Supporting Information for Fluorinated Click-Derived Tripodal Ligands Drive Spin Crossover in both Iron(II) and Cobalt(II) Complexes

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Content

Magnetometric Measurements

Figure S 1: Preperation of the samples. Top: compound in eicosan-matrix in plastic capsule. Bottom: compound ground and pressed into a pellet.

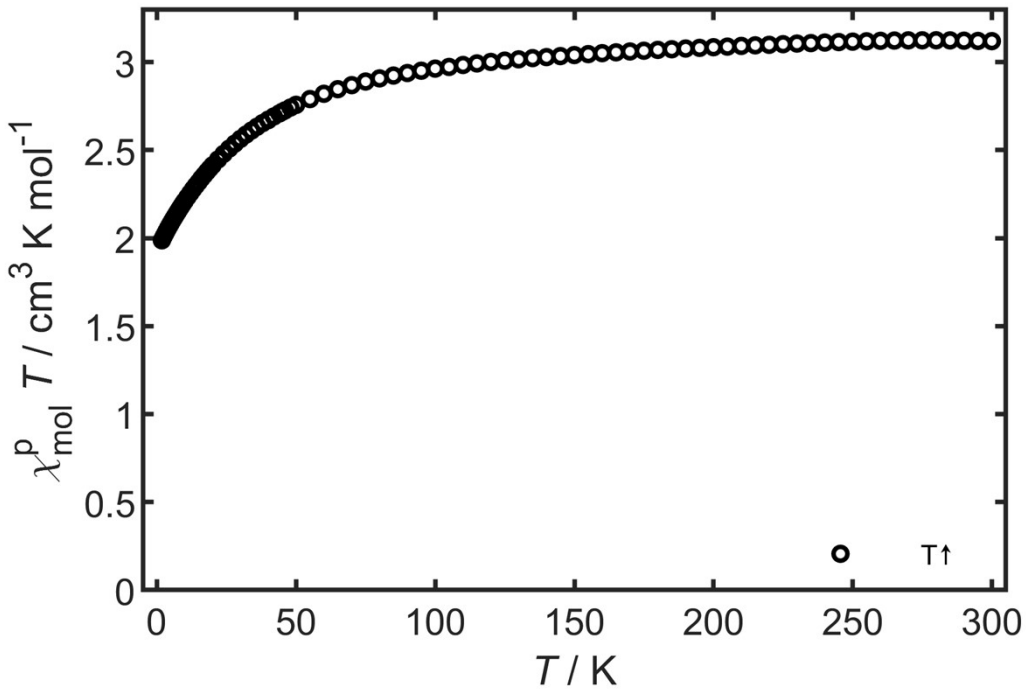

Figure S 2: χ_MT vs. T of complex **1** pressed in a pellet.

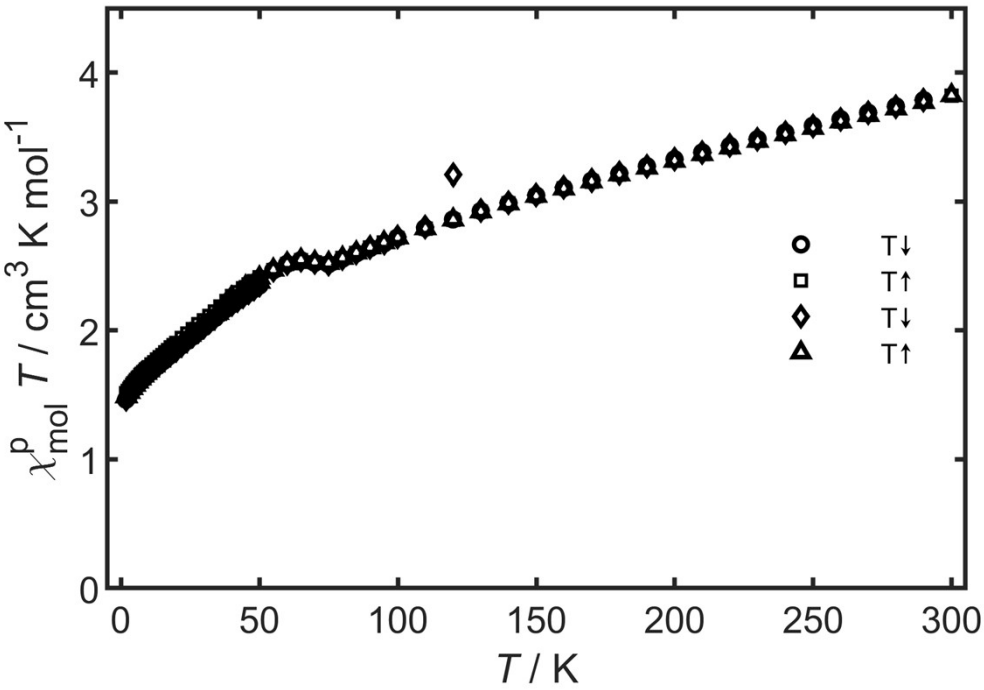

Figure S 3: Susceptibility-temperature product of complex **2** from 1.8 to 300 K. The sample was prepared in an eicosan matrix.

Mössbauer Spectroscopy

Mössbauer spectra at 80 and 292 K were recorded for Complex **3**.

