

Supporting Information for

A simple and efficient synthesis of [MCl(NHC)] (M = Au, Ag) complexes

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1. Experimental details

All reactions were performed under air atmosphere and solvents were used as received without purification or drying. $[\text{AuCl}(\text{tht})]^1$ and imidazolium salts² were prepared according to published procedures. AgNO_3 and K_2CO_3 were commercially available from PANREAC. ^1H , NMR experiments were recorded at room temperature on a BRUKER AVANCE 400 (^1H , 400 MHz) or on a BRUKER AVANCE II 300 spectrometer (^1H , 300 MHz) with chemical shifts (δ , ppm) reported relative to the solvent peaks of the deuterated solvent.³

2. General procedure for the synthesis of $[\text{NHC}\cdot\text{H}][\text{AuCl}_2]$ salts

A mixture of $\text{NHC}\cdot\text{HCl}$ (0.35 mmol) and $[\text{AuCl}(\text{tht})]$ (0.35 mmol) in dichloromethane (10 mL) was stirred for 15 min. The solvent was removed until 2 mL (c.a.) and then the product was precipitated with ether (15 mL) and washed (3x5 mL) to give **1** (96%), **2** (95%), **3** (97%) and **4** (95%) as a white solids.

$[\text{IPr}\cdot\text{H}][\text{AuCl}_2]$ **1**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 9.12 (s, 1H, im), 7.88 (s, 2H, im), 7.63 (t, $J = 7.8$ Hz, 2H, Ph), 7.39 (d, $J = 7.8$ Hz, 4H, Ph), 2.45 (sept, $J = 6.7$ Hz, 4H, CH), 1.32 (d, $J = 6.7$ Hz, 12H, CH_3), 1.22 (d, $J = 6.7$ Hz, 12H, CH_3).

$[\text{SIPr}\cdot\text{H}][\text{AuCl}_2]$ **2**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 8.05 (s, 1H, im), 7.49 (t, $J = 7.5$ Hz, 2H, Ph), 7.29 (d, $J = 7.8$ Hz, 4H, Ph), 4.76 (s, 4H, im), 3.04 (sept, $J = 6.7$ Hz, 4H, CH), 1.42 (d, $J = 6.8$ Hz, 12H, CH_3), 1.26 (d, $J = 6.8$ Hz, 12H, CH_3).

$[\text{IMes}\cdot\text{H}][\text{AuCl}_2]$ **3**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 9.58 (s, 1H, im), 7.63 (s, 2H, im), 7.06 (s, 4H, Ph), 2.37 (s, 6H, CH_3), 2.17 (s, 12H, CH_3).

$[\text{SIMes}\cdot\text{H}][\text{AuCl}_2]$ **4**: ^1H NMR (CDCl_3 , 400 MHz, 294 K): δ 8.35 (s, 1H, im), 7.00 (s, 4H, Ph), 4.60 (s, 4H, im), 2.40 (s, 12H, CH_3), 2.32 (s, 6H, CH_3).

3. General procedure for the synthesis of $[\text{AuCl}(\text{NHC})]$ complexes

A mixture of $\text{NHC}\cdot\text{HCl}$ (0.35 mmol) and $[\text{AuCl}(\text{tht})]$ (0.35 mmol) in dichloromethane (15 mL) was stirred for 15 min and then K_2CO_3 (5 mmol) was added. After 1.5 h, the mixture was filtered through Celite and the solvent was removed in vacuo until 2 mL (c.a.). The product was precipitated with ether (10 mL) and washed (3x5 mL) to give **1a** (93%), **2a** (93%), **3a** (91%) and **4a** (94%) as a white solids. NMR data were compared to published data.⁴

$[\text{AuCl}(\text{IPr})]$ **1a**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.59 (t, $J = 7.8$ Hz, 2H, Ph), 7.38 (d, $J = 7.8$ Hz, 4H, Ph), 7.26 (s, 2H, im), 2.59 (sept, $J = 6.7$ Hz, 4H, CH), 1.37 (d, $J = 6.9$ Hz, 12H, CH_3), 1.26 (d, $J = 6.9$ Hz, 12H, CH_3).

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[AuCl(SIPr)] **2a**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.41 (t, $J = 7.5$ Hz, 2H, Ph), 7.23 (d, $J = 7.7$ Hz, 4H, Ph), 4.04 (s, 4H, im), 3.05 (sept, $J = 6.7$ Hz, 4H, CH), 1.42 (d, $J = 6.8$ Hz, 12H, CH_3), 1.34 (d, $J = 6.9$ Hz, 12H, CH_3).

[AuCl(IMes)] **3a**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.09 (s, 2H, im), 6.99 (s, 4H, Ph), 2.34 (s, 6H, CH_3), 2.10 (s, 12H, CH_3).

[AuCl(SIMes)] **4a**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 6.94 (s, 4H, Ph), 3.98 (s, 4H, im), 2.31 (s, 12H, CH_3), 2.29 (s, 6H, CH_3).

4. General procedure for the synthesis of [AgCl(NHC)] complexes

A mixture of NHC•HCl (0.3 mmol) and AgNO_3 (0.3 mmol) in dichloromethane (15 mL) was stirred for 2 min and then K_2CO_3 (5 mmol) was added. After 1.5 h, the mixture was filtered through Celite and the solvent was removed in vacuo until 2 mL (c.a.). The product was precipitated with ether (10 mL) and washed (3x5mL) to give **1b** (91%), **2b** (90%), **3b** (92%) and **4b** (92%) as a white solids. NMR data were compared to published data.⁵

[AgCl(IPr)] **1b**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.50 (t, $J = 7.8$ Hz, 2H, Ph), 7.30 (d, $J = 7.8$ Hz, 4H, Ph), 7.21 (s, 2H, im), 2.55 (sept, $J = 6.7$ Hz, 4H, CH), 1.29 (d, $J = 6.9$ Hz, 12H, CH_3), 1.23 (d, $J = 6.9$ Hz, 12H, CH_3).

[AgCl(SIPr)] **2b**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.41 (t, $J = 7.6$ Hz, 2H, Ph), 7.25 (d, $J = 7.8$ Hz, 4H, Ph), 4.06 (s, 4H, im), 3.05 (sept, $J = 6.7$ Hz, 4H, CH), 1.35 (d, $J = 6.8$ Hz, 12H, CH_3), 1.33 (d, $J = 6.9$ Hz, 12H, CH_3).

[AgCl(IMes)] **3b**: ^1H NMR (CDCl_3 , 300 MHz, 294 K): δ 7.14 (s, 2H, im), 6.98 (s, 4H, Ph), 2.33 (s, 6H, CH_3), 2.06 (s, 12H, CH_3).

[AgCl(SIMes)] **4b**: ^1H NMR (CDCl_3 , 400 MHz, 294 K): δ 6.92 (s, 4H, Ph), 3.99 (s, 4H, im), 2.28 (s, 12H, CH_3), 2.27 (s, 6H, CH_3).

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