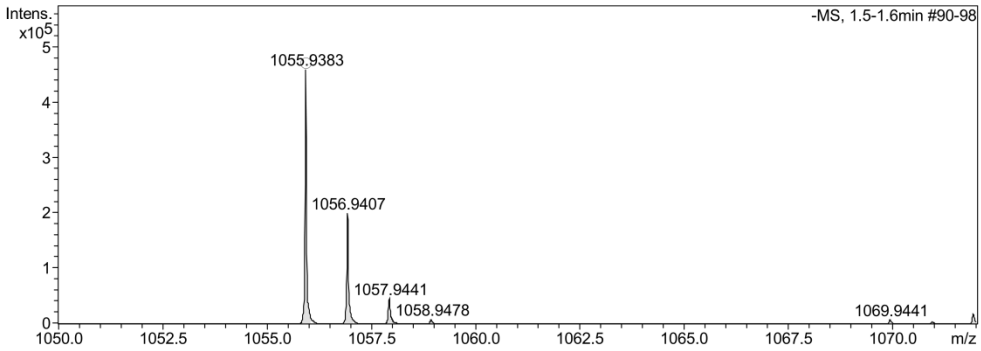

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
1055.9383	1	C40H5CoF24N4	1055.9463	7.6	7.1	1	25.10	28.5	even	-	8.0
	2	C36H5CoF24N4O3	1055.9310	-6.9	15.4	2	100.00	24.5	even	-	7.2
	3	C32H5CoF24N4O6	1055.9158	-21.3	36.9	3	0.00	20.5	even	-	22.5

Gr_4296p000002.d

Bruker Compass DataAnalysis 4.2 printed: 1/12/2017 5:17:08 PM by: Larisa Panz Page 1 of 1

Fig. S8: High resolution APCI mass spectra of **(((CF$_3$)$_3$-tpfc)Co(py)$_2$**.

Compound Spectrum SmartFormula Report

Analysis Info

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Comment			

Acquisition Parameter

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Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	200 °C

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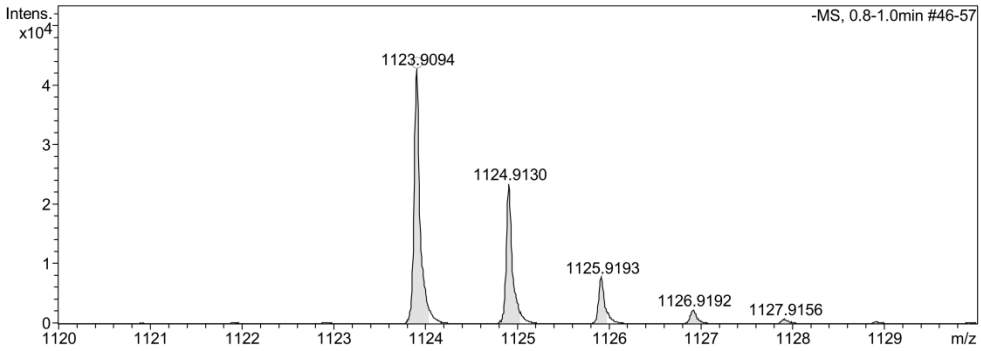


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
1123.9094	1	C41H4CoF27N4	1123.9337	21.6	63.7	1	100.00	28.5	even	-	24.3

Fig. S9: High resolution APCI mass spectra of **(($(CF_3)_4$-tpfc)Co(py)$_2$**

Table S1: ^{1}H NMR spectroscopy data of 6-coordinate CF_3-substituted cobalt(III)corroles

	^{1}H NMR chemical shift in δ ppm, spin multiplicity, (J_{H-H} coupling constant in Hz).								
	C_{18}-H	C_2-H	C_{12}-H	C_8-H	C_{13}-H	C_7-H	*para*-H_{py}	*meta*-H_{py}	*ortho*-H_{py}
[a]$((CF_3)_2$-tpfc)$(py)_2$	9.40 *s*		8.70 d, (4.8)		8.56 d, (4.8)		6.07 t	5.11 t	1.55 d
[b]$((CF_3)_3$-tpfc)$(py)_2$	9.62 *s*		8.49 d,(4.92)	8.46 d,(4.98)	8.33 d, (4.92)	8.35 d,(4.98)	4.70 t	4.09 t	1.75 d
[b]$((CF_3)_4$-tpfc)$(py)_2$			8.15 d, (4.9)		8.02 d, (4.9)		4.88 t	4.23 t	2.37 d

a = 400 MHz in $CDCl_3$; b = 600 MHz in C_6D_6

Table S2: ^{19}F NMR spectroscopy data of 6-coordinate CF_3-substituted cobalt(III)corroles

	^{19}F NMR chemical shift in δ ppm, spin multiplicity, (J_{F-F} coupling constant in Hz).											
	C_{18}- CF_3	C_2-CF_3	C_{17}- CF_3	C_3-CF_3	*Ortho*-F			para-F			meta-F	
a$((CF_3)_2$-tpfc)$(py)_2$			-52.75 s		-138.01 dd,(24.4, 8.3)		-138.39 dd,(24.4,6.8)	-153.11 t, (20.9)		-153.36 t, (20.6)	-162.31 td,(23.8, 7.5)	-163.60 td,(24.0, 7.2)
b$((CF_3)_3$-tpfc)$(py)_2$	-44.21 q, (10.9)		-46.17 q, (10.9)	-49.02 s	-134.94 dd,(24.1, 6.3)	-135.14 dd,(24.3, 6.9)	-135.25 dd,(25.0,8.1)	-147.20 t, (21.7)	-147.30 t, (23.2)	-147.39 t, (22.2)	-157.82 td,(24.4, 8.1)	-159.11 – -159.36 2td
b$((CF_3)_4$-tpfc)$(py)_2$	-44.60 s		-44.78 s		-135.16 dd, (18.4)		-135.39 dd,(24.7, 7.9)	-146.54 t, (21.8)		-146.81 t, (21.4)	-157.82 td,(24.1, 7.9)	-158.88 td,(23.7, 7.0)

