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## The influence of the ligand chelate effect on iron-amine-catalysed Kumada cross-coupling

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### SUPPORTING INFORMATION

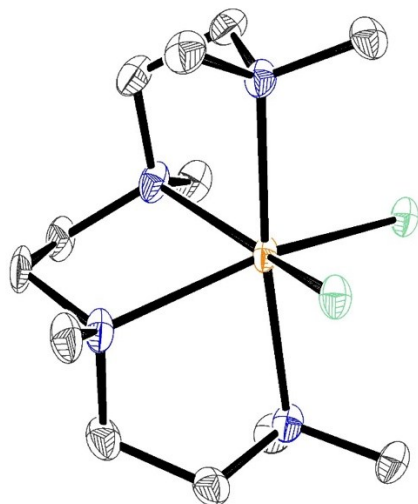
#### Crystallographic Experimental

X-ray diffraction experiments on single crystal of **9** were carried out at 100K on a Bruker Proteum Microstar diffractometer using Cu-K<sub>α</sub> radiation ( $\lambda = 1.54178 \text{ \AA}$ ) and on **8** at 100K on a Bruker APEX II diffractometer using Mo-K<sub>α</sub> radiation ( $\lambda = 0.71073 \text{ \AA}$ ). Data collections were performed using a CCD area detector from a single crystal mounted on a glass fibre. Intensities were integrated<sup>S1</sup> from several series of exposures measuring 0.5° in  $\omega$  or  $\varphi$ . Absorption corrections were based on equivalent reflections using SADABS.<sup>S2</sup> The structures were solved using SHELXS and refined against all Fo2 data with hydrogen atoms riding in calculated positions using SHELXL.<sup>S3</sup> The structures have been deposited at the Cambridge Crystallographic Data Centre, CCDC numbers for **8** and **9**, CCDC 1478297 and CCDC 1478298 respectively.

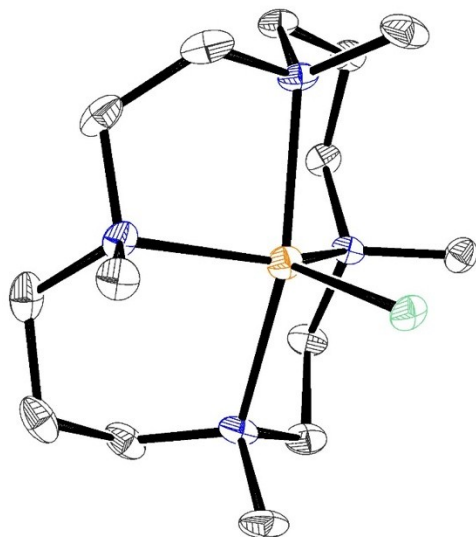
## Crystallographic Data

Identification code	<b>8</b>	<b>9·3CH<sub>3</sub>CN</b>
Empirical formula	C <sub>12</sub> H <sub>30</sub> Cl <sub>2</sub> FeN <sub>4</sub>	C <sub>20</sub> H <sub>41</sub> Cl <sub>2</sub> FeN <sub>7</sub>
Formula weight	357.15	506.35
Temperature/K	100	100
Crystal system	monoclinic	triclinic
Space group	C2/c	P-1
a/Å	14.884(3)	8.4114(17)
b/Å	7.9168(16)	13.145(3)
c/Å	14.972(3)	13.243(3)
α/°	90	65.49(3)
β/°	104.91(3)	81.50(3)
γ/°	90	81.42(3)
Volume/Å <sup>3</sup>	1704.7(6)	1311.5(6)
Z	4	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.392	1.282
μ/mm <sup>-1</sup>	1.192	0.799
F(000)	760.0	540.0
Crystal size/mm <sup>3</sup>	0.24 × 0.2 × 0.15	0.6 × 0.4 × 0.4
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54178)
2θ range for data collection/°	5.632 to 54.964	3.396 to 51.728
Index ranges	-19 ≤ h ≤ 19 -10 ≤ k ≤ 10 -18 ≤ l ≤ 19	-6 ≤ h ≤ 9 -15 ≤ k ≤ 15 -15 ≤ l ≤ 15
Reflections collected	11668	8897
Independent reflections	1951 [R <sub>int</sub> = 0.0560, R <sub>sigma</sub> = 0.0429]	4071 [R <sub>int</sub> = 0.0353, R <sub>sigma</sub> = 0.0508]
Data/restraints/parameters	1951/0/90	4071/0/278
Goodness-of-fit on F <sup>2</sup>	0.891	1.206
Final R indexes [I >= 2σ (I)]	R <sub>1</sub> = 0.0383, wR <sub>2</sub> = 0.1083	R <sub>1</sub> = 0.0512, wR <sub>2</sub> = 0.1239
Final R indexes [all data]	R <sub>1</sub> = 0.0588, wR <sub>2</sub> = 0.1245	R <sub>1</sub> = 0.0515, wR <sub>2</sub> = 0.1240
Largest diff. peak/hole / e Å <sup>-3</sup>	0.47/-0.58	0.61/-0.49

**Figure S1.** Structure of complex **8**, thermal ellipsoids set at 50% probability, hydrogen atoms omitted for clarity.



**Figure S2.** Structure of complex **9**, thermal ellipsoids set at 50% probability, hydrogen atoms and three molecules of MeCN omitted for clarity.



## References

- S1. Bruker-AXS SAINT V7.68A, Madison, Wisconsin.
- S2. G. M. Sheldrick, SADABS V2008/1, University of Göttingen, Germany.
- S3. G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.