Supporting Information

Detailed structural, spectroscopic and electro-chemical trends of halido mono- and bis(NHC) complexes of Au(I) and Au(III)

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Table SI-1. Selected X-ray crystallographic data for complexes **2**, **3**, **5**–**9.**

	2	**3**	**5**	**6**
Formula	$C_{13}H_{18}AuBrN_2$	$C_{13}H_{18}AuIN_2$	$C_{13}H_{18}AuCl_3N_2$	$C_{13}H_{18}AuBr_3N_2$
Formula weight	479.17	526.16	505.61	638.99
Colour, habit	Yellow, block	Colorless, block	Yellow, block	Gold, block
Crystal size/mm	0.36 × 0.20 × 0.10	0.50 × 0.24 × 0.12	0.60 × 0.48 × 0.28	0.28 × 0.28 × 0.20
T/K	100(2)	100(2)	100(2)	223(2)
Crystal system	Monoclinic	Monoclinic	Tetragonal	Tetragonal
Space group	$P2_1/n$	$P2_1/c$	$P4_12_12$	$P4_32_12$
a/Å	9.6791(11)	10.5679(14)	8.7682(7)	9.0114(3)
b/Å	7.8592(9)	10.6108(15)	8.7682(7)	9.0114(3)
c/Å	19.129(2)	13.2940(18)	20.718(3)	21.0622(16)
α/°	90	90	90	90
β/°	100.293(3)	93.197(3)	90	90
γ/°	90	90	90	90
V/Å^3	1431.7(3)	1488.4(4)	1592.8(3)	1710.36(15)
Z	4	4	4	4
D_c/g cm^{-3}	2.223	2.348	2.108	2.482
Radiation used	Mo-Kα	Mo-Kα	Mo-Kα	Mo-Kα
μ/mm^{-1}	13.047	11.940	9.727	15.599
θ range/°	2.16 to 27.50	1.93 to 27.49	2.52 to 27.50	2.46 to 27.49
Reflection collected	9793	10345	11256	11963
Max., min. transmission	0.2679, 0.1768	0.3283, 0.0658	0.1715, 0.0677	0.1464, 0.0972
Final R indices	R_1 = 0.0427,	R_1 = 0.0346,	R_1 = 0.0248,	R_1 = 0.0210,
R indices (all data)	R_1 = 0.0487,	R_1 = 0.0369,	R_1 = 0.0257,	R_1 = 0.0221,
Goodness-of-fit	1.074	1.095	1.162	1.074
Peak/hole/e Å^{-3}	4.547/–3.736	4.335/–1.600	2.561/–1.081	0.706/–0.723

Table SI-1. (Continued).

	7	**8**·0.67$CHCl_3$	**9**·0.67CH_2Cl_2
Formula	$C_{13}H_{18}AuI_3N_2$	$C_{26.67}H_{36.67}$ $AuBCl_4F_4N_4$	$C_{26.67}H_{37.33}AuBBr$ $Cl_{1.33}F_4N_4$
Formula weight	779.96	838.84	904.80
Colour, habit	Red, block	Colorless, block	Yellow, plate
Crystal size/mm	0.60 × 0.40 × 0.20	0.30 × 0.24 × 0.08	0.40 × 0.30 × 0.10
T/K	100(2)	223(2)	223(2)
Crystal system	Tetragonal	Monoclinic	Monoclinic
Space group	$P4_32_12$	$C2/c$	$C2/c$
a/Å	9.3135(12)	40.5846(15)	40.65(3)
b/Å	9.3135(12)	10.9152(4)	10.902(8)
c/Å	21.152(4)	25.3892(9)	25.010(18)
α/°	90	90	90
β/°	90	116.7480(10)	116.24(3)
γ/°	90	90	90
V/Å^3	1834.8(5)	10043.6(6)	9941(13)
Z	4	12	12
D_c/g cm^{-3}	2.824	1.664	1.814
Radiation used	Mo-Kα	Mo-Kα	Mo-Kα
μ/mm^{-1}	13.057	4.759	7.004
θ range/°	2.39 to 27.47	1.80 to 27.50	1.66 to 27.50
Reflection collected	12445	34858	34744
Max., min. transmission	0.1799, 0.0473	0.7020, 0.3294	0.5410, 0.1660
Final R indices	R_1 = 0.0267,	R_1 = 0.0405,	R_1 = 0.0471,
R indices (all data)	R_1 = 0.0269,	R_1 = 0.0553,	R_1 = 0.0693,
Goodness-of-fit	1.146	1.017	0.993
Peak/hole/e Å^{-3}	1.281/–2.390	1.506/–0.676	1.713/–1.436