a = 400 MHz in $CDCl_3$; b = 600 MHz in C_6D_6

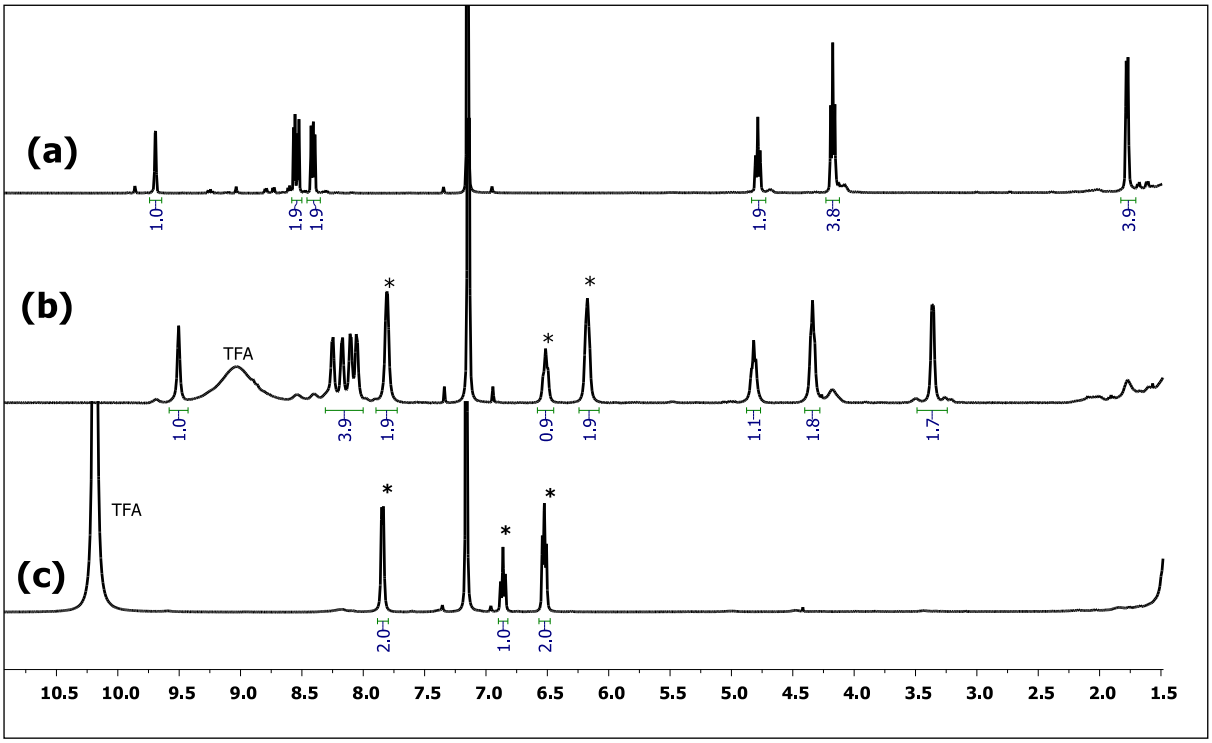


Fig. S10: ^{1}H NMR spectra of (a) **$((CF_3)_3$-tpfc)Co(py)$_2$** (5 x 10^{-5} M) (b) **$((CF_3)_3$-tpfc)Co(py)$_2$ + TFA** (20 mM)**,** (C) **pyridine** and **TFA**; were recorded at 400 MHz in C_6D_6. * indicates non-coordinated protonated pyridine species.

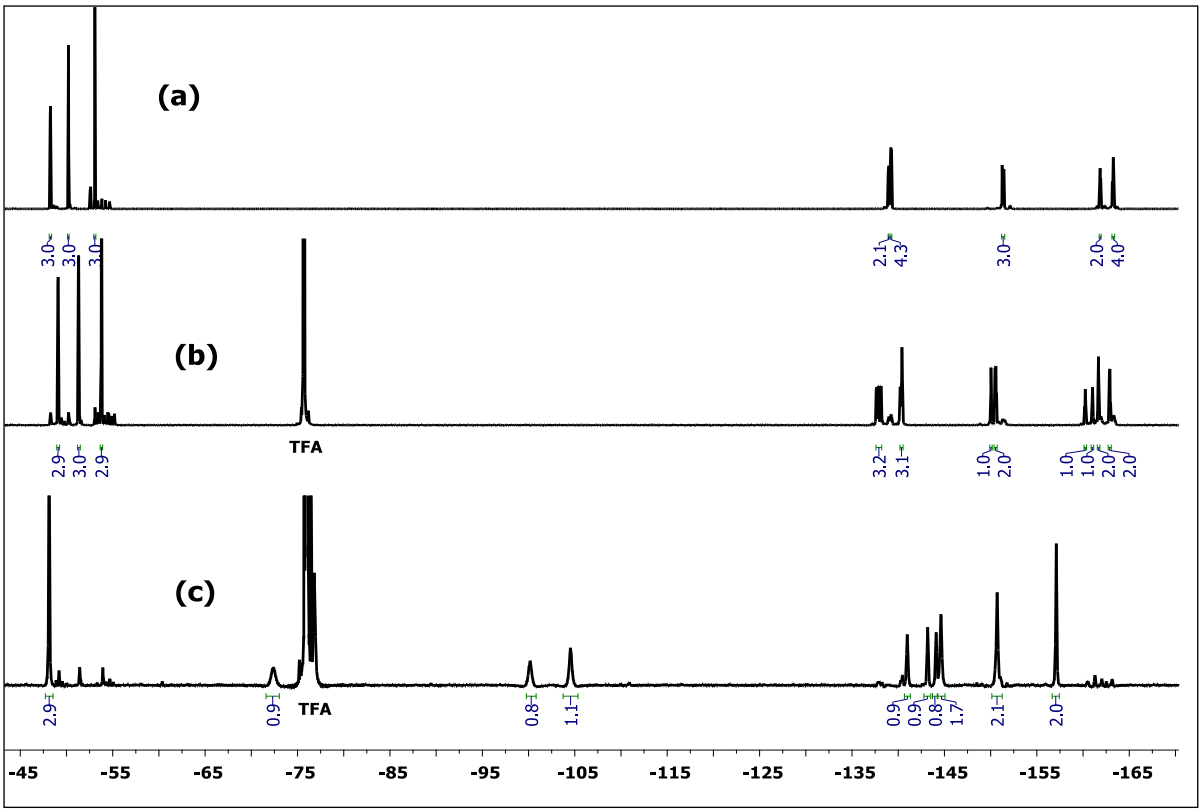


Fig. S11: ^{19}F NMR spectra of (a) **((CF$_3$)$_3$-tpfc)Co(py)$_2$** (5 x 10^{-5} M) (b) **((CF$_3$)$_3$-tpfc)Co(py)$_2$ + TFA** (20 mM), (C) **((CF$_3$)$_3$-tpfc)Co(py)$_2$** and **TFA** (100 mM) were recorded at 377 MHz in C_6D_6.

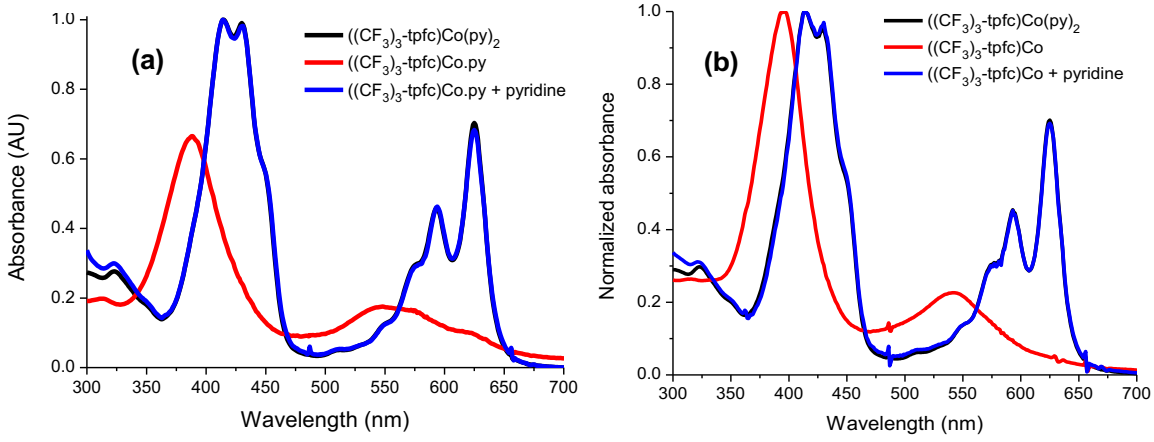


Fig. S12: Overlapped absorption spectra of mono-pyridine, without-pyridine complexes were regenerated to bis-pyridine complexes by addition of pyridine; a) from ((CF$_3$)$_3$-tpfc)Co.py to ((CF$_3$)$_3$-tpfc)Co(py)$_2$; b) from ((CF$_3$)$_3$-tpfc)Co to ((CF$_3$)$_3$-tpfc)Co(py)$_2$.

