

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

Identification code	ZA27
Empirical formula	$C_{14}H_{24}Au_2N_8P_2$
Formula weight	760.29
Temperature	293 (2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cc_{cm}
Unit cell dimensions	$a = 6.011 (1) \text{ \AA}$ $b = 23.877 (6) \text{ \AA}$ $c = 6.914 (1) \text{ \AA}$
Volume, Z	$V = 992.3 (3) \text{ \AA}^3, 2$
Density (calculated)	$D_x = 2.544 \text{ Mg m}^{-3}$
Absorption coefficient	14.945 mm^{-1}
Crystal size	0.35 x 0.15 x 0.10 mm
Theta range for data collection	8.5 - 12.5
Limiting indices	$-1 \leq h \leq 7, 0 \leq k \leq 30, -8 \leq l \leq 0$
Reflections collected	726
Independent reflections	620 [R(int) = 0.0281]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9680 and 0.375
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	620 / 0 / 62
Goodness-of-fit on F^2	1.031

Final R indices [$I > 2\sigma(I)$] $R_1 = 0.0337$, $wR_2 = 0.0791$

Largest diff. peak and hole 1.436 and -1.141 e.Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Au1	0.0000	0.0000	0.0000	0.0449 (2)
P1	-0.1570 (8)	0.0879 (2)	0.0000	0.0324 (9)
N1	-0.5350 (27)	0.1502 (8)	0.0000	0.046 (5)
N2	-0.2130 (24)	0.1892 (5)	0.1753 (19)	0.045 (3)
N3	-0.4148 (55)	0.0829 (22)	0.0000	0.065
C1	-0.4774 (55)	0.0898 (19)	0.0000	0.049 (8)
C2	-0.0991 (33)	0.1355 (6)	0.2040 (19)	0.043 (3)
C3	-0.4562 (22)	0.1811 (7)	0.1772 (27)	0.042 (4)
C4	-0.1439 (44)	0.2178 (8)	0.0000	0.046 (5)
C5	-0.2629 (42)	0.0527 (11)	0.0000	0.068

Table 3. Bond lengths [Å] and angles [deg] for **1**.

Au1-C5 ⁱ	2.02 (3)
Au1-C5	2.02 (3)
Au1-P1	2.302 (5)
Au1-P1 ⁱ	2.302 (5)
P1-C5	1.06 (2)
P1-N3	1.55 (3)
P1-C1	1.93 (3)
P1-C2	1.844 (14)
P1-C2 ⁱⁱ	1.844 (14)
N1-C3	1.51 (2)
N1-C3 ⁱⁱ	1.51 (2)
N1-C1	1.48 (5)
N1-N3	1.76 (5)
N1-C4	1.45 (2)
N1-C2	1.47 (2)
N1-C3	1.47 (2)
N3-C5	1.16 (4)
C1-C5	1.56 (5)
C2-C2 ⁱⁱⁱ	1.35 (4)
C3-C3 ^{iv}	1.14 (3)
C4-N2 ⁱⁱ	1.45 (2)
C4-C4 ^v	2.00 (5)
C5 ⁱ -Au1-C5	179.998 (2)
C5 ⁱ - Au1-P1	152.7 (7)
C5-Au1-P1	27.3 (7)
C5 ⁱ -Au1-P1 ⁱ	27.3 (7)
C5-Au1-P1 ⁱ	152.7 (7)
P1-Au1-P1 ⁱ	180.0
C5-P1-N3	48.5 (22)
C5-P1-C1	54.2 (20)
N3-P1-C1	5.7 (30)
C5-P1-C2	127.3 (7)
N3-P1-C2	103.6 (14)
C1-P1-C2	100.1 (11)
C5-P1-C2 ⁱⁱ	127.3 (7)
N3-P1-C2 ⁱⁱ	103.6 (14)
C1-P1-C2 ⁱⁱ	100.1 (11)
C2-P1-C2 ⁱⁱ	99.7 (9)
C5-P1-Au1	61.3 (14)
N3-P1-Au1	109.8 (19)
C1-P1-Au1	115.5 (14)
C2-P1-Au1	119.0 (5)
C2 ⁱⁱ -P1-Au1	119.0 (5)
C3-N1-C3 ⁱⁱ	108.9 (18)
C3-N1-C1	113.7 (11)
C3 ⁱⁱ -N1-C1	113.7 (11)
C3-N1-N3	108.5 (11)
C3 ⁱⁱ -N1-N3	108.5 (11)
C1-N1-N3	10.7 (18)

C4-N2-C2	112.9 (14)
C4-N2-C3	110.7 (16)
C2-N2-C3	110.3 (13)
C5-N3-P1	42.8 (16)
C5-N3-N1	152.5 (36)
P1-N3-N1	109.8 (28)
C5-C1-N1	138.0 (26)
C5-C1-P1	33.2 (11)
N1-C1-P1	104.8 (21)
C2 ⁱⁱⁱ -C2-N2	118.4 (8)
C2 ⁱⁱⁱ -C2-P1	121.8 (14)
N2-C2-P1	110.3 (10)
C3 ^{iv} -C3-N2	117.9 (23)
C3 ^{iv} -C3-N1	125.1 (15)
N2-C3-N1	111.6 (12)
N2 ⁱⁱ -C4-N2	113.2 (17)
N2 ⁱⁱ -C4-C4 ^v	100.3 (15)
N2-C4-C4 ^v	100.3 (15)
P1-C5-N3	88.8 (29)
P1-C5-C1	92.6 (22)
N3-C5-C1	3.8 (34)
P1-C5-Au1	91.4 (16)
N3-C5-Au1	179.8 (25)
C1-C5-Au1	176.0 (21)

Symmetry codes: (i) $-x; -y; -z$; (ii) $x; y; -z$; (iii) $-x; y; \frac{1}{2}-z$; (iv) $-1-x; y; \frac{1}{2}-z$;
(v) $-\frac{1}{2}-x; \frac{1}{2}-y; -z$.

Table 4. Anisotropic displacement parameters (A^2) for **1**.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Au1	0.0534 (3)	0.0276 (3)	0.0535 (3)	0.0070 (4)	0.000	0.000
P1	0.037 (2)	0.024 (2)	0.037 (2)	0.004 (2)	0.000	0.000
N1	0.048 (13)	0.034 (8)	0.057 (10)	0.017 (8)	0.000	0.000
N2	0.062 (7)	0.031(6)	0.041(5)	0.002(6)	- 0.001(6)	0.001 (5)
C1	0.032 (12)	0.063 (18)	0.052 (11)	- 0.014 (18)	0.000	0.000
C2	0.063 (8)	0.030 (6)	0.037 (7)	0.005 (7)	- 0.010 (6)	0.006 (5)
C3	0.043 (10)	0.037 (7)	0.046 (5)	0.002 (5)	0.019 (5)	- 0.012 (6)
C4	0.065 (14)	0.024 (9)	0.048 (10)	-0.012 (9)	0.000	0.000