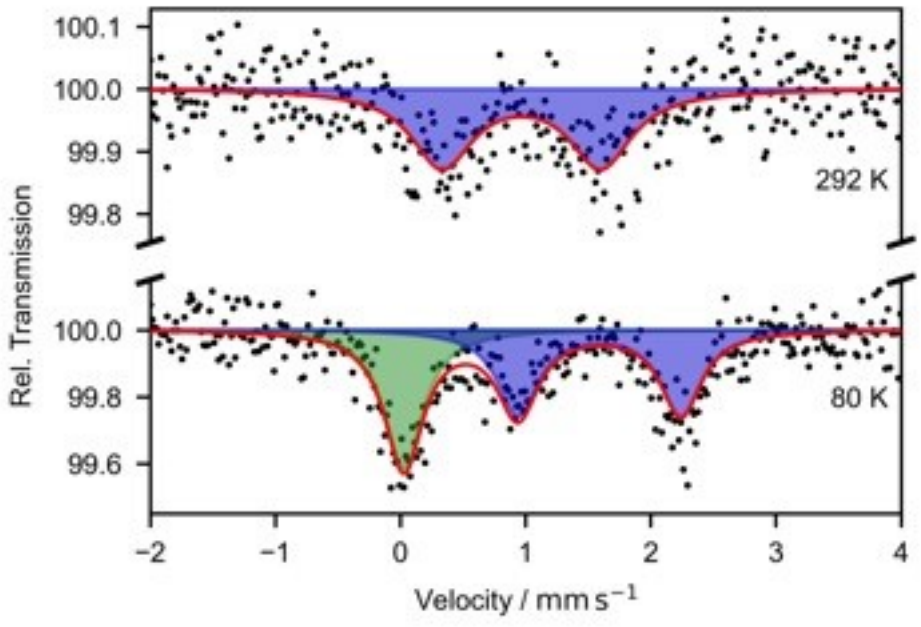

Figure S4: Mössbauer spectra of complex **3** at the indicated temperatures. Measurements were done on the same sample as in the case of the magnetometry. Fits are shown as red solid lines. The contribution of each spin species is shown in green (low spin) and blue (high spin).

Table S1: Overview of the fit parameters from the temperature dependent Mössbauer measurements of **3**.

System		**80 K**	**292 K**
***S* = 2**	δ_{IS} **/ mm s^{-1}**	1.59(1)	0.97(1)
	ΔE_{QS} **/ mm s^{-1}**	1.30(1)	1.27(1)
	Γ **/ mm s^{-1}**	0.40(1)	0.60(1)
***S* = 0**	δ_{IS} **/ mm s^{-1}**	0.03(1)	-
	Γ **/ mm s^{-1}**	0.38(1)	-
	HS molar fraction	0.56	1

EPR Spectroscopy

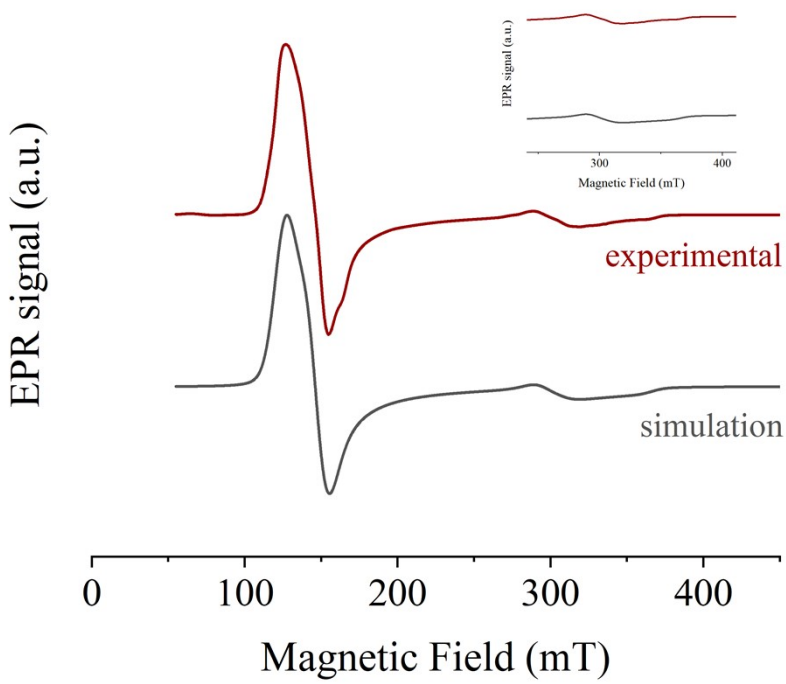

Figure S5: EPR Spectrum of **2** at 13K.

X-Ray Crystallography

Table S2: Crystallographic data of **1**, **2** and **3**.

	1	**2**	**3**
Chemical formula	$C_{62}H_{62}B_2CoF_{14}N_{20}O_2$	$C_{60}H_{54}B_2CoF_{14}N_{20}$	$C_{62}H_{53}B_2CoF_{14}N_{20}O$
M_r	1465.86	1401.78	1437.71
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	P-1	$P2_1/n$
a (Å)	7.7391(3)	14.384(6)	7.8403(4)
b (Å)	20.7813(8)	14.984(6)	20.397(1)
c (Å)	20.1509(9)	15.384(6)	19.7649(9)
α(°)	90	91.16(1)	90
β (°)	98.408(3)	107.86(1)	97.184(2)
γ (°)	90	93.21(1)	90
V (Å^3)	3206.0(2)	3148(2)	3136.0(3)
Z	2	2	2
Densitiy (g cm^{-3})	1.518	1.479	1.523
F(000)	1506	1434	1470

Radiation Type	MoK_α	MoK_α	MoK_α
μ (mm^{-1})	3.003	0.372	0.344
Crystal size	0.18 x 0.08 x 0.08	0.14 x 0.13 x .0.1	0.08x0.06x0.02
Meas. Refl.	21514	38191	89633
Indep. Refl.	5786	11473	5774
Obsvd. [$I > 2\sigma(I)$] refl.	4420	7519	5036
R_{int}	0.0634	0.0602	0.0725
R [$F^2 > 2\sigma(F^2)$], wR(F^2), S	0.0928, 0.2274, 1.094	0.0597, 0.1607, 1.066	0.0655, 0.1679, 1.130
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.882, -0.660	0.644, -0.543	0.537, -1.058