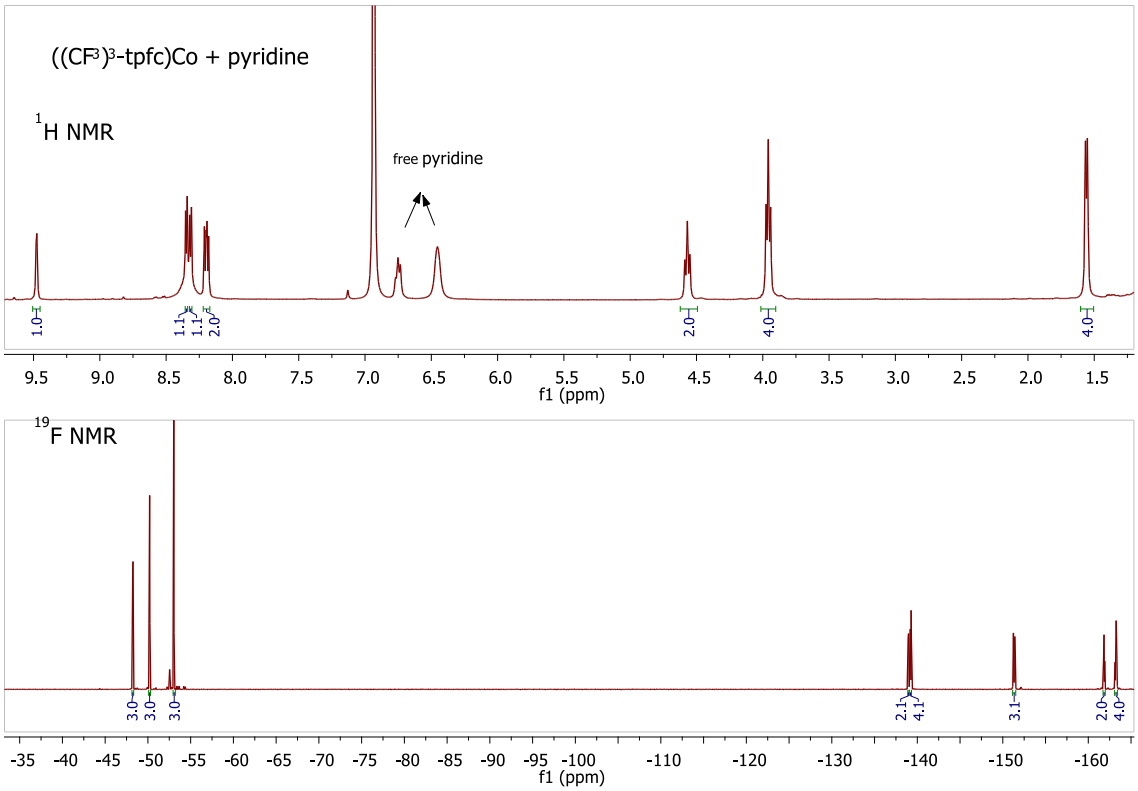


Fig. S13: ^{1}H & ^{19}F NMR spectra were recorded for $((CF_3)_3$-tpfc)Co treated with pyridine which results **$((CF_3)_3$-tpfc)Co(py)$_2$** was regenerated, at 400 MHz in C_6D_6 solvent.

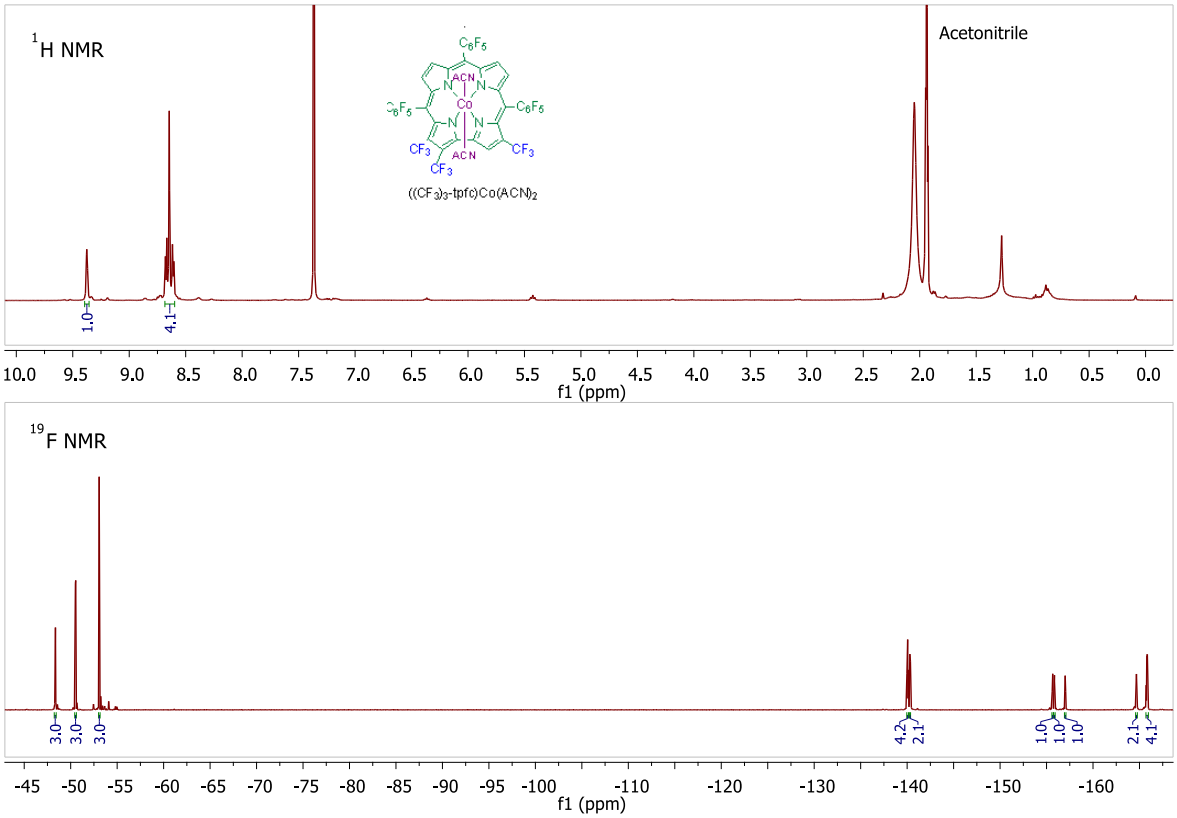


Fig. S14: ^{1}H NMR & ^{19}F NMR spectra of **$((CF_3)_3$-tpfc)Co** were recorded in acetonitrile-d_3 solvent at 400 MHz., which indicates formation of diamagnetic **$((CF_3)_3$-tpfc)Co$(CD_3CN)_2$**.

