

Supporting Information

Reactions of Pyridyl Side-Chain-Functionalized Cyclopentadienes with Metal Carbonyl: Intramolecular C-H Activation of Pyridine

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Table 2. Crystal Data and Summary of X-ray Data Collection for 4 and 8

	4	8
formula	C ₃₂ H ₃₂ Fe ₂ N ₂ O ₄	C ₃₂ H ₃₂ N ₂ O ₄ Ru ₂
fw	620.30	710.74
T, K	293(2)	293(2)
Radiation (λ), Å	Mo Ka (0.71073)	Mo Ka (0.71073)
cryst syst	Triclinic	Triclinic
space group	P-1	P-1
a, Å	7.093(9)	7.786(3)
b, Å	7.925(10)	8.564(3)
c, Å	10.999(13)	12.065(4)
α , deg	103.839(19)	104.075(5)
β , deg	99.014(19)	100.816(5)
γ , deg	107.913(19)	107.401(5)
V, Å ³	553.3(12)	714.6(4)
Z	1	1
D_{calc} , g·cm ⁻³	1.862	1.651
μ , mm ⁻¹	1.362	1.097
F(000)	322	358
cryst size, mm	0.22x0.18x0.14	0.20x0.16x0.12
2 θ range, deg	5.68-52.64	3.62-52.62
no. of reflns collected	3210	4128
no. of indep reflns/R _{int}	2207/ 0.0189	2872/ 0.0200
no. of params	183	184
goodness-of-fit on F^2	1.026	1.145
R_I , wR ₂ [$I > 2\sigma(I)$]	0.0371, 0.0945	0.0313, 0.0740
R_I , wR ₂ (all data)	0.0502, 0.1017	0.0406, 0.0906

Figure 5. ORTEP diagram of **4**. Thermal ellipsoids are shown at the 30% level.

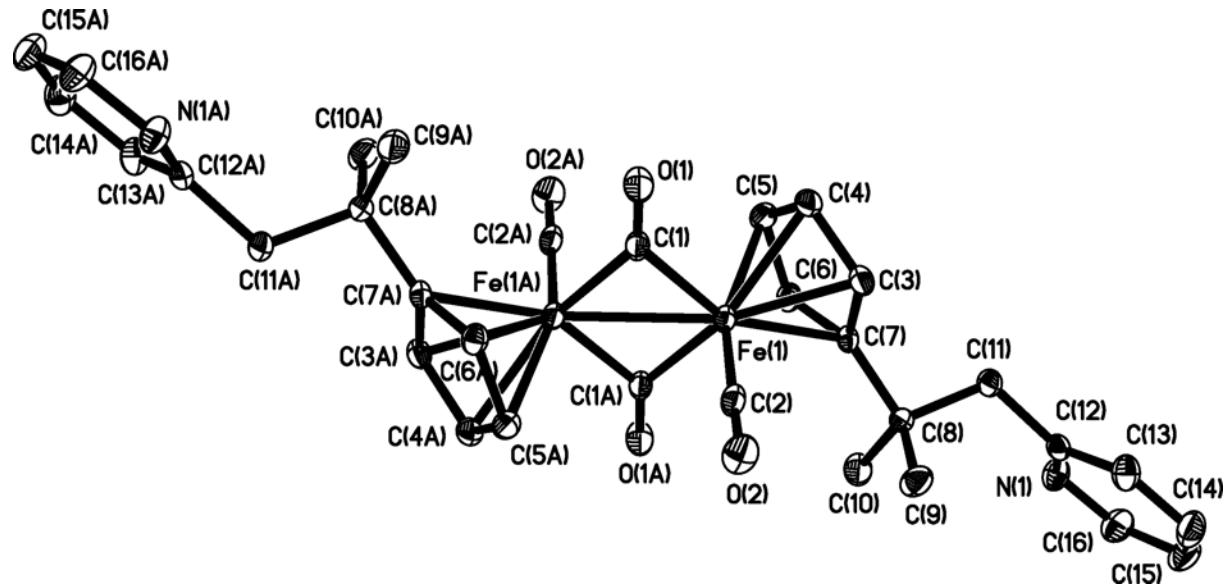


Figure 6. ORTEP diagram of **8**. Thermal ellipsoids are shown at the 30% level.