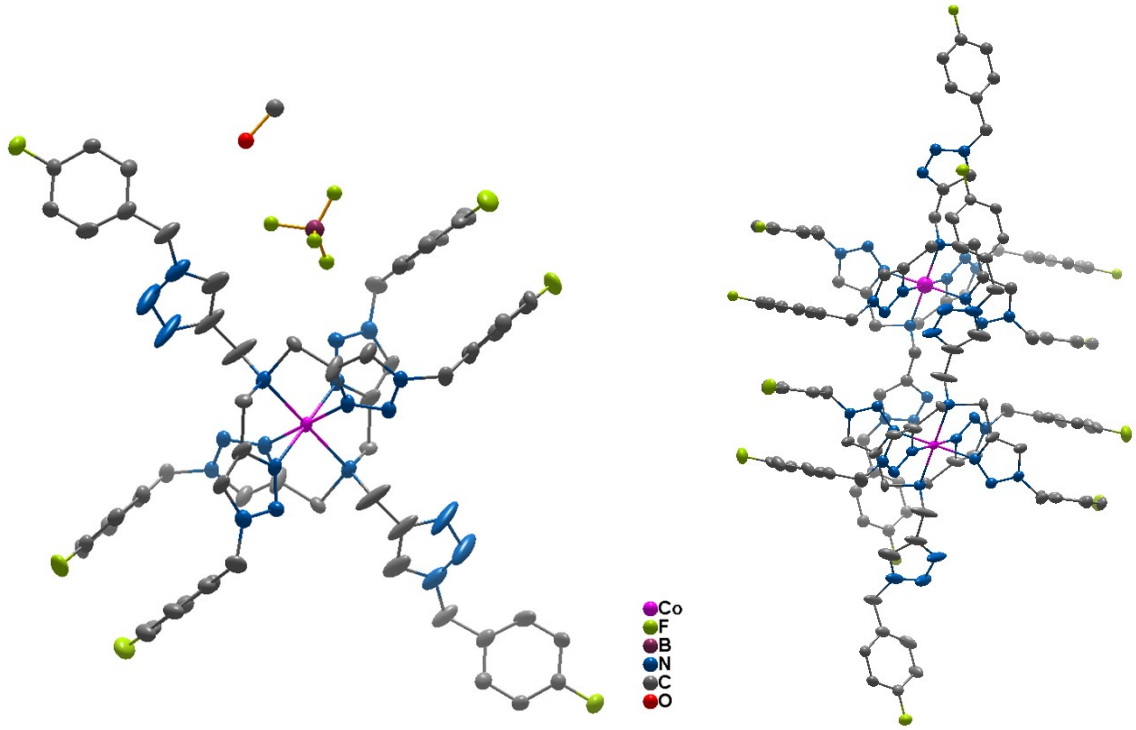

Figure S6: Perspective view of **1**, left with solvent molecule and anion, right: stacking of two molecules. Ellipsoids are at a probability level of 50%. H atoms, anions and solvent molecules are omitted for clarity.

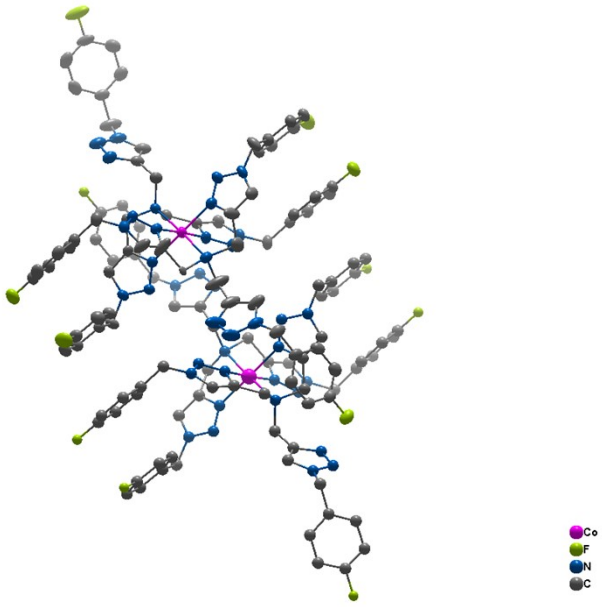

Figure S7: Perspective view of **2**, stacking of two molecules. Ellipsoids are at a probability level of 50%. H atoms, anions and solvent molecules are omitted for clarity.