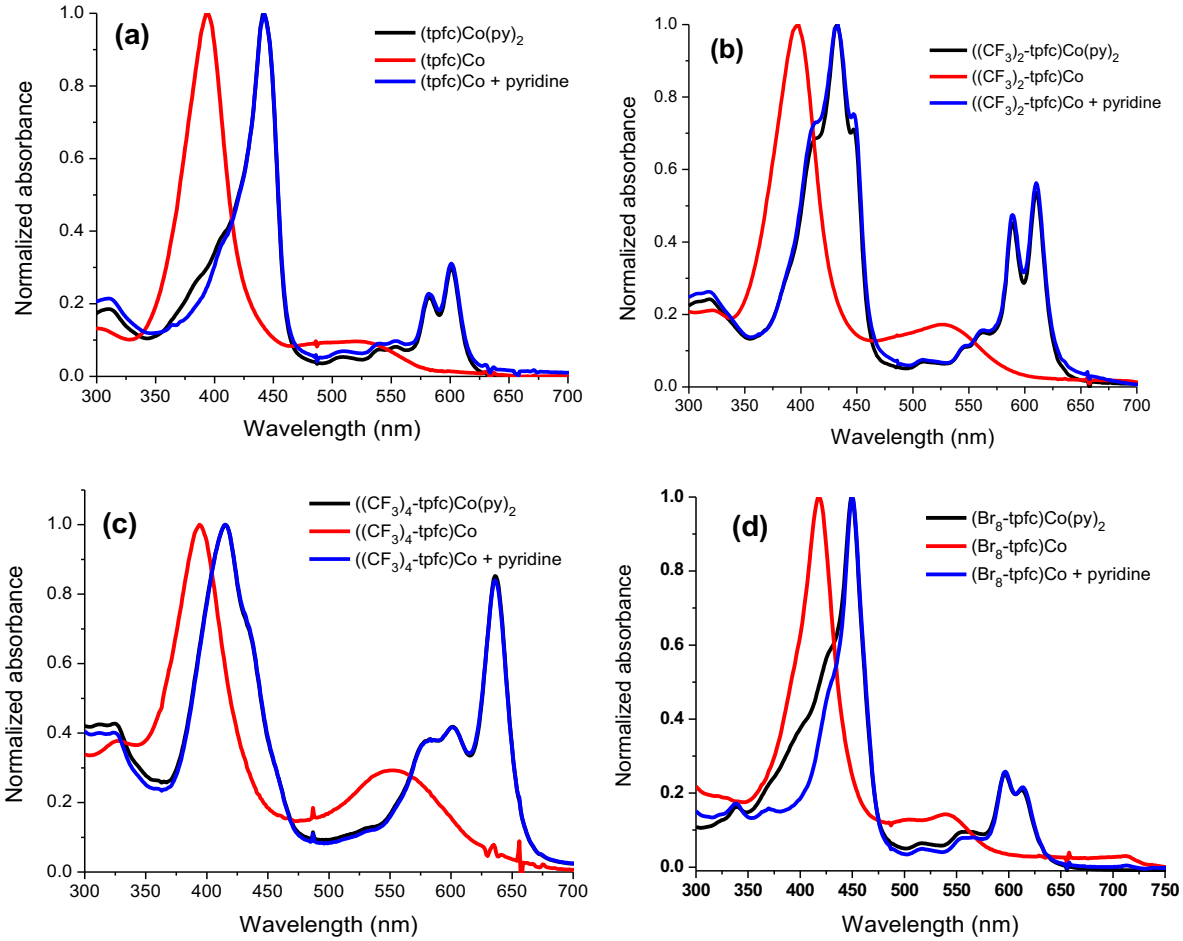
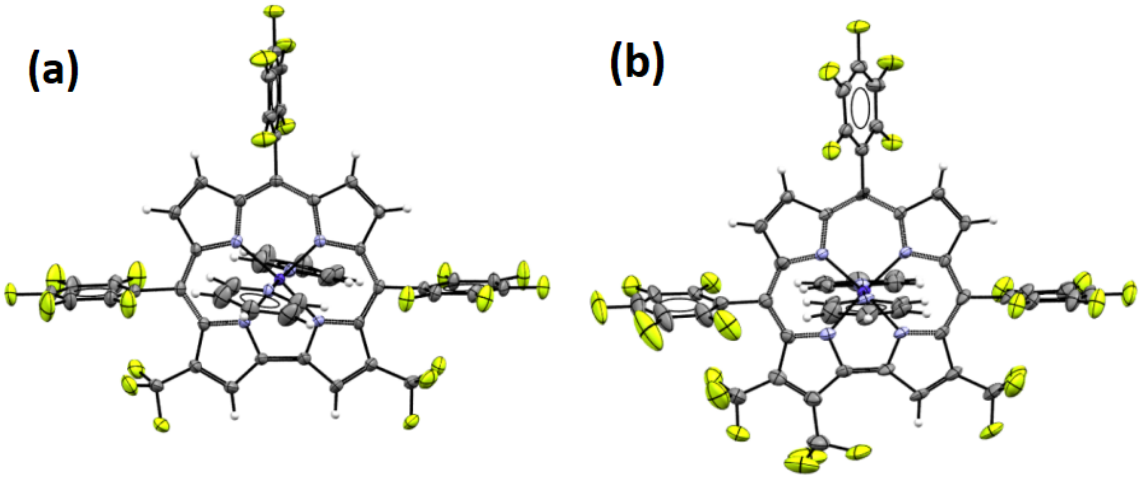


Fig. S15: Overlapped absorption spectra of bis-pyridine, non-pyridine and added pyridine to non-pyridine cobalt corroles; a) (tpfc)Co(py)$_2$, (tpfc)Co, (tpfc)Co with pyridine; b) ((CF$_3$)$_2$-tpfc)Co(py)$_2$, ((CF$_3$)$_2$-tpfc)Co, ((CF$_3$)$_2$-tpfc)Co with pyridine; c) ((CF$_3$)$_4$-tpfc)Co(py)$_2$, ((CF$_3$)$_4$-tpfc)Co, ((CF$_3$)$_4$-tpfc)Co with pyridine; d) (Br$_8$-tpfc)Co(py)$_2$, (Br$_8$-tpfc)Co, (Br$_8$-tpfc)Co with pyridine in toluene at RT.



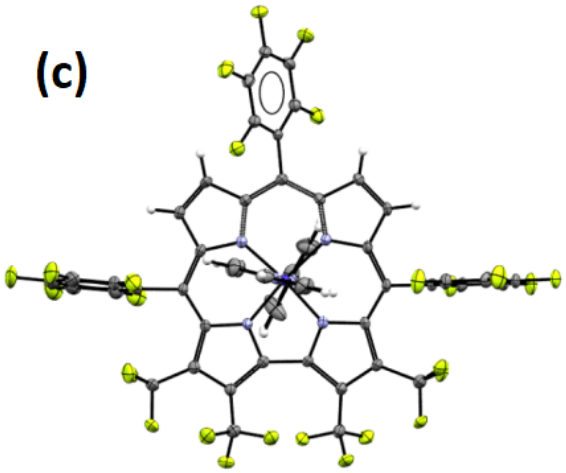


Fig. S16: ORTEP view of X-ray crystal structures of (a) $((CF_3)_2$-tpfc)Co(py)$_2$, (b) $((CF_3)_3$-tpfc)Co(py)$_2$, (c) $((CF_3)_4$-tpfc)Co(py)$_2$.

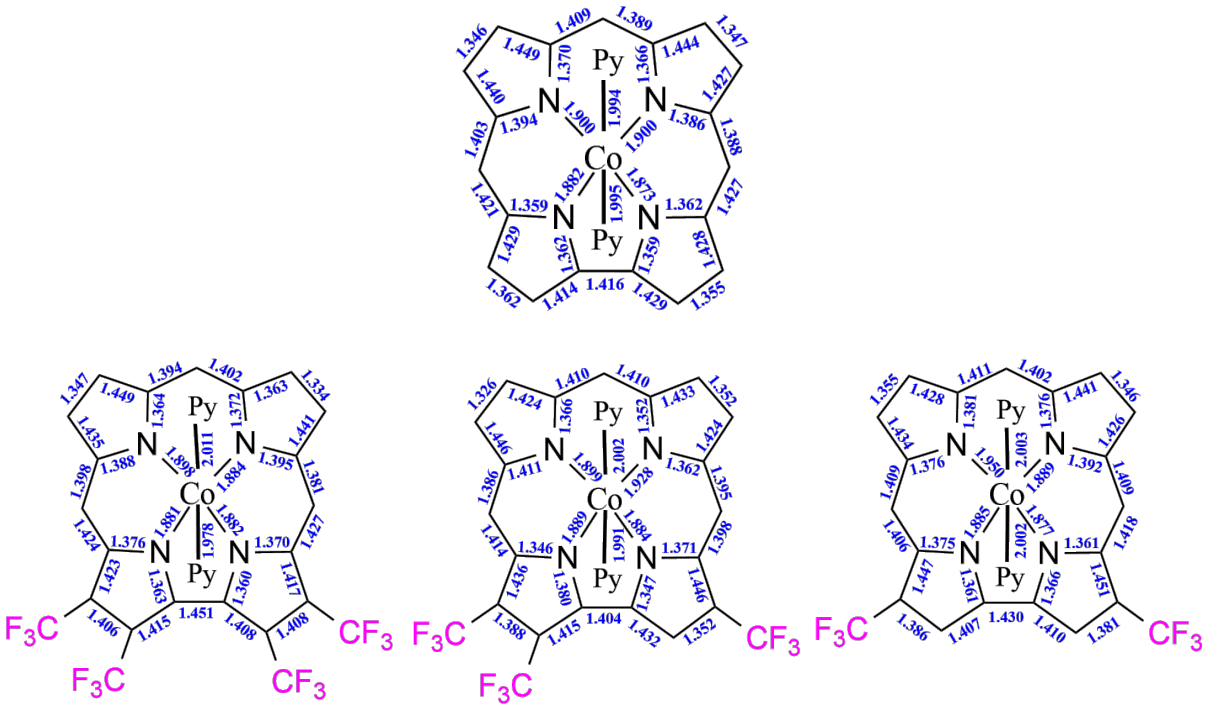
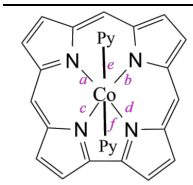


