Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Non-covalent interactions in coinage metal complexes of 1,2,4-triazole-based *N*-heterocyclic carbenes

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Table S1. Crystallographic data for **2**, **3**, **4**, **5**, **7**, **8** and **9**

Compound	**2**	**3**·C_7H_8	**4**·C_6H_6	**5**·0.5 C_6H_6
chem formula	$C_{42}H_{52}AgIN_8$	$C_{21}H_{26}AuClN_4$ ·C_7H_8	$C_{21}H_{26}AuBrN_4$ ·C_6H_6	$C_{21}H_{26}AuIN_4$ ·0.5 C_6H_6
cryst syst	monoclinic	monoclinic	orthorhombic	monoclinic
space group	*C*2/*c*	$P2_1/c$	$Pca2_1$	$P2_1/c$
a/Å	21.4227(11)	14.5680(4)	19.9850(5)	13.95419(10)
b/Å	8.8240(4)	11.8901(10)	8.5330(18)	14.5710(5)
c/Å	23.7341(6)	17.570(1)	31.1480(12)	14.1930(8)
α/deg	90	90	90	90
β/deg	111.380(3)	118.093(4)	90	119.557(5)
γ/deg	90	90	90	90
Z	4	4	8	4
unit cell volume/$Å^3$	4177.8(3)	2684.8(3)	5311.7(11)	2436.1(3)
density/g.cm^{-3}	1.437	1.630	1.724	1.901
abs coeff, μ/mm^{-1}	1.26	5.60	7.07	7.32
F(000)	1840	1304	2688	1332
h; k; l – min, max	-27, 25; -10, 11; -30, 30	-18, 18; -14, 15; -22, 19	-25, 19; -10, 10; -38, 36	-17, 14; -18, 18; -17, 18
$\theta_{min;\ max}$/deg	1.8; 27.5	2.2; 27.5	4.1; 26.4	1.7; 27.5
reflections	19021	26335	46503	20514
total (R_{int}) [a]	4705 (0.038)	6121 (0.110)	10365 (0.152)	5559 (0.060)
observed [I>2σ(I)]	3950	5108	9472	4762
no. of parameters	236	307	569	271
max/min ρ/e$Å^{-3}$	1.15; -1.08	4.33; -2.44	2.17; -2.15	6.43; -2.28
goodness of fit on F^2 [b]	1.10	1.13	1.09	1.08
final R1 values (I>2σ(I)) [c]	0.040	0.041	0.047	0.044
final wR2 values (I>2σ(I))	0.087	0.117	0.121	0.113

[a] $R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$. [b] $S = [\sum(w(F_o^2 - F_c^2)^2) / (N_{diffr.} - N_{param.})]^{½}$. [c] Weighting scheme : $w = [\sigma^2(F_o^2) + (w_1P)^2 + w_2P]^{-1}$, where $P = [\max(F_o^2) + 2F_c^2]$, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2) / (\sum w(F_o^2)^2)]^{½}$

Table S1 continued

Compound	**7**	**8**	**9Cu/Br**·C_4H_8O
chem formula	$C_{19}H_{21}AgClN_3$	$C_{19}H_{21}AuClN_3$	$C_{19}H_{21}Br_{0.5}Cl_{0.5}CuN_3$ ·1.5 C_4H_8O
cryst syst	triclinic	triclinic	monoclinic
space group	*P*-1	*P*-1	$P2_1/c$
a/Å	8.9450(3)	8.9260(3)	9.2450(9)
b/Å	10.9861(7)	11.0071(6)	16.2720(14)
c/Å	10.9950(6)	11.0108(8)	17.9170(5)
α/deg	62.599(4)	62.047(5)	90
β/deg	72.338(3)	71.966(6)	111.442(4)
γ/deg	80.124(3)	80.177(5)	90
Z	2	2	4
unit cell volume/Å^3	913.39(8)	908.82(10)	2508.8(3)
density/g.cm^{-3}	1.581	1.914	1.283
abs coeff, μ/mm^{-1}	1.25	8.25	1.74
F(000)	440	504	1004
h; k; l – min, max	-10, 11; -14, 14; -14, 14	-11, 11; -14, 14; -14, 14	-12, 11; -21, 20; -23, 23
$\theta_{min;\ max}$/deg	2.1; 27.5	3.2; 28.5	4.2; 26.4
reflections	19018	19132	23685
total (R_{int}) [a]	4169 (0.035)	4560 (0.060)	5080 (0.049)
observed [I>2σ(I)]	3963	4364	4206
no. of parameters	217	217	281
max/min ρ/e Å^{-3}	1.84; -0.86	1.48; -2.22	0.48; -0.45
goodness of fit on F^2 [b]	1.07	1.13	1.09
final R1 values (I>2σ(I)) [c]	0.032	0.024	0.042
final wR2 values (I>2σ(I))	0.092	0.062	0.102

[a] $R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$. [b] $S = [\sum(w(F_o^2 - F_c^2)^2) / (N_{diffr.} - N_{param.})]^{½}$. [c] Weighting scheme : $w = [\sigma^2(F_o^2) + (w_1P)^2 + w_2P]^{-1}$, where $P = [\max(F_o^2) + 2F_c^2]$, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2) / (\sum w(F_o^2)^2)]^{½}$