Table 1. Crystal data and structure refinement for **2**.

Identification code	ZA33
Empirical formula	$C_6H_{12}N_3PAuCl$
Formula weight	389.6
Temperature	298 (2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	*R-3*
Unit cell dimensions	a = 22.587(2)Å
	c = 9.814(2) Å
Volume, Z	V = 4336(1)Å ^{3}, 18
Density (calculated)	D_x = 2.686 Mg m^{-3}
Absorption coefficient	15.638 mm^{-1}
Crystal size	0.40 x 0.08 x 0.08 mm
Theta range for data collection	4 - 45
Limiting indices	0<=h<=21, 0<=k<=21, -10<=l<=10
Reflections collected	4140
Independent reflections	1274 [R(int) = 0.0287]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
F(000)	3240
Goodness-of-fit on F^2	1.02
Final R indices [I>2sigma(I)]	R1 = 0.0283, wR2 = 0.0274
Largest diff. peak and hole	0.57 and –0.83 e.A^-3

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Au1	0.343720	0.026690	0.177030	0.0372
Cl1	0.436460	0.014790	0.124550	0.0570
P1	0.253650	0.039000	0.218460	0.0305
N3	0.181240	0.102500	0.146580	0.0292
N2	0.114790	-0.017580	0.219810	0.0412
N1	0.180850	0.073570	0.387620	0.0517
C1	0.168230	-0.034990	0.191630	0.0459
C2	0.242920	0.099940	0.111950	0.0398
C3	0.240950	0.065960	0.386060	0.0388
C4	0.119540	0.007510	0.361550	0.0577
C5	0.120550	0.035650	0.125490	0.0395
C6	0.183530	0.123750	0.289700	0.0410

Table 3. Bond lengths [A] and angles [deg] for **2**.

Au1-Cl1	2.299 (4)
Au1-P1	2.224 (4)
C1-P1	1.833 (9)
C2-P1	1.838 (13)
C3-P1	1.826 (11)
C2-N3	1.463 (16)
C5-N3	1.460 (11)
C6-N3	1.477 (13)
C6-N3	1.477 (13)
C1-N2	1.471 (18)
C4-N2	1.486 (15)
C3-N1	1.451 (19)
C4-N1	1.464 (13)
C6-N1	1.464 (16)
P1-C1	1.833 (9)
N1-C1	1.471 (18)
P1-C2	1.838 (13)
N3-C2	1.463 (16)
P1-C3	1.826 (11)
N1-C3	1.451 (19)
N1-C4	1.486 (15)
N1-C4	1.464 (13)
N3-C5	1.460 (11)
N1-C5	1.471 (15)
N3-C6	1.477 (13)
N1-C6	1.464 (16)
Cl1 -Au -P1	177.6 (1)
Au -P1 -C2	117.4 (4)
C1 -P1 -C2	97.4 (5)
Au -P1 -C3	120.8 (4)
C1 -P1 -C3	99.4 (5)
C2 -P1 -C3	99.3 (6)
C2 -N3 -C5	110.3 (9)
C2 -N3 -C6	110.8 (8)
C5 -N3 -C6	109.5 (7)
C1 -N2 -C4	111.4 (1)
C1 -N2 -C5	110.6 (9)
C4 -N2 -C5	108.5 (1)
C3 -N1 -C4	110.0 (1)
C3 -N1 -C6	113.9 (8)
C4 -N1 -C6	109.0 (9)
P1 -C1 -N2	111.1 (7)
P1 -C2 -N3	112.5 (7)
P1 -C3 -N1	111.2 (7)
N2 -C4 -N1	113.8 (8)
N3 -C5 -N2	114.2 (9)
N3 -C6 -N1	113.1 (1)

Table 4. Anisotropic displacement parameters (A^2) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Au1	0.03370	0.03517	0.04284	-0.00275	-0.00094	0.02175
Cl1	0.04180	0.06877	0.06060	-0.01940	-0.00955	0.03679
P1	0.03462	0.02647	0.03064	-0.00153	0.00030	0.01679
N3	0.02405	0.03250	0.03108	0.00119	-0.00302	0.01650
N2	0.03156	0.02464	0.06757	0.01356	-0.00369	0.00740
N1	0.05449	0.07122	0.02958	-0.00224	0.00120	0.04330
C1	0.05931	0.01864	0.06003	0.00146	-0.01746	0.01971
C2	0.03946	0.03570	0.04453	0.01201	0.00156	0.02234
C3	0.04121	0.04843	0.02699	-0.00429	-0.00782	0.02963
C4	0.04597	0.08157	0.04560	0.04244	0.02563	0.04252
C5	0.03592	0.03711	0.04558	0.00144	-0.01170	0.01412
C6	0.03728	0.04540	0.04052	-0.00251	-0.00034	0.02343