Fig. S17: Bond distances in Å units of 6-coordinated cobalt(III) corroles, from the X-ray crystal structures.

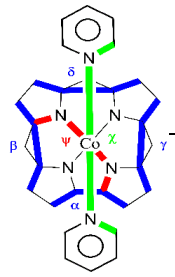
Table S3: X-ray structural bond length data.



	Co-N bond distance (Å)						
	a	*b*	*c*	*d*	*(a+b+c+d)/4*	*e*	*f*
[i](tpfc)Co(py)$_2$	1.900	1.900	1.882	1.873	1.885	1.994	1.995
$((CF_3)_2$-tpfc)Co(py)$_2$	1.950	1.889	1.885	1.877	1.900	2.003	2.002
$((CF_3)_3$-tpfc)Co(py)$_2$	1.899	1.928	1.889	1.884	1.900	2.002	1.991
$((CF_3)_4$-tpfc)Co(py)$_2$	1.898	1.884	1.881	1.882	1.886	2.011	1.978

i = X-ray data from reference 1.

Table S4: X-ray structural parameters and data relevant for appreciating deviation from planarity.



	Torsional Angle (degrees)						Mean plane deviation (Å)	
	Saddle				Ruffle	py-Co-py		
	α	β	γ	δ	ψ	χ	Average of 23 ring atoms	Cobalt
[i](tpfc)Co(py)$_2$	2.12	28.73	1.77	20.09	5.60	7.09	1.448	0.005
((CF$_3$)$_2$-tpfc)Co(py)$_2$	1.91	1.02	2.89	3.91	1.37	3.44	0.911	0.006
((CF$_3$)$_3$-tpfc)Co(py)$_2$	1.65	6.65	2.81	4.60	2.11	1.68	1.222	0.018
((CF$_3$)$_4$-tpfc)Co(py)$_2$	16.92	16.91	5.96	8.04	4.57	77.11	3.605	0.039

i = from reference 1

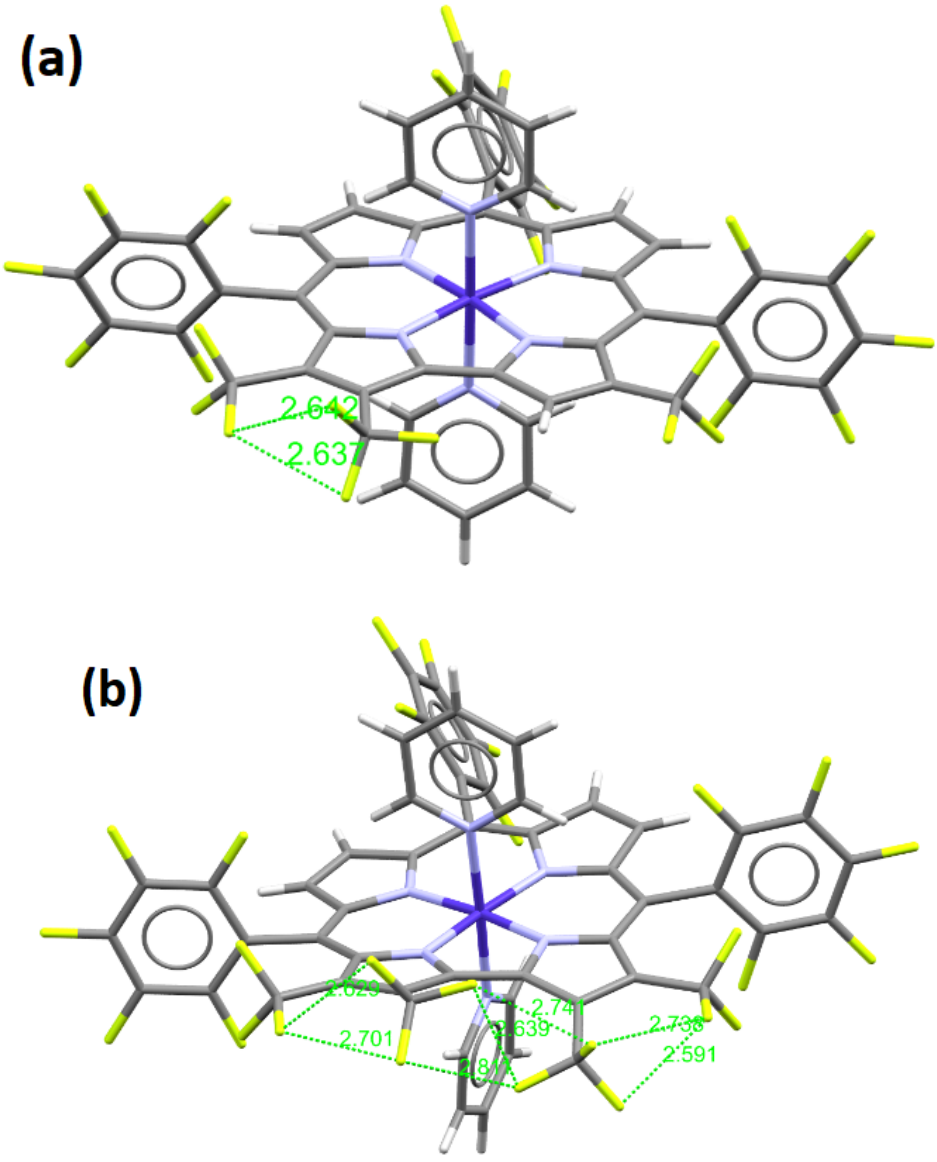


Fig. S18: Distance in Å between F···F atoms of (a) ((CF$_3$)$_3$-tpfc)Co(py)$_2$ and (b) ((CF$_3$)$_4$-tpfc)Co(py)$_2$ from X-ray crystal structures.

