Synthesis and Characterization of M(II) (M = Mn, Fe, and Co) Azafulvene-amine Complexes and their Psuedohalide Derivatives

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Supporting Information Table of Contents:

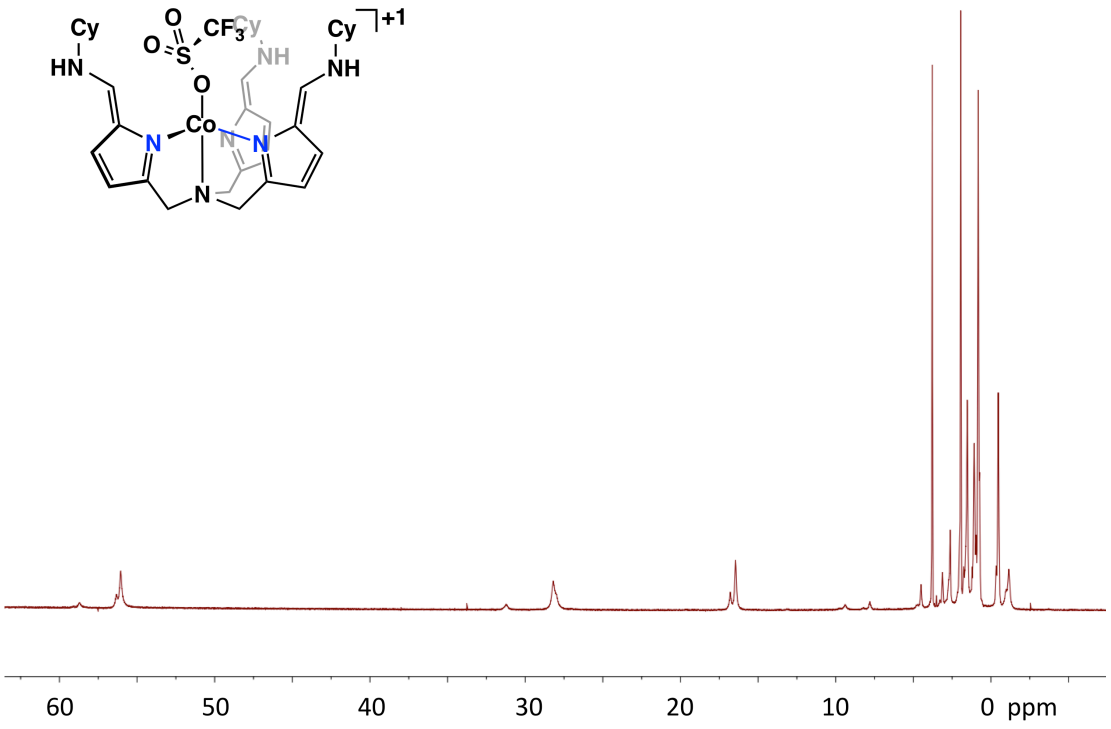
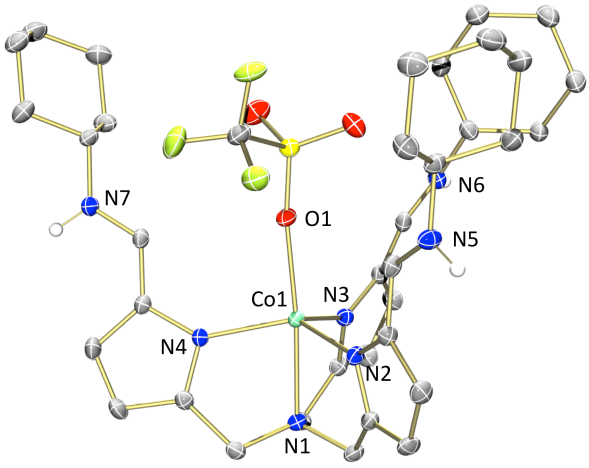


Figure S1. ^{1}H NMR spectrum of **3** (CD_3CN, 25 °C).



