

SUPPLEMENTARY MATERIAL

Low-valent Iron Complexes Stabilised by a Bulky Guanidinate Ligand: Synthesis and Reactivity Studies*

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Table S1. Summary of crystallographic data for **6**, **7** and **8**·(hexane)

	6	7	8 ·(hexane)
empirical formula	C ₃₅ H ₄₈ FeN ₃ O ₃	C ₆₅ H ₉₆ Fe ₂ N ₆ S ₂	C ₉₀ H ₁₄₀ Fe ₂ N ₁₂
formula weight	614.61	1137.30	1501.84
crystal system	monoclinic	triclinic	tetragonal
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 4 ₂ / <i>n</i>
a (Å)	11.2420(6)	15.6492(9)	25.258(4)
b (Å)	18.8185(10)	17.9642(11)	25.258(4)
c (Å)	16.0197(8)	19.0189(11)	14.101(3)
α (°)	90	106.366(3)	90
β (°)	97.064(2)	109.517(2)	90
γ (°)	90	95.129(3)	90
V (Å ³)	3363.4(3)	4734.7(5)	8996(3)
Z	4	3	4
T (K)	123(2)	123(2)	100(2)
ρ _{calcd} (g·cm ³)	1.214	1.197	1.109
μ (mm ⁻¹)	0.485	0.568	0.371
F(000)	1316	1836	3264
reflns collected	24918	47301	57897
unique reflns	7694	16469	7810
R _{int}	0.0320	0.0453	0.1089
R1 indices [I > 2σ(I)]	0.0435	0.0509	0.0922
wR2 indices (all data)	0.1108	0.1232	0.2883
largest peak and hole (e·Å ⁻³)	0.32, -0.51	1.00, -0.48	1.00, -0.47
CCDC no.	991289	991290	991291