Table S5: X-ray crystal parameters of $((CF_3)_4$-tpfc)Co(py)$_2$, $((CF_3)_3$-tpfc)Co(py)$_2$ and $((CF_3)_2$-tpfc)Co(py)$_2$.

entry	**$((CF_3)_4$-tpfc)Co(py)$_2$**	**$((CF_3)_3$-tpfc)Co(py)$_2$**	**$((CF_3)_2$-tpfc)Co(py)$_2$**
CCDC number	1580471	1580472	1580473
Empirical formula	$C_{52}H_{16}Cl_2CoF_{27}N_6$	$C_{106}H_{40}Co_2F_{48}N_{12}$	$C_{55}H_{30}CoF_{21}N_6$
Formula weight	1367.54	2561.33	1232.78
Dimensions [mm]	0.24 x 0.18 x 0.15	0.27 x 0.24 x 0.15	0.33 x 0.18 x 0.12
Crystal system	Monoclinic	Monoclinic	Monoclinic
a [Å]	17.15 (3)	32.9730 (5)	14.295 (4)
b [Å]	22.56 (11)	17.0890 (4)	15.8010 (19)
c [Å]	25.63 (5)	23.2410 (5)	26.668 (3)
V [Å^3]	9925 (6)	10638.1(4)	5105.5 (17)
F(000)	5392.0	4984.0	2472.0
Space group	C 2/c	C 2	P 21/c
Z	8	4	4
M(Mo-K$_\alpha$) [mm^{-1}]	0.9050	0.9253	0.9370
R_1	0.0858	0.0984	0.0765
Reflections measured	8087	8181	7499
$2\theta_{max}$ [^{o}]	24	24	24
Temperature (K)	200 (2)	200 (2)	200 (2)

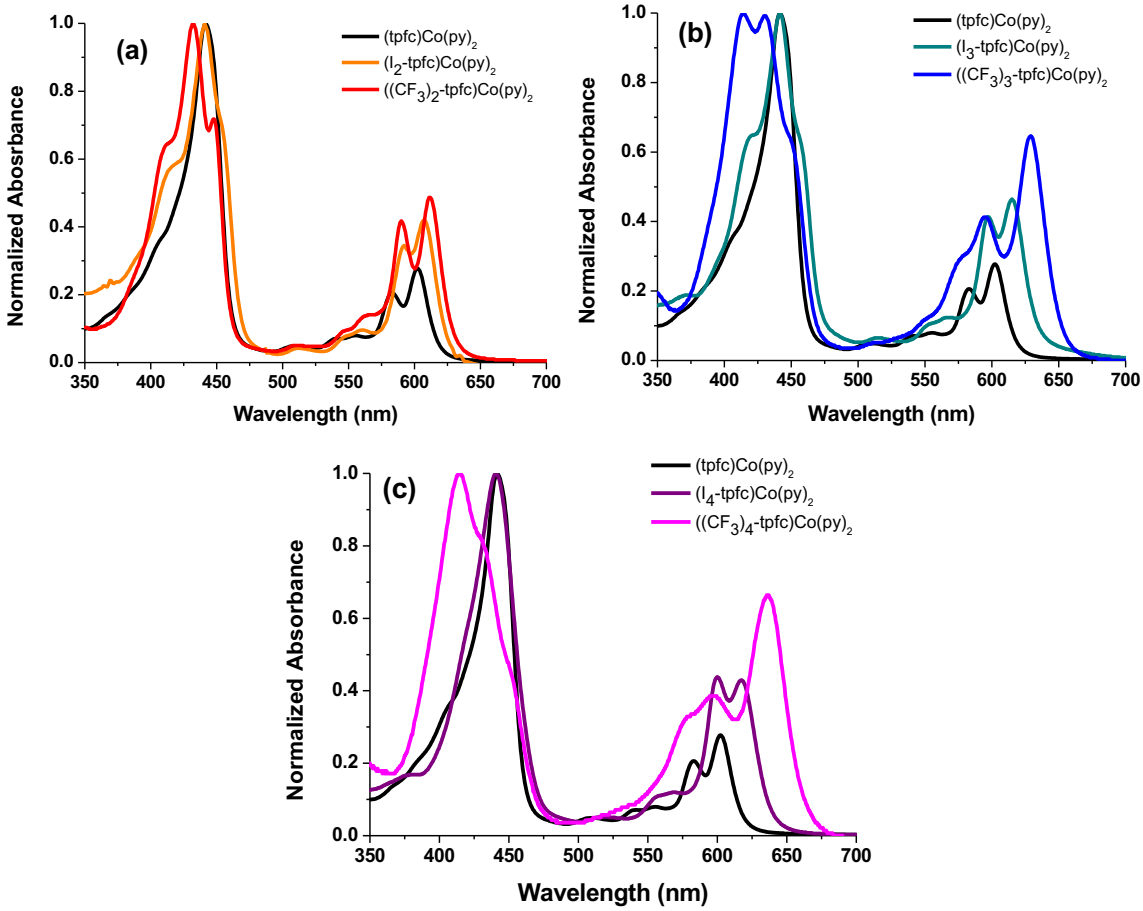


Fig. S19: Overlapped absorption spectra of bis-pyridine cobalt corroles: a) (tpfc)Co(py)$_2$, (I$_2$-tpfc)Co(py)$_2$, ((CF$_3$)$_2$-tpfc)Co(py)$_2$; b) (tpfc)Co(py)$_2$, (I$_3$-tpfc)Co(py)$_2$, ((CF$_3$)$_3$-tpfc)Co(py)$_2$; c) (tpfc)Co(py)$_2$, (I$_4$-tpfc)Co(py)$_2$, ((CF$_3$)$_4$-tpfc)Co(py)$_2$ in toluene at RT.

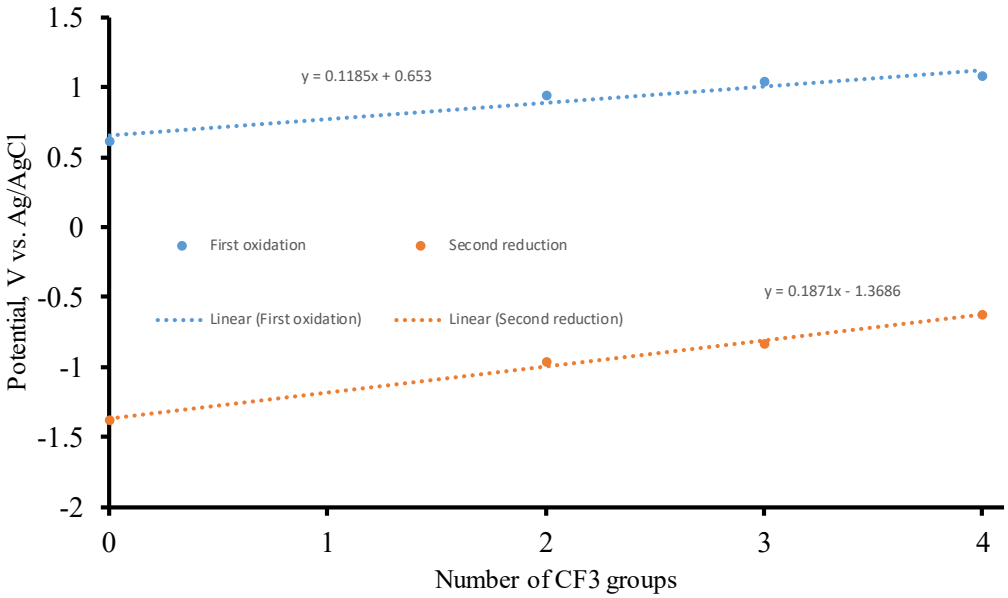


Fig. S20: Linear plot of half-wave potentials ($E_{1/2}$) of the first electron oxidation (blue) and the second electron reduction (red) of 6-coordinate cobalt(III)corrole bis-pyridine (0.1 M TBAP, glassy carbon, Ag/AgCl, Pt wire in Acetonitrile).

Table S6: Cartesian coordinates of (tpfc)Co and ($(CF_3)_2$-tpfc)Co by B3LYP/6-311G(d,p).

