Supplementary Material (ESI) for Dalton Transactions

Chemical and Biological Studies of Gold(III) Complexes with Uninegative Bidentate N-N Ligands

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Electronic Supplementary Information:

Table S1. Important least-squares planes and dihedral angles for **2**.

A	Equations of planes in the form $lX + mY + nZ = p$ where X, Y, Z are orthogonal coordinates in Å. Deviations (Å) of atoms from the planes are given in square brackets.
Plane (1)	Au(2), Cl(3), Cl(4), N(2), N(3); $-0.4295X + 0.7905Y + 0.4367Z = 6.3216$ [Au(1) -2.2793, Cl(1) -3.7534, Cl(2) -3.9686, N(1) -0.7614, N(4) -0.9758, C(1) -0.3497, C(2) 0.7439, C(3) 0.9625, C(4) 0.8288, C(5) 0.4342, C(6) -0.6751]
Plane (2)	Au(1), Cl(1), Cl(2), N(1), N(4); $0.6046X + 0.7331Y - 0.3115Z = -0.1343$ [Au(2) -2.2648, Cl(3) -3.8717, Cl(4) -3.7618, N(2) -0.9191, N(3) -0.7695, C(1) 0.8603, C(2) 0.4573, C(3) -0.6519, C(4) -0.3198, C(5) 0.7300, C(6) 0.9175]
Plane (3)	C(3), C(1), N(1), N(2); $0.4271X + 0.6906Y + 0.5836Z = 4.8313$ [Au(1) 0.0129, Au(2) 0.2578, Cl(1) -1.8289, Cl(2) 0.0507, Cl(3) -1.5296, Cl(4) 0.6123, N(3) 1.7993, N(4) 1.6626, C(2) -0.0091, C(4) 3.1152, C(5) 3.7887, C(6) 2.8781]
Plane (4)	Au(2), C(3), C(1), Au(1), N(1), N(2); $0.4425X + 0.7238Y + 0.5295Z = 4.6326$ [Cl(1) -1.7793, Cl(2) -0.0224, Cl(3) -1.7502, Cl(4) 0.2678, N(3) 1.6286, N(4) 1.5471, C(2) 0.0510, C(4) 2.9163, C(5) 3.6274, C(6) 2.7682]
Plane (5)	Au(2), C(6), C(4), Au(1), N(3), N(4); $-0.2447X + 0.8851Y - 0.3960Z = -0.5576$
Plane (6)	C(4), C(6), N(3), N(4); $-0.2416X + 0.8470Y - 0.4736Z = -1.3445$
Plane (7)	N(1), N(2), N(3), N(4); $0.1315X + 0.9876Y + 0.0858Z = 3.4705$ [Au(1) -0.9153, Au(2) -0.9424, Cl(1) -1.8712, Cl(2) -1.9689, Cl(3) -2.0372, Cl(4) -1.8782, C(1) 0.8628, C(2) 1.2889, C(3) 0.7077, C(4) 0.9091, C(5) 1.3566, C(6) 0.7603]
B	Dihedral angles (º) between planes
	(1)-(2): 79.4; (1)-(3): 51.9; (1)-(4): 52.2; (1)-(7): 40.4; (2)-(3): 54.4; (2)-(7): 39.0; (3)-(4): 3.7; (3)-(6): 78.1; (3)-(7): 38.0; (4)-(5): 71.2; (5)-(6): 5.0; (6)-(7): 40.2;

Table S2. ^{1}H NMR Data for Picolinamide, $[Au(Hpla)Cl_2]Cl$, and **1**.

Compound	Solvent	Hydrogen atoms on pyridine				NH
Picolinamide	$CDCl_3$	8.57(d)	8.19(d)	7.85(t)	7.44(t)	6.15(b)
$[Au(Hpla)Cl_2]Cl$	D_2O	8.84(d)	8.60(t)	8.42(d)	8.12(t)	
1	$CDCl_3$	9.44(d)	8.40(t)	8.15(d)	7.92(t)	6.46(b)
1	$(CD_3)_2CO$	9.40(d)	8.67(t)	8.19(t)	8.08(d)	7.78(b)
1	D_2O	9.38(d)	8.48(t)	8.16(t)	8.02(d)	
1	$(CD_3)_2SO$	9.21(d)	8.52(t)	8.04(t)	7.94(d)	8.90(s)

Table S3. ^{1}H and ^{13}C Data for complexes **2** and **3** (δ, in $CDCl_3$)

Compound	Atoms on Pyrazoyl Ring	CH_3
^{1}H		
Pyrazole	12.59, 7.64(d), 6.36(q)	
2	7.99(d), 6.72(t)	
3-methylpyrazole	12.22, 7.51(d), 6.08(d)	2.36(s)
3	7.79(d), 6.48(d); 7.75(d), 6.49(d)	2.55(s)
^{13}C		
Pyrazole	136.5, 133.8, 104.8	
2	150.4, 142.1	
3-methylpyrazole	142.9, 134.7, 104.2	11.8
3	151.2, 141.4, 109.1; 150.9, 140.8, 109.4	14.4