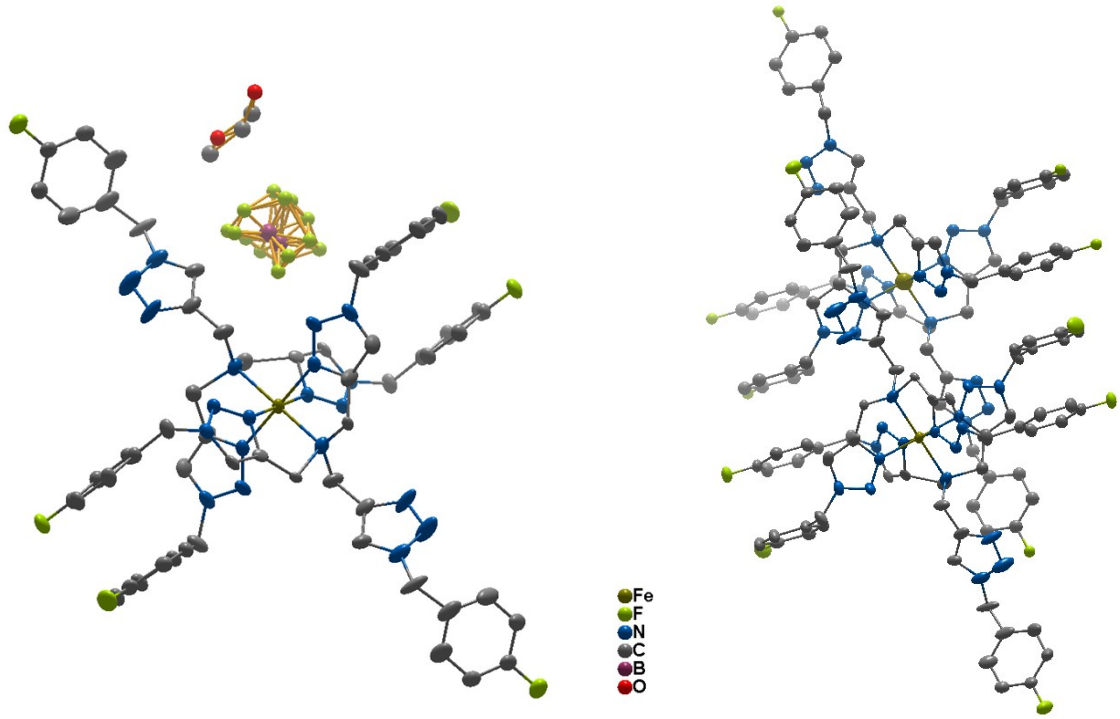

Figure S8: Perspective view of **3**, left with solvent molecule and anion, right: stacking of two molecules. Ellipsoids are at a probability level of 50%. H atoms, anions and solvent molecules are omitted for clarity.

IR Spectroscopy

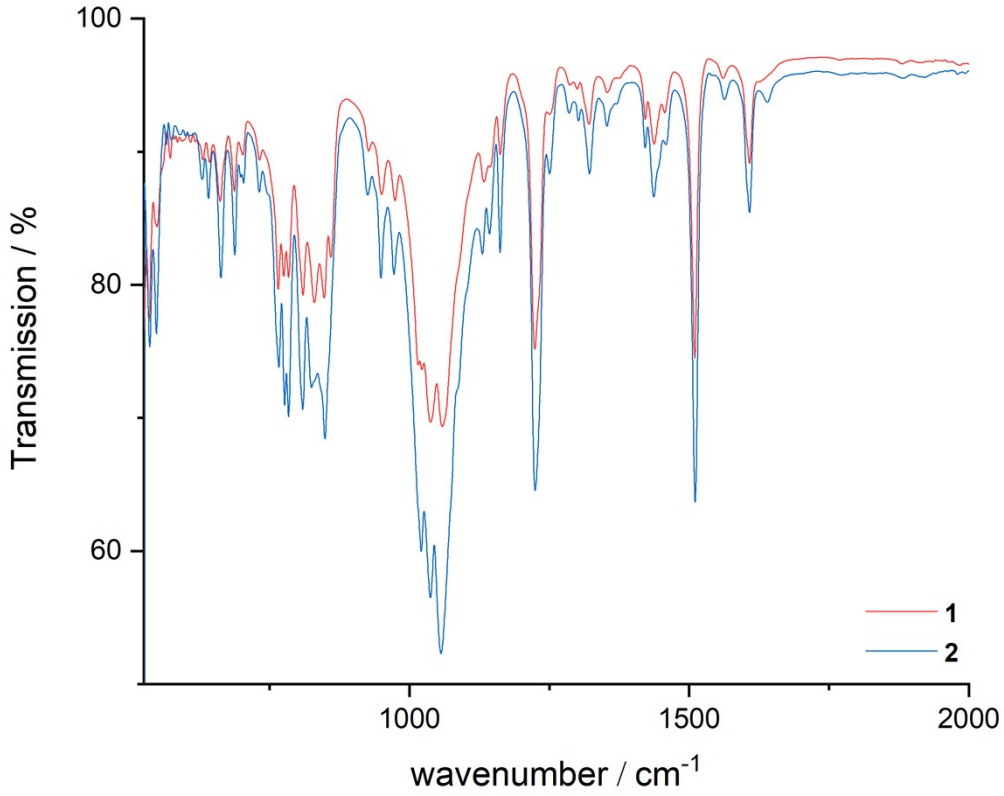

Figure S 9: IR spectra of **1** and **2**.