(tpfc)Co, neutral, triplet				($(CF_3)_2$-tpfc)Co, neutral, triplet			
	X	Y	Z		X	Y	Z
C	1.23317800	-1.60320800	-0.01820100	C	-1.22948900	-2.14777800	0.00848400
C	2.52875600	-2.21287400	-0.06337600	C	-2.52608400	-2.75516500	0.02962200
C	3.45881600	-1.21429800	-0.07195400	C	-3.45294400	-1.75550100	0.03339700
C	2.76510500	0.03605400	-0.03219400	C	-2.75686800	-0.50386500	0.01689700
N	1.38724300	-0.23232700	-0.00279800	N	-1.37947900	-0.77596900	0.00230300
H	2.71397400	-3.27492700	-0.09415400	C	3.45295600	-1.75547700	-0.03339600
H	4.53082400	-1.32585000	-0.11162000	C	2.75687200	-0.50384600	-0.01689500
H	-4.53082400	-1.32585000	0.11162000	C	2.52610400	-2.75514700	-0.02962000
C	-3.45881600	-1.21429900	0.07195400	N	1.37948500	-0.77595900	-0.00230000
C	-2.76510500	0.03605400	0.03219200	C	1.22950500	-2.14776900	-0.00848100
C	-2.52875600	-2.21287400	0.06337500	C	0.70278500	3.14386100	-0.00297200
N	-1.38724300	-0.23232700	0.00279500	C	1.75262900	4.07378100	-0.00538700
C	-1.23317800	-1.60320800	0.01820000	N	1.23803600	1.86814300	-0.00737200
H	-2.71397300	-3.27492700	0.09415400	C	2.93492900	3.34370100	-0.01110400
C	-0.70246200	3.70216200	0.00813300	C	2.60225200	1.94291700	-0.01249900
C	-1.78062700	4.61378100	0.00439900	C	-2.93495300	3.34367700	0.01110800
N	-1.21976000	2.41300800	0.02401200	C	-2.60226300	1.94289700	0.01250100
C	-2.94474700	3.85977900	0.01503600	C	-1.75265900	4.07376700	0.00538900
C	-2.57889200	2.47827300	0.02765200	N	-1.23804700	1.86813300	0.00737100
C	2.94474600	3.85977900	-0.01503400	C	-0.70280700	3.14385500	0.00297100
C	2.57889200	2.47827300	-0.02765500	C	0.00001500	-4.30518200	0.00000000
C	1.78062600	4.61378100	-0.00441100	C	0.28632400	-5.03320700	1.15561000
N	1.21976000	2.41300800	-0.02401600	C	-0.28628800	-5.03320700	-1.15561200
C	0.70246100	3.70216200	-0.00813900	C	0.29147400	-6.42282700	1.16755200
C	0.00000000	-3.75711500	0.00000000	C	-0.29142900	-6.42282600	-1.16755700
C	-0.30130300	-4.48622100	-1.15123400	C	0.00002500	-7.11863200	-0.00000400
C	0.30130400	-4.48622000	1.15123400	C	4.85510000	0.78545600	-0.03028400
C	-0.30668900	-5.87590400	-1.16310300	C	5.58746700	0.78023500	1.15537400
C	0.30669000	-5.87590400	1.16310300	C	5.56927700	0.79418900	-1.22695100
C	0.00000000	-6.57198700	0.00000000	C	6.97583900	0.78960000	1.15762100
C	-4.83696300	1.42372100	0.04608200	C	6.95744700	0.80347400	-1.25023200
C	-5.60726800	1.11364800	-1.07651800	C	7.66104000	0.80193600	-0.05158700
C	-5.51908500	1.87677300	1.17696700	C	-4.85510400	0.78543100	0.03028400
C	-6.99120600	1.23885800	-1.07734000	C	-5.58746900	0.78022500	-1.15537500

C	-6.90148200	2.01511600	1.19763900
C	-7.63945700	1.69292100	0.06502500
C	4.83696200	1.42372200	-0.04608200
C	5.60726600	1.11364900	1.07652000
C	5.51908800	1.87677300	-1.17696600
C	6.99120400	1.23885900	1.07734400
C	6.90148500	2.01511600	-1.19763500
C	7.63945700	1.69292200	-0.06502000
C	0.00000000	-2.26510100	-0.00000100
C	3.35322700	1.30215200	-0.03451700
C	-3.35322700	1.30215100	0.03451400
F	5.01542100	0.68288700	2.19725100
F	7.70053400	0.93408100	2.16801800
F	8.96695800	1.81972500	-0.07433800
F	7.52503200	2.44848400	-2.29729200
F	4.83961800	2.19042400	-2.28746800
F	-4.83961400	2.19042500	2.28746700
F	-7.52502800	2.44848500	2.29729600
F	-8.96695800	1.81972500	0.07434600
F	-7.70053800	0.93408000	-2.16801200
F	-5.01542600	0.68288600	-2.19725000
F	0.59894500	-3.84677000	2.28920800
F	0.59908100	-6.54589100	2.28208500
F	-0.59894400	-3.84677100	-2.28920900
F	-0.59908000	-6.54589200	-2.28208500
F	0.00000100	-7.90591500	0.00000000
H	-1.70567500	5.69011800	-0.00732500
H	1.70567400	5.69011800	0.00730800
H	3.95509200	4.23919700	-0.00824600
H	-3.95509300	4.23919600	0.00825200
Co	0.00000000	1.02630100	-0.00000200
C	-5.56928300	0.79415800	1.22695000
C	-6.97584100	0.78959400	-1.15762400
C	-6.95745200	0.80344600	1.25022900
C	-7.66104400	0.80192000	0.05158200
C	0.00001000	-2.81321100	0.00000100
C	-3.36328300	0.75238400	0.01897800
C	3.36327900	0.75240800	-0.01897700
F	-4.95030800	0.76900700	-2.33169500
F	-7.65451600	0.78777000	-2.30831400
F	-8.99399600	0.81131300	0.06184100
F	-7.61855800	0.81463700	2.41109800
F	-4.91414900	0.79598900	2.39356600
F	4.91414200	0.79603100	-2.39356600
F	7.61855100	0.81467200	-2.41110200
F	8.99399200	0.81132600	-0.06184700
F	7.65451600	0.78776300	2.30831000
F	4.95030700	0.76900600	2.33169400
F	-0.57031000	-4.39160900	-2.29576400
F	-0.56948500	-7.09210900	-2.28942300
F	0.57034100	-4.39161000	2.29576300
F	0.56953400	-7.09211100	2.28941600
F	0.00002900	-8.45144000	-0.00000500
Co	-0.00000100	0.47951700	0.00000000
H	-4.52529800	-1.86438700	0.04833700
H	-2.71284000	-3.81710600	0.04523900
H	2.71286800	-3.81708700	-0.04523700
H	4.52531200	-1.86435400	-0.04833600
C	-4.27599500	4.00213600	0.01403200
C	4.27596300	4.00217700	-0.01402500
F	-5.02096500	3.67216300	-1.06663400
F	-5.00922100	3.68610900	1.10694800
F	-4.15109500	5.34499300	0.00486200
F	4.15104300	5.34503200	-0.00484800
F	5.00919300	3.68616900	-1.10694300
F	5.02093700	3.67221200	1.06664100
H	1.66806800	5.14809000	-0.00292500
H	-1.66810700	5.14807700	0.00292800

Table S7: Cartesian coordinates of ((CF_3)$_3$-tpfc)Co and ((CF_3)$_4$-tpfc)Co by B3LYP/6-311G(d,p).

