Supplementary Information

Silver(I), gold(I) and palladium(II) complexes of a NHC-pincer ligand with an aminotriazine core: a comparison with pyridyl analogues

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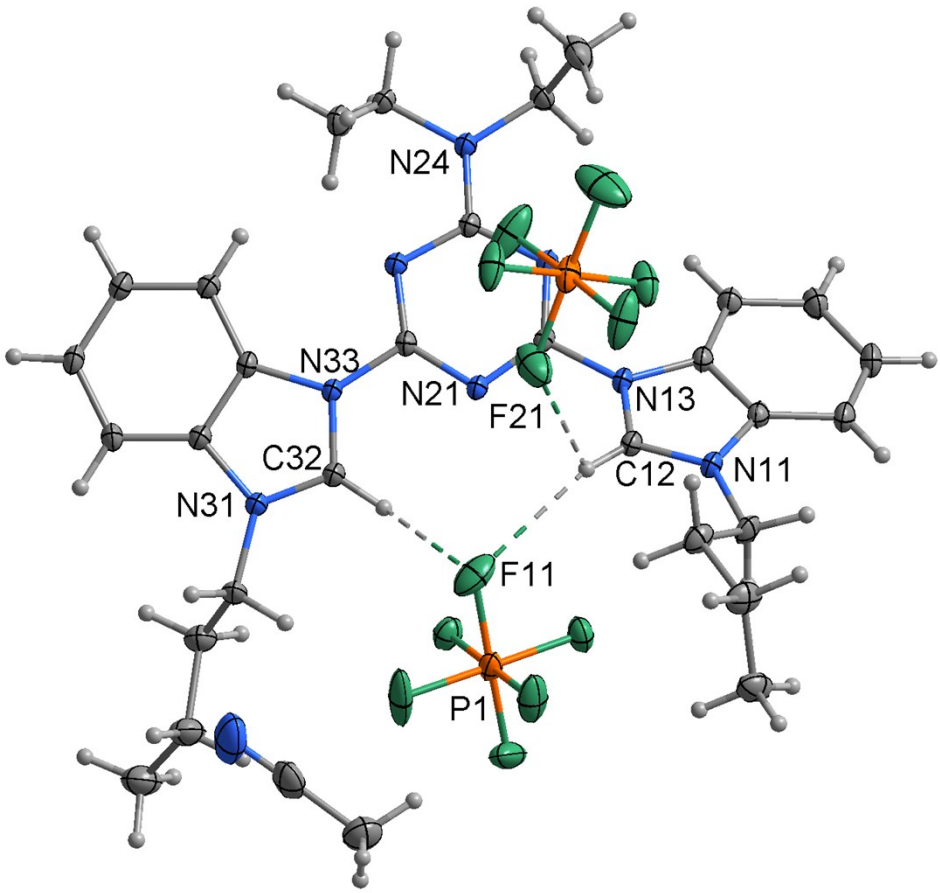
Table S1. Crystal data and structure refinement.

	5·2PF$_6$	**6**·2PF$_6$	**7**·2PF$_6$
Empirical formula	$C_{31}H_{41}F_{12}N_9P_2$	$C_{60}H_{75}Ag_2F_{12}N_{17}P_2$	$C_{60}H_{75}Au_2F_{12}N_{17}P_2$
Formula weight	829.67	1540.05	1718.24
Crystal system	Monoclinic	Triclinic	Triclinic
space group	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
a (Å)	8.5126(3)	11.8333(4)	11.826(2)
b (Å)	25.0522(8)	16.5871(5)	16.6381(18)
c (Å)	17.3391(5)	18.7892(6)	19.0617(19)
α (°)	90	70.639(3)	71.356(9)
β (°)	93.315(3)	75.383(3)	75.241(11)
γ (°)	90	69.878(3)	70.279(12)
V (Å^3)	3691.5(2)	3227.0(2)	3299.6(7)
Z	4	2	2
ρ (g cm^{-3})	1.493	1.585	1.729
μ (mm^{-1})	0.216	0.745	4.577
$T_{max/min}$	0.970/0.944	0.954/0.895	0.703/0.444
Crystal dimensions (mm)	0.34 x 0.26 x 0.15	0.189 x 0.181 x 0.071	0.34 x 0.20 x 0.085
θ_{max} (°)	34.49	32.65	31.0
Reflections collected	97461	43244	43785
Unique reflections	15185	21262	21024
R_{int}	0.0659	0.0579	0.0456
Reflections (I>2σ(I))	9874	11934	12661
Data/restraints/parameters	15185 / 0 / 492	21262 / 0 / 847	21024 / 21 / 847
G.O.F. (F^2)	0.950	0.860	0.817
$R1$, $wR2$ [I>2σ(I)]	0.0476, 0.1186	0.0463, 0.0796	0.0383, 0.0687
$R1$, $wR2$ [all data]	0.0791, 0.1262	0.1031, 0.0889	0.0725, 0.0736
$\Delta\rho_{max,min}$ (e.Å^{-3})	0.710, -0.502	1.471, -0.819	2.001, -2.151