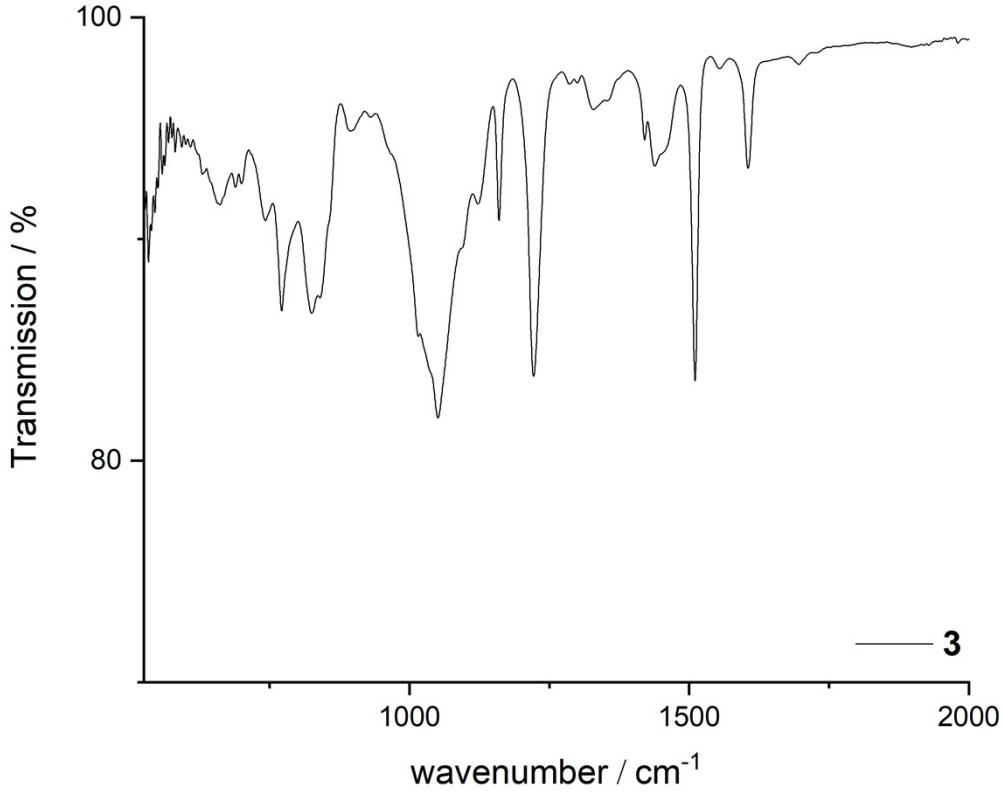

Figure S 10: IR spectrum of **3**.

NMR Spectra

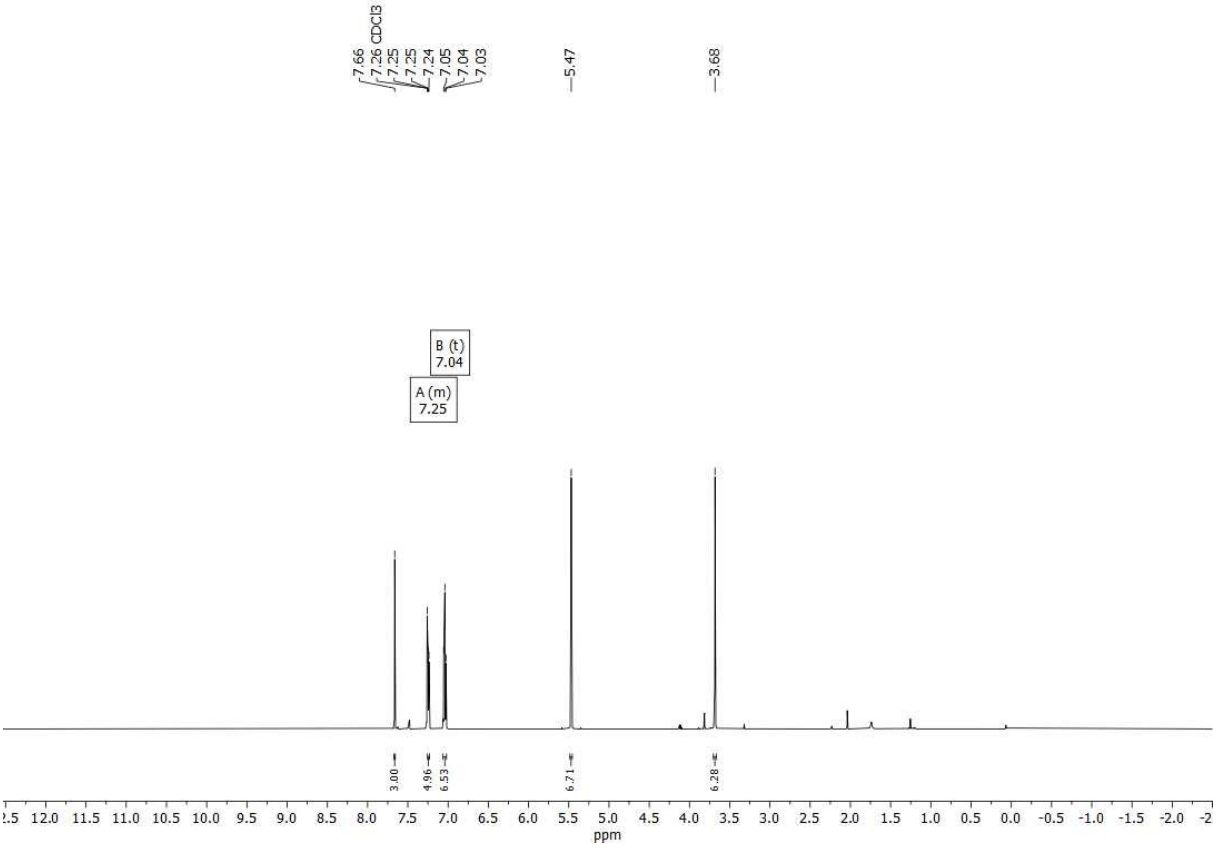

Figure S 11: ^{1}H NMR of TFTA in $CDCl_3$.

