Electronic Supplementary Information

Polymorphism and "reverse" spin transition in the spin crossover system $[Co(4\text{-terpyridone})_2](CF_3SO_3)_2 \cdot 1H_2O$

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Table S1. Crystal data for **1** at 293 K and 120 K.

	1	
	293 K	**120 K**
Empirical formula	$C_{32}H_{24}N_6O_9S_2F_6Co$	
*M*r	873.62	
Crystal system	triclinic	
Space group	P-1	
a (Å)	9.1020(5)	9.0803(2)
b (Å)	9.2410(5)	9.1039(3)
c (Å)	21.3860(18)	21.1499(7)
α (°)	94.896(2)	94.899(3)
β (°)	94.487(2)	94.810(2)
γ (°)	90.730(6)	91.322(2)
V (Å^3)	1786.4(2)	1735.05(9)

Selected bond lengths [Å] and angles [°] for **1** at 120 K.

Co(1)-N(1)	2.099(9)
Co(1)-N(2)	1.922(9)
Co(1)-N(3))	2.097(12)
Co(1)-N(4)	2.074(11)
Co(1)-N(5)	1.909(10)
Co(1)-N(6)	2.079(10)
N(1)-Co-N(2)	79.1(4)
N(1)-Co-N(3)	158.3(4)
N(1)-Co-N(4)	93.7(4)
N(1)-Co-N(5)	100.8(4)
N(1)-Co-N(6)	89.4(4)
N(2)-Co-N(3)	79.2(4)
N(2)-Co-N(4)	101.1(4)
N(2)-Co-N(5)	179.2(4)
N(2)-Co-N(6)	99.2(4)
N(3)-Co-N(4)	91.5(4)
N(3)-Co-N(5)	100.9(4)
N(3)-Co-N(6)	93.0(4)
N(4)-Co-N(5)	79.7(4)
N(4)-Co-N(6)	159.7(4)
N(5)-Co-N(6)	79.9(4)

Table S2. Crystal data for **2** at 293 K, 180 K and 120 K.

	2		
	293 K	**180 K**	**120 K**
Empirical formula	$C_{32}H_{24}N_6O_9F_6S_2Co$		
*M*r	873.62		
Crystal system	triclinic		
Space group	P-1		
a (Å)	9.5700(4)	18.6610(6)	9.2500(4)
b (Å)	14.3510(9)	14.2520(4)	14.2320(7)
c (Å)	14.9540(8)	14.8710(5)	14.8280(10)
α	75.456(4)	75.246(2)	75.209(2)
β (°)	71.982(4)	72.662(1)	72.982(3)
γ	72.274(2)	72.439(1)	72.315(2)
V (Å^3)	1832.19(17)	3539.92(19)	1748.45(16)