	8·2PF$_6$	**9**·2PF$_6$	**11**.2BPh$_4$
Empirical formula	$C_{91}H_{114}Au_4BrClF_{12}N_{26}P_2$	$C_{31}H_{39}ClF_6N_9PPd$	$C_{102}H_{98}Au_2B_2N_{10}$
Formula weight	2765.25	824.53	1879.45
Crystal system	Monoclinic	Triclinic	Monoclinic
space group	$P2_1/n$	$P\bar{1}$	$P2_1/c$
a (Å)	16.7514(2)	10.7399(2)	13.4178(2)
b (Å)	15.6398(2)	11.5769(2)	17.8673(3)
c (Å)	39.1287(10)	15.0394(3)	17.5027(2)
α (°)	90	106.461(2)	90
β (°)	91.285(2)	107.735(2)	100.730(1)
γ (°)	90	90.060(2)	90
V (Å^3)	10248.7(3)	1700.22(5)	4122.73(10)
Z	4	2	2
ρ (g cm^{-3})	1.792	1.611	1.514
μ (mm^{-1})	6.235	0.743	3.61
$T_{max/min}$	0.484/0.221	0.892/0.723	1.00/803
Crystal dimensions (mm)	0.41 x 0.26 x 0.16	0.63 x 0.43 x 0.15	0.245x0.189x0.126
θ_{max} (°)	29.00	38.63	32.04
Reflections collected	109934	66083	51745
Unique reflections	27241	18811	13579
R_{int}	0.0488	0.0336	0.0572
Reflections (I>2σ(I))	18091	15338	9061
Data/restraints/parameters	27241 / 21 / 1250	18811 / 0 / 447	13579 / 0 / 525
G.O.F. (F^2)	1.023	0.976	0.844
$R1$, $wR2$ [I>2σ(I)]	0.0657, 0.1469	0.0276, 0.0658	0.0281,0.0462
$R1$, $wR2$ [all data]	0.1038, 0.1569	0.0379, 0.0680	0.0589, 0.0497
$\Delta\rho_{max,min}$ (e.Å^{-3})	4.498, -2.442	0.768, -0.671	2.516, -0.833

Figure S1. Projection of **5**·2PF_6. Ellipsoids displayed at the 50% probablilty level.



Extended discussion of the structure of 8

The orientations of the ligand are such that the triazine group of each ligand is approximately parallel to a benzimidazolyl ring of an adjacent ligand. The closest contacts between the triazine group (12n) of ligand (1) are to ring (23n) (C(124)···C(234) 3.46(1), N(123)···C(234) 3.51(1) Å, inter-planar angle 4.1(3)°); between the triazine group (22n) of ligand (2) and ring (11n) (N(113)...C(226) 3.67(1) Å, inter-planar angle 9.9(3)°); and between triazine (32n) and ring (21n) (N(211)···N(323) 3.28(1), C(212)···C(322) 3.30(1) and C(214)···C(324) 3.43(1) Å, inter-planar angle 5.2(3)°). The cations lie in sheets parallel to the (-101) plane as shown in Figure 7(b). There appears to be significant interaction from the coordinated halide Br(2),Cl(2) to the π electrons of the

adjacent molecule with the distance between Br(2), Cl(2) and the centroid of the ring (32n) of the centrosymmetrically related molecule at (1-x,1-y,1-z) being 3.17 Å.