Supplementary Material (ESI) for New Journal of Chemistry

Supporting information for:

A cytotoxic bis(carbene)gold(I) complex of ferrocenyl complexes: synthesis and structural characterisation

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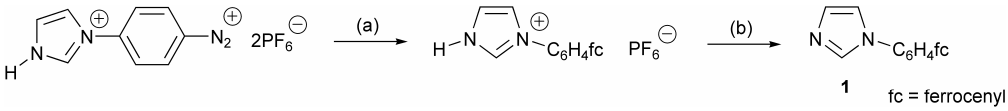
General Procedures

Reactions were carried out under argon using standard Schlenk and vacuum-line techniques. All solvents were dried according to standard literature methods under nitrogen atmosphere.[1] The infrared spectra were recorded on a Nicolet Avatar 330 FT-IR with ATR (attenuated total reflection) accessory (Smart Performer) or on a Nicolet 5700 FT-IR with ATR diamond window. Starting materials are commercially available and were used without further purification.

Alternative prepeartion of 1-(4-ferrocenylphenyl)imidazole, 1



Scheme S1. Alternative synthetic method for **1**: (a) Ferrocene, DMSO/acetone; (b) $NaHCO_3$.

Compound **1** was also prepared by the portionwise addition of 4-(1*H*-imidazolyl)phenyldiazonium bishexafluorophosphate (2.06 g, 4.45 mmol) to a solution of ferrocene (3.31 g, 17.8 mmol) in a mixture of DMSO and acetone (1:3) (50 ml). Upon ultrasonication, gas evolution and a darkening of the reaction mixture was observed. After complete addition of the diazonium salt, the mixture was ultrasonically radiated for another 30 min. Acetone was removed *in vacuo* to yield a precipitate, which was filtered off. The filtrate was washed several times with *n*-hexane to remove residual ferrocene, followed by addition of a saturated $NaHCO_3$ solution (200 ml). The mixture was extracted with CH_2Cl_2 (3 x 30 ml), washed with H_2O (1 x 100 ml) and dried over Na_2SO_4. The crude product solution was reduced to 2 ml and chromatographed on a column, charged with silica gel 60 (50 g), with diethyl ether/CH_2Cl_2 (1:1) as eluent. The dark orange fraction was collected and dried *in vacuo*, to yield red-brown, microcrystalline material (0.34 g, 16%).

IR spectrum (KBr) of 1-[*(E)*-2-butenyl]-3-(4-ferrocenylphenyl)imidazolium bromide, 2

ν_{max}(KBr)/cm^{-1} 3165m, 3090s, 3066s, 2964s, 2854m, 1614s, 1552vs, 1412s, 1203s, 1105s, 1068s, 1030s, 974m, 887m, 845s, 825vs, 808s, 737s, 640s, 619s, 540m, 507s and 490s;

IR spectrum (KBr) of 1-[*(E)*-2-butenyl]-3-(4-ferrocenylphenyl)imidazolium tetrafluoroborate, 3

ν_{max}(KBr)/cm^{-1} 3165s, 3090s, 3028s, 2854m, 1616m, 1566s, 1556s, 1402s, 1107vs, 1070vs, 1032vs, 887w, 835m, 812m, 752m, 627m, 532m, 520m, 509m, 486m and 463m.

IR spectrum (KBr) of bis{1-[*(E)*-2-butenyl]-3-(4-ferrocenylphenyl)-2*H*-imidazol-2-ylidene}gold(I) tetrafluoroborate, 4

ν_{max}(KBr)/cm^{-1} 3167w, 3136w, 2983m, 2964m, 1606w, 1529s, 1491m, 1460m, 1423m, 1261m, 1174s, 1105vs, 1084vs, 1030vs, 968m, 887m, 820s, 800s, 743m and 520s;

References

1 R. J. Errington, *Advanced Practical Inorganic and Metalorganic Chemistry*, Chapman & Hall, London, 1997, pp. 296.