Magnesium amido N-heterocyclic carbene complexes

Supplementary Material (ESI) for Dalton Transactions

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Electronic Supplementary Information.

Reaction of 1 with pyridine

In the search for alternative syntheses of the purple complex **2**, we treated a suspension of **1** in thf with 2 equivalents of pyridine at room temperature, which led to the formation of a red solution and a colourless solid (identified as $MgCl_2$) after 22 hours. Filtration and removal of volatiles from the solution affords a red solid. The ^{1}H NMR spectrum of a d_5-pyridine solution of the red solid contains four resonances due to the protons on the two imidazole rings observed at 7.63, 6.76, 6.24 and 5.89 ppm, one set of resonances due to a bound pyridine molecule, shifted very slightly to lower frequency in comparison to free pyridine. The ^{13}C NMR spectrum contains two separate carbene resonances at 171.3 and 164.1 ppm, which are at considerably lower frequencies than the carbene resonance observed for **1** (194.0 ppm).

To a suspension of **1** (0.55 g, 0.63 mmol) in thf (5 cm^3) was added a solution of pyridine (0.1 cm^3, 2.0 equiv.) in thf (5 cm^3). The resulting mixture was stirred at room temperature for 22 hours to yield a red solution and white precipitate. The solution was filtered and volatiles were removed under reduced pressure to afford a red solid (0.42 g). ^{1}H NMR (C_5D_5N): 8.70 (s, 2Hs, pyr), 7.63 (d, 1H, ^{3}J = 2.2 Hz, C*H*), 7.52 (s, 1H, pyr), 7.15 (s, 2Hs, pyr), 6.82 (s, 4Hs, Ar), 6.76 (s, 1H, C*H*), 6.24 (d, 1H, ^{3}J = 1.2 Hz, C*H*), 5.88 (d, 1H, ^{3}J = 1.2 Hz, C*H*), 3.41 (br, 2Hs, CH_2), 2.84 (m, 4Hs, CH_2), 2.65 (br, 2Hs, CH_2), 2.17 (s, 6Hs, CH_3), 2.13 (d, 6Hs, CH_3), 2.06 (s, 6Hs, CH_3). ^{13}C{^{1}H} NMR (C_5D_5N): 171.3 (N*C*N), 164.1 (N*C*N), 138.2, 137.7, 137.3, 134.9, 132.1 (All Ar), 129.9 (*C*H), 129.6 (*C*H), 129.0, 127.2 (both Ar), 114.5 (*C*H), 113.4 (*C*H), 56.7 (*C*H$_2$), 55.7 (*C*H$_2$), 43.4 (*C*H$_2$), 39.4 (*C*H$_2$), 20.7 (*p*-*C*H$_3$), 18.5 (*o*-*C*H$_3$).