((CF_3)$_3$-tpfc)Co, neutral, triplet				((CF_3)$_4$-tpfc)Co, neutral, triplet			
	X	Y	Z		X	Y	Z
C	0.95835100	2.55778900	-0.00729200	C	0.95041100	2.57968400	0.00862100
C	2.21317100	3.24942300	0.03813600	C	2.20177200	3.29306100	0.07808100
C	3.20112000	2.31505300	0.04327600	C	3.19494400	2.36238900	0.08374100
C	2.58870600	1.01690700	-0.00571700	C	2.57691600	1.05753900	0.00954700
N	1.19675000	1.19771700	-0.03187900	N	1.20034900	1.22757200	-0.02684000
C	-3.68086200	1.86220600	-0.05043400	C	-3.70965500	1.85619300	-0.05064900
C	-2.90359200	0.66064000	-0.02194300	C	-2.90648200	0.66095600	-0.01958100
C	-2.82143500	2.92026000	-0.05274500	C	-2.86124000	2.92510400	-0.05186800
N	-1.54650300	1.02037600	-0.00793400	N	-1.56886600	1.02757600	-0.00137900
C	-1.48932800	2.39777300	-0.02453600	C	-1.52144100	2.40052700	-0.01591300
C	-0.62201100	-2.86122100	0.02361700	C	-0.60763100	-2.85622400	0.00677600
C	-1.62384600	-3.84511300	0.02385600	C	-1.60380500	-3.86111800	-0.00651600
N	-1.23021800	-1.61659600	0.01122600	N	-1.21537800	-1.62717900	0.00834400
C	-2.84308000	-3.18256200	0.01260100	C	-2.82949400	-3.21291900	-0.01154700
C	-2.58916000	-1.76914700	0.00470000	C	-2.57434100	-1.78927400	-0.00277300
C	3.04837200	-2.79995400	-0.10384500	C	3.07477200	-2.78022300	-0.14223300
C	2.60468600	-1.43911800	-0.05353500	C	2.61063900	-1.41902200	-0.06571300
C	1.91312800	-3.62501800	-0.03772500	C	1.94351200	-3.61003100	-0.07240100
N	1.23870400	-1.46509400	-0.00166700	N	1.24459500	-1.45525900	-0.00989000
C	0.79165800	-2.77347600	0.00855800	C	0.81305700	-2.75604000	-0.01304100
C	-0.40459100	4.63319900	-0.00356500	C	-0.43804300	4.63737300	0.00948100

C	-0.76151800	5.33037100	1.15160600	C	-0.95518600	5.33419000	1.10913200
C	-0.14633000	5.38851600	-1.14836000	C	-0.02856600	5.41445700	-1.08173900
C	-0.86184900	6.71612900	1.17324800	C	-1.06779200	6.72253200	1.12615500
C	-0.23574700	6.77530100	-1.15030000	C	-0.11925400	6.80456000	-1.08310400
C	-0.59626700	7.43979800	0.01636400	C	-0.64450900	7.46142700	0.02549700
C	-4.91166500	-0.75951700	-0.02406800	C	-4.89627300	-0.79355800	-0.02573500
C	-5.64241100	-0.79843700	1.16170700	C	-5.63197700	-0.86063000	1.15989600
C	-5.62286500	-0.81096100	-1.22122700	C	-5.61779900	-0.83017900	-1.22146600
C	-7.02755500	-0.89262300	1.16352200	C	-7.02061300	-0.96132100	1.16346900
C	-7.00775200	-0.90495200	-1.24481700	C	-7.00622500	-0.92995000	-1.24416700
C	-7.71029000	-0.94635500	-0.04607900	C	-7.70902700	-0.99643300	-0.04511700
C	4.76837600	-0.08990700	0.05588100	C	4.75803300	-0.06518700	0.08533000
C	5.54596600	0.17884300	-1.06914900	C	5.54824300	0.35827300	-0.98800600
C	5.42645300	-0.20637800	1.27844900	C	5.42255100	-0.35381800	1.28020000
C	6.92463800	0.31659400	-0.98941400	C	6.92984000	0.48685400	-0.88553000
C	6.80443900	-0.07231800	1.38409400	C	6.80479500	-0.23904200	1.40591500
C	7.55426200	0.18919700	0.24382200	C	7.56061400	0.18333300	0.31775300
C	-0.30670900	3.14492500	-0.01394700	C	-0.33065300	3.15117100	-0.00067200
C	3.28095100	-0.18890100	-0.02365900	C	3.27232600	-0.16046200	-0.01801800
C	-3.42491800	-0.63080600	-0.01243900	C	-3.40908100	-0.65146200	-0.01468300
F	4.96277500	0.30505200	-2.26650300	F	4.98074500	0.65239900	-2.16547300
F	7.64827200	0.56759200	-2.08389100	F	7.65966600	0.89393800	-1.93657600
F	8.87757900	0.31958700	0.33228200	F	8.89147800	0.30259400	0.42772900
F	7.41078400	-0.18983400	2.56814700	F	7.41093900	-0.52280600	2.56901000
F	4.72415400	-0.45219400	2.39062700	F	4.72993700	-0.74881100	2.35555600
F	-4.96736800	-0.77126300	-2.38687500	F	-4.97711700	-0.76538400	-2.39518700
F	-7.66643100	-0.95582000	-2.40553400	F	-7.67101700	-0.96147800	-2.40990500
F	-9.03975000	-1.03686200	-0.05671300	F	-9.04618500	-1.09109500	-0.05453000
F	-7.70507100	-0.93199400	2.31371700	F	-7.69908600	-1.02284000	2.31998700
F	-5.00622700	-0.74715100	2.33730500	F	-5.00554600	-0.82566900	2.34226000
F	0.20223900	4.77680400	-2.28694300	F	0.46897900	4.82650200	-2.17819900
F	0.01705600	7.47112800	-2.26144200	F	0.28233200	7.51376700	-2.14915200
F	-1.02225700	4.66070300	2.28114100	F	-1.36089800	4.66776800	2.19863500
F	-1.20624300	7.35516600	2.29387400	F	-1.56631000	7.35389900	2.20027800
F	-0.68718100	8.76899200	0.02594500	F	-0.74199000	8.79822000	0.03336000
Co	-0.08917100	-0.15025800	-0.00670200	Co	-0.08868900	-0.14440500	-0.00307500
H	4.26295100	2.49465900	0.07834300	H	4.25775700	2.54634900	0.14046100
H	2.32870000	4.32100200	0.07087300	H	2.30944200	4.36687900	0.13141400
H	-3.07590900	3.96770200	-0.07822500	H	-3.12484600	3.97234200	-0.08427900
H	-4.75795100	1.89915900	-0.06848600	H	-4.78982600	1.87953200	-0.07316500
C	4.46577600	-3.26903800	-0.27436500	C	4.47985000	-3.24691300	-0.32692100
C	1.86431300	-5.12625000	0.00637600	C	1.90866800	-5.10260900	-0.05513800
C	-4.14426200	-3.91946700	0.00940600	C	-4.11982100	-3.94684900	-0.02521000
F	5.07408900	-2.62734400	-1.29948900	F	5.14067400	-2.51598400	-1.26486500
F	5.21568100	-3.05314200	0.83088700	F	5.22568900	-3.17072000	0.81025400
F	4.54542200	-4.57796500	-0.54849500	F	4.55503300	-4.52870000	-0.74197000
F	2.67790000	-5.63226900	0.94975200	F	2.79682200	-5.63217000	0.81950900
F	0.61586700	-5.55633200	0.31064500	F	0.69028800	-5.56599800	0.32594800
F	2.18828700	-5.69322000	-1.16968700	F	2.16442300	-5.66079000	-1.26302500
F	-3.94128600	-5.25082300	0.02112300	F	-3.92733200	-5.28725800	-0.03572200
F	-4.89229900	-3.64729400	-1.08534600	F	-4.88846000	-3.66464400	-1.11414900
F	-4.90772700	-3.63029500	1.08886300	F	-4.90058800	-3.68334700	1.05986100
H	-1.48363400	-4.90979400	0.02934900	H	-1.44734100	-4.92583200	-0.01686900

References

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