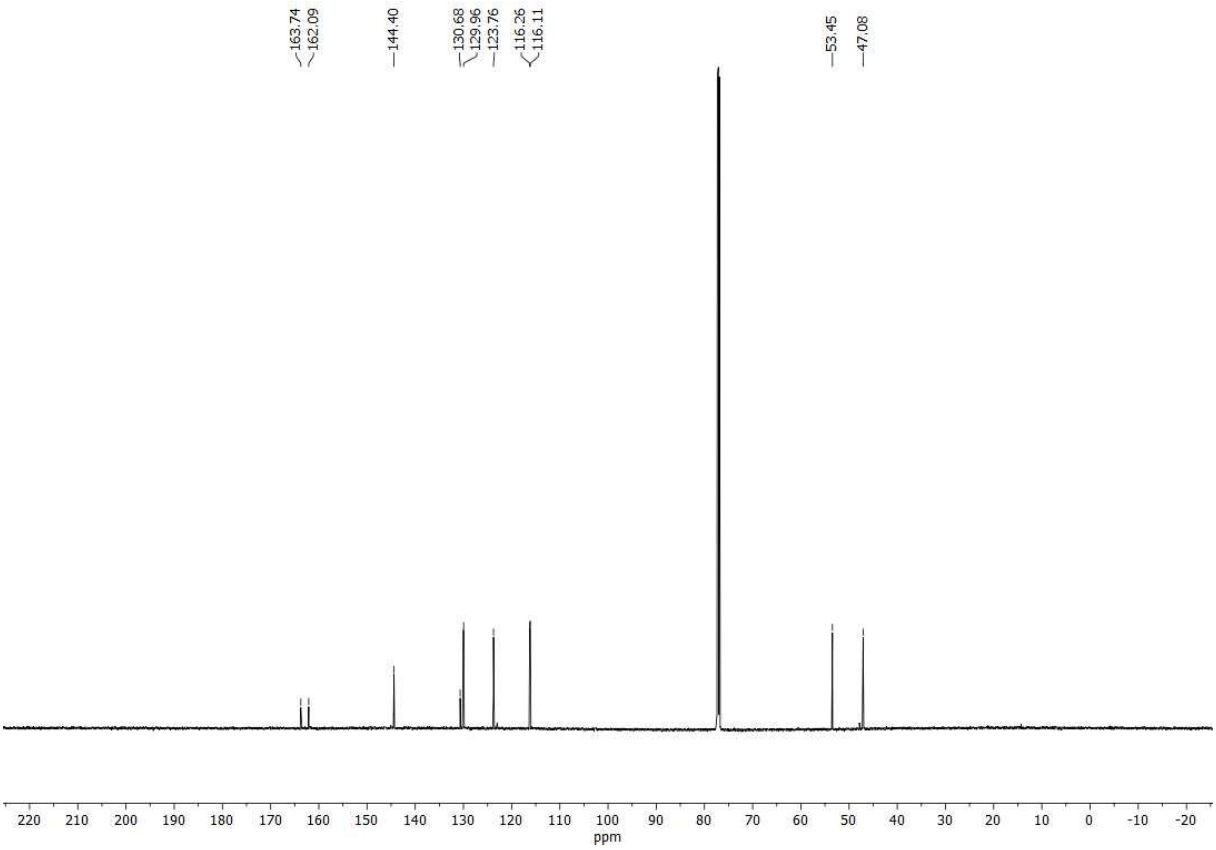

Figure S 12:^{13}C NMR of TFTA in $CDCl_3$.

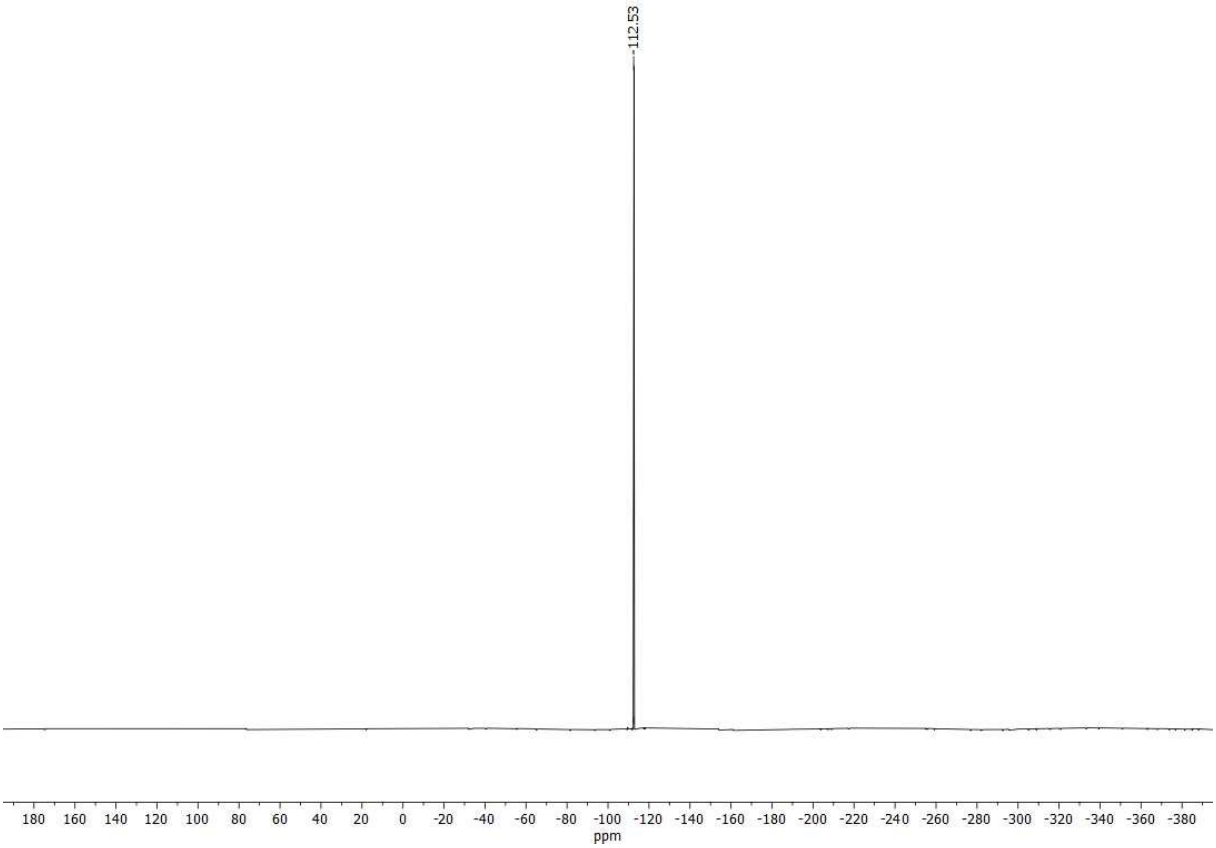

Figure S 13:^{19}F NMR of TFTA in $CDCl_3$.

