

[(1,10-Phenanthrolin-5-yl)ethynyl]- (triphenylphosphine-κP)gold(I)

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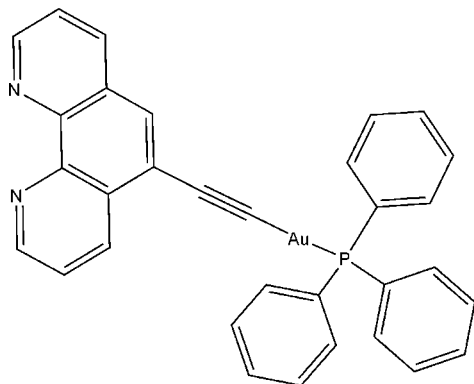
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.038; wR factor = 0.094; data-to-parameter ratio = 17.9.

The title compound, $[\text{Au}(\text{C}_{14}\text{H}_7\text{N}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$, was synthesized by the reaction of $[\text{AuCl}(\text{PPh}_3)]$ and 5-ethynyl-1,10-phenanthroline. The coordination geometry of gold(I) is two-coordinate (linear) and no intermolecular $\text{Au}\cdots\text{Au}$ interactions are observed.

Related literature

For related literature, see: McAuliffe *et al.* (1979); Pomestchenko *et al.* (2005); Xu *et al.* (2006); Yam *et al.* (1999); Ziessel *et al.* (1996, 1998).



Experimental

Crystal data

$[\text{Au}(\text{C}_{14}\text{H}_7\text{N}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$	$V = 2553.9$ (3) Å ³
$M_r = 662.45$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.6927$ (7) Å	$\mu = 5.85$ mm ⁻¹
$b = 18.9137$ (11) Å	$T = 293$ (2) K
$c = 16.0457$ (13) Å	$0.46 \times 0.35 \times 0.20$ mm
$\beta = 104.512$ (4)°	

Data collection

Rigaku Mercury 70 CCD diffractometer	18982 measured reflections
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 2000)	5803 independent reflections
$T_{\min} = 0.461$, $T_{\max} = 1.000$	4969 reflections with $I > 2\sigma(I)$
(expected range = 0.143–0.311)	$R_{\text{int}} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	325 parameters
$wR(F^2) = 0.094$	H-atom parameters constrained
$S = 1.10$	$\Delta\rho_{\text{max}} = 1.18$ e Å ⁻³
5803 reflections	$\Delta\rho_{\text{min}} = -1.75$ e Å ⁻³

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2351).

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supplementary materials

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[(1,10-Phenanthrolin-5-yl)ethynyl](triphenylphosphine- κ P)gold(I)

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Comment

Acetylide-functionalized diimines have been used widely in the design of multi-component transition metal complexes composed of discrete redox and/or photoactive sub-units. (Pomestchenko *et al.*, 2005; Ziessel *et al.*, 1998) We have focused on such bridging ligands for the design of d–f bimetallic arrays by introducing d-block chromophores and f-block lumino-phores bound to acetylide and bipyridine/phenanthroline, respectively.

As shown in Fig. 1, the coordination geometry of Gold(I) is two-coordinate (linear), the Gold(I) atom is bound to (1,10-phenanthrolin-5-yl)ethynyl as well as coordinated to P atom from triphenylphosphine. The bond distance [2.013 (5) Å] of gold(I)–alkynyl is comparable to those observed in other Gold (I) acetylide complexes (Yam *et al.*, 1999). The structure of (1,10-phenanthrolin-5-yl)ethynyl is normal compared to the platinum compound (Xu *et al.*, 2006). Unlike some Gold (I) acetylide complexes (Yam *et al.*, 1999), no intermolecular Au...Au interaction is observed.

Experimental

[AuCl(PPh₃)] (McAuliffe *et al.*, 1979) (100 mg, 0.202 mmol) and 5-Ethynyl-1,10-phenanthroline (Ziessel *et al.*, 1996) (40.4 mg, 0.02 mmol) were stirred in a solution of CH₃ONa in MeOH (0.1 M, 15 ml) for 8 h. After filtration, the solid precipitate was washed with 2 ml MeOH and recrystallized by diffusion of n-hexane into its dichloromethane solution. Yellow crystals suitable for single-crystal X-ray analysis were obtained after 5 days.

Refinement

All H atoms were included in calculated positions with C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

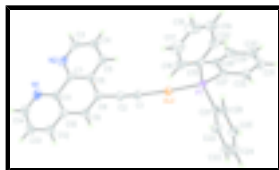


Fig. 1. A view of the compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

[(1,10-Phenanthrolin-5-yl)ethynyl](triphenylphosphine- κ P)gold(I)

Crystal data

[Au(C₁₄H₇N₂)(C₁₈H₁₅P)]

$M_r = 662.45$

$F_{000} = 1288$

$D_x = 1.723 \text{ Mg m}^{-3}$

supplementary materials

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.6927$ (7) Å

$b = 18.9137$ (11) Å

$c = 16.0457$ (13) Å

$\beta = 104.512$ (4)°

$V = 2553.9$ (3) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5853 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 5.85$ mm⁻¹

