Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Influences on the Rotated Structure of the Diiron Dithiolate Complexes: Electronic Asymmetry vs. Secondary Coordination Sphere Interaction

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Table S1. X-ray Crystallographic Data after SQUEEZE refinement

	[**4**](TFA)$_2$	[**5**](OTf)$_2$
Empirical formula	$C_{78}H_{80}F_6Fe_4N_2O_{12}P_4S_4$	$C_{78}H_{84}F_6Fe_4N_2O_{14}P_4S_6$
Formula weight	1826.96	1927.11
T, K	150(2)	150(2)
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/n$	P-1
a, Å	17.133(3)	16.4839(5)
b, Å	13.281(2)	17.0452(5)
c, Å	23.904(4)	21.2654(4)
α, °	90	94.2320(2)
β, °	107.252(8)	108.7318(14)
γ, °	90	113.5410(11)
V, Å^3	5194.5(15)	5045.1(2)
Z	2	2
ρ_{calcd}, Mg m^{-3}	1.168	1.269
μ, mm^{-1}	0.747	0.814
F (000)	1880	1984
Reflections collected	20998	63604
Independent reflections	9021	17651
R_{int}	0.0900	0.0826
Goodness-of-fit on F^2	1.006	1.064
R1 [$I > 2\sigma(I)$] (all data)[a]	0.0759 (0.1371)	0.0791 (0.1309)
wR2 [$I > 2\sigma(I)$] (all data)[b]	0.1645 (0.1808)	0.2196 (0.2346)

[a] $R1 = (\Sigma||F_o|-|F_c||)/(\Sigma|F_o|)$. [b] $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.