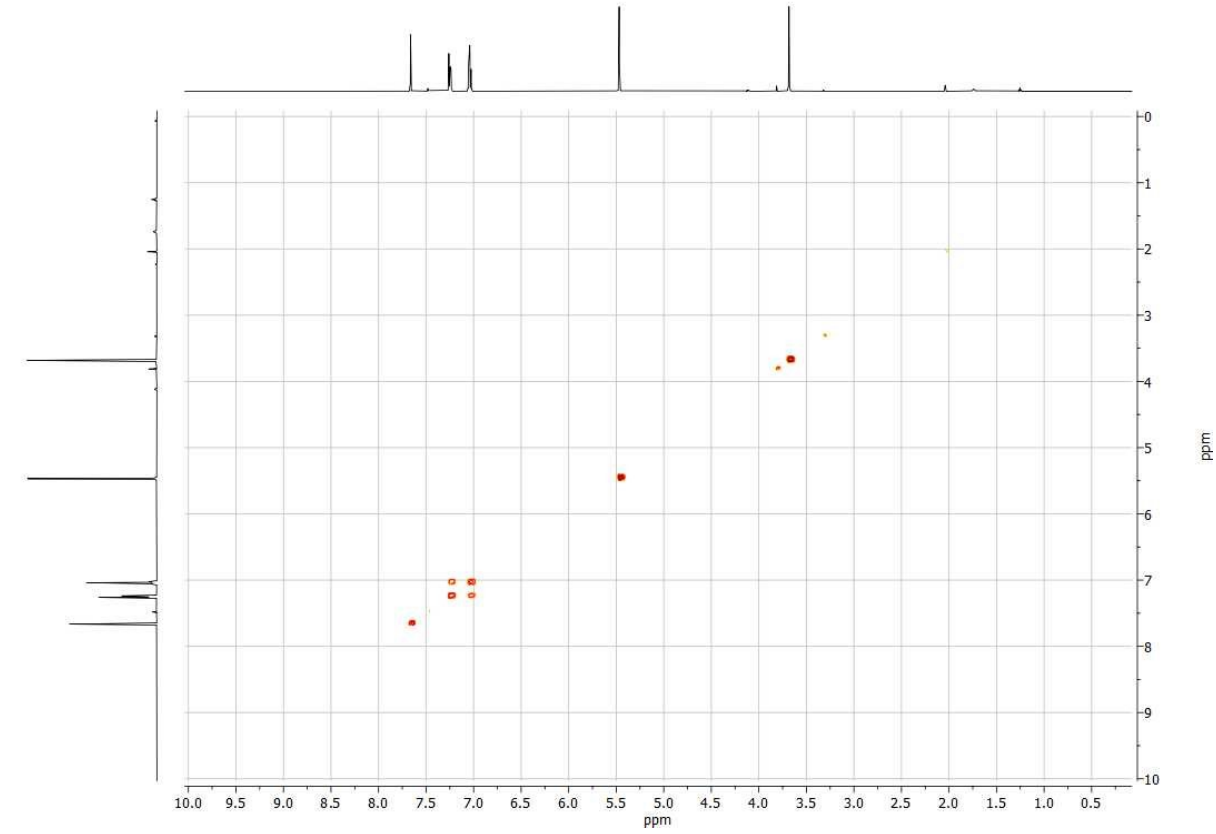

Figure S 14:^{1}H ^{1}H Cosy NMR of TFTA in $CDCl_3$.