[(afa^{NCy})Co](OTf)$_2$ (3)

Figure S2. Molecular structure of **3** shown with 50% probability ellipsoids. Select hydrogen atoms, counter ions and solvent molecules have removed for clarity. Selected bond lengths (Å): Co1-N1: 2.236(2), Co1-N2: 2.039(3), Co1-N3: 2.017(2), Co1-N4: 2.048(3), Co1-O1: 2.178(2).

Table S1. Crystallographic Parameters for complexes **3-4**, **6-8**, and **11-12** (L = [N(afa^{Cy})$_3$]).

	$[LCo]^{2+}$(**3**)	$[LMn(NCS)]^{1+}$ (**4**)	$[LCo(NCS)]^{1+}$ (**6**)	$[LMn(NCO)]^{1+}$ (**7**)	$[LFe(NCO)]^{1+}$ (**8**)	$[LFe(N_3)]^{1+}$ (**11**)	$[LCo(N_3)]^{1+}$ (**12**)
Empirical formula	$C_{42}H_{59}CoF_6N_7O_7S_2$	$C_{79}H_{105}F_6Mn_2N_{16}O_6S_4$	$C_{37}H_{51}CoF_3N_8O_3S_2$	$C_{42}H_{60}F_3MnN_8O_5S$	$C_{42}H_{61}F_3FeN_8O_5S$	$C_{44}H_{69}F_3FeN_{12}O_5S$	$C_{83}H_{111}Co_2F_6N_{20}O_6S_2$
Formula weight	1011.01	1726.91	847.91	827.48	902.89	991.02	1780.89
Temperature	176 K	183 K	100 K	183 K	175 K	173 K	166 K
Wavelength	0.71073	1.54178	0.71073	1.54178	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic
Space group	P 212121	P 2(1)/c	P bca	-P 2ac 2ab	P bca	P bca	P 2(1)/c
Unit cell	a = 10.718(2) Å	a = 15.6420(3) Å	a = 15.3462(4) Å	a = 15.0279(13) Å	a = 14.860(3) Å	a = 15.225(2) Å	a = 15.471(4) Å
dimensions	b = 16.199(3) Å	b = 23.493(4) Å	b = 23.0779(5) Å	b = 23.222(2) Å	b = 23.493(4) Å	b = 23.068(3) Å	b = 23.427(6) Å
	c = 27.605(6) Å	c = 25.1862(6) Å	c = 26.5156(7) Å	c = 26.969(2) Å	c = 26.472(5) Å	c = 26.462(4) Å	c = 24.935(7) Å
	α = 90°	α = 90°	α = 90°	α= 90°	α = 90°	α = 90°	α= 90°
	β = 90°	β = 101.847(1)°	β = 90°	β = 90°	β = 90°	β = 90°	β = 101.761(3)°
	γ = 90°	γ = 90°	γ = 90°	γ = 90°	γ = 90°	γ = 90°	γ = 90°
Volume	4792.8(16)	9075.6(3)	9390.7(4)	9411.6(14)	9241(3)	9294(2)	8848(4)
Z	4	4	8	8	8	8	4
Reflections collected	10200	16070	10288	8372	8512	8582	16701
Independent reflections	8543	13635	8080	6071	6461	6167	13176
Goodness-of-fit on F2	1.015	1.047	1.039	1.078	1.027	1.074	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0373 wR2 = 0.0827	R1 = 0.0407 wR2 = 0.1047	R1 = 0.0402 wR2 = 0.1063	R1 = 0.0690 wR2 = 0.1634	R1 = 0.0445 wR2 = 0.1201	R1 = 0.0479 wR2 = 0.1220	R1 = 0.0366 wR2 = 0.0901
R indices	R1 = 0.0524 wR2 = 0.0881	R1 = 0.0483 wR2 = 0.1090	R1 = 0.0563 wR2 = 0.1130	R1 = 0.0972 wR2 = 0.1785	R1 = 0.0624 wR2 = 0.1340	R1 = 0.0741 wR2 = 0.1334	R1 = 0.0524 wR2 = 0.0995