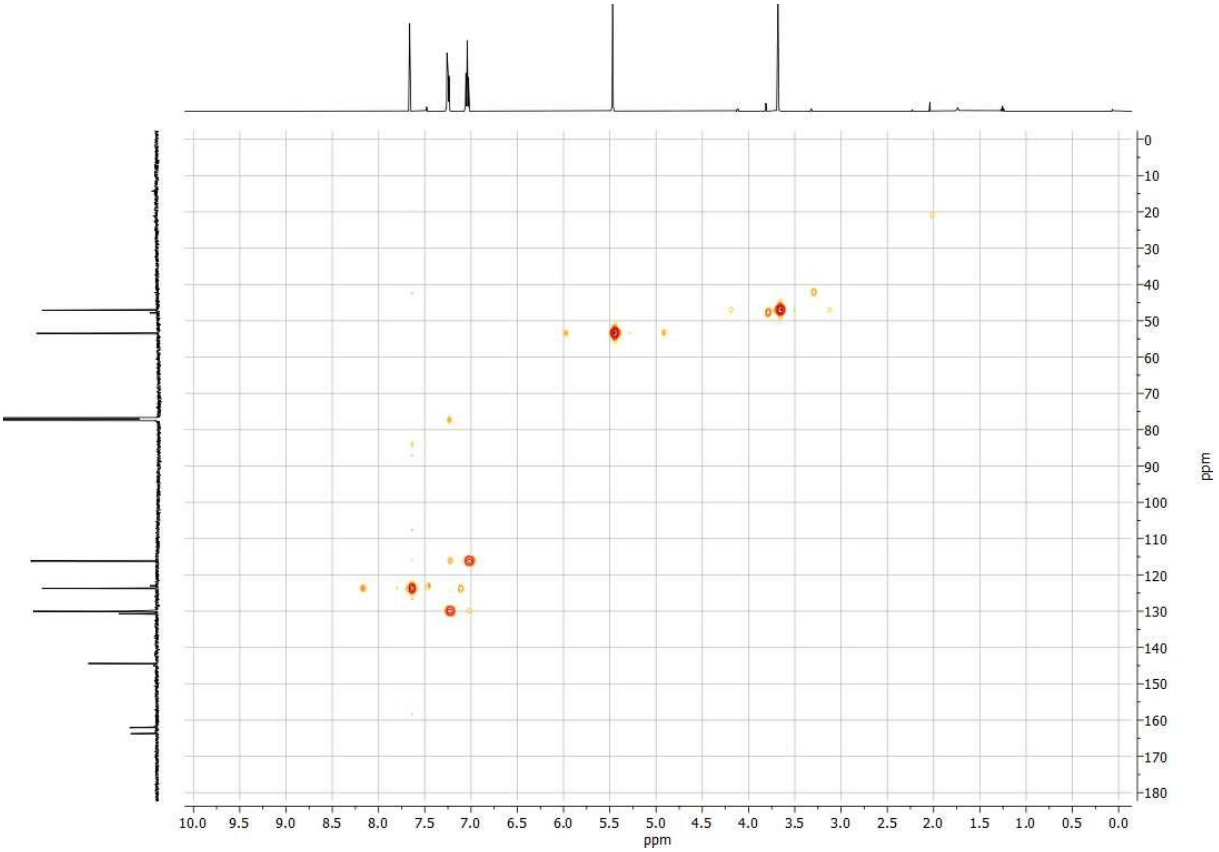

Figure S 15:^{1}H ^{13}C HMBC NMR of TFTA in $CDCl_3$.

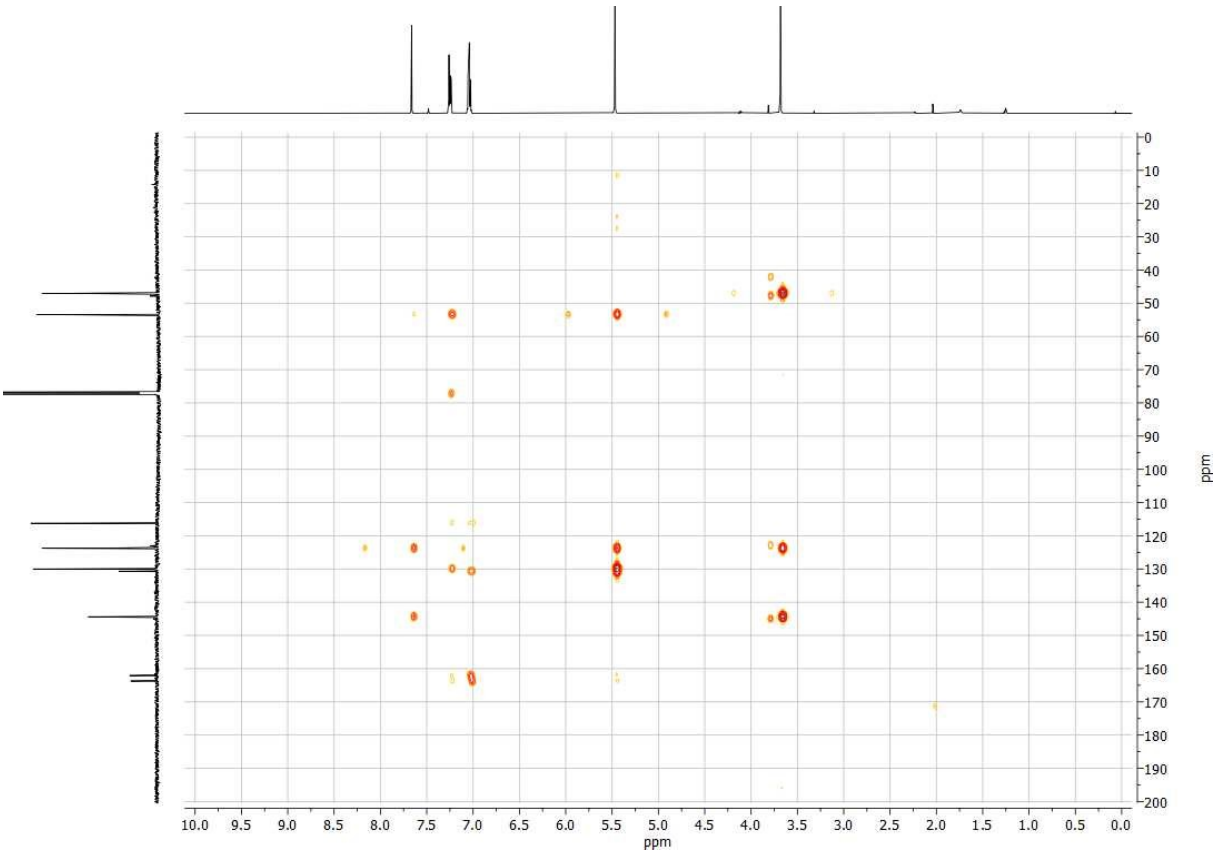

Figure S 16:^{1}H ^{13}C HMQC NMR of TFTA in $CDCl_3$.