$T = 293$ (2) K

Prism, yellow

$0.46 \times 0.35 \times 0.20$ mm

Data collection

Rigaku Mercury 70 CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 14.6306 pixels mm⁻¹

$T = 293$ (2) K

ω scans

Absorption correction: multi-scan
(CrystalClear; Rigaku, 2000)

$T_{\min} = 0.461$, $T_{\max} = 1.000$

18982 measured reflections

5803 independent reflections

4969 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.0$ °

$h = -11 \rightarrow 11$

$k = -24 \rightarrow 24$

$l = -20 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.094$

$S = 1.10$

5803 reflections

325 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 4.4814P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.18$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.74$ e Å⁻³

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -

factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.89976 (2)	0.047965 (11)	0.329679 (12)	0.04690 (8)
P1	0.94614 (14)	0.01607 (7)	0.20171 (8)	0.0399 (3)
N1	0.5643 (6)	0.2381 (3)	0.7534 (3)	0.0597 (12)
N2	0.3701 (6)	0.1515 (2)	0.6332 (3)	0.0568 (11)
C1	0.8451 (6)	0.0855 (3)	0.4361 (3)	0.0482 (12)
C2	0.8054 (7)	0.1118 (3)	0.4934 (3)	0.0505 (12)
C3	0.2785 (7)	0.1123 (3)	0.5744 (4)	0.0597 (14)
H3A	0.1747	0.1047	0.5780	0.072*
C4	0.3268 (7)	0.0810 (3)	0.5065 (4)	0.0576 (14)
H4A	0.2562	0.0541	0.4656	0.069*
C5	0.4785 (7)	0.0907 (3)	0.5011 (3)	0.0486 (12)
H5A	0.5133	0.0699	0.4566	0.058*
C6	0.5826 (6)	0.1320 (2)	0.5627 (3)	0.0425 (11)
C7	0.5225 (6)	0.1622 (3)	0.6278 (3)	0.0446 (11)
C8	0.7466 (6)	0.1438 (3)	0.5600 (3)	0.0447 (11)
C9	0.8397 (7)	0.1859 (3)	0.6210 (3)	0.0518 (12)
H9A	0.9449	0.1933	0.6198	0.062*
C10	0.7807 (7)	0.2192 (3)	0.6868 (3)	0.0500 (12)
C11	0.6247 (7)	0.2078 (3)	0.6917 (3)	0.0484 (12)
C12	0.8761 (8)	0.2647 (3)	0.7469 (4)	0.0635 (15)
H12A	0.9801	0.2741	0.7448	0.076*
C13	0.8153 (9)	0.2951 (3)	0.8081 (4)	0.0682 (17)
H13A	0.8767	0.3254	0.8487	0.082*
C14	0.6605 (9)	0.2801 (3)	0.8090 (4)	0.0676 (17)
H14A	0.6208	0.3010	0.8518	0.081*
C15	0.8246 (5)	0.0706 (3)	0.1168 (3)	0.0438 (11)
C16	0.8142 (7)	0.1420 (3)	0.1320 (5)	0.0646 (16)
H16A	0.8686	0.1611	0.1846	0.077*
C17	0.7230 (8)	0.1852 (3)	0.0693 (6)	0.085 (2)
H17A	0.7166	0.2333	0.0798	0.102*
C18	0.6428 (9)	0.1581 (4)	-0.0075 (5)	0.089 (2)
H18A	0.5856	0.1880	-0.0502	0.106*
C19	0.6458 (8)	0.0874 (4)	-0.0221 (4)	0.0752 (19)
H19A	0.5861	0.0688	-0.0738	0.090*
C20	0.7374 (7)	0.0429 (3)	0.0393 (4)	0.0560 (14)
H20A	0.7403	-0.0054	0.0286	0.067*
C21	1.1503 (5)	0.0309 (3)	0.1981 (3)	0.0396 (10)
C22	1.2703 (6)	0.0017 (3)	0.2625 (4)	0.0552 (13)
H22A	1.2441	-0.0255	0.3052	0.066*
C23	1.4268 (6)	0.0123 (4)	0.2641 (4)	0.0643 (16)
H23A	1.5061	-0.0082	0.3072	0.077*
C24	1.4665 (7)	0.0532 (3)	0.2022 (5)	0.0638 (16)

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H24A	1.5727	0.0611	0.2037	0.077*
C25	1.3492 (7)	0.0825 (4)	0.1377 (4)	0.0600 (14)
H25A	1.3764	0.1096	0.0952	0.072*
C26	1.1918 (6)	0.0719 (3)	0.1359 (3)	0.0486 (12)
H26A	1.1130	0.0925	0.0926	0.058*
C27	0.9016 (6)	-0.0739 (3)	0.1666 (3)	0.0435 (11)
C28	0.7915 (6)	-0.1114 (3)	0.1980 (3)	0.0505 (12)
H28A	0.7497	-0.0915	0.2405	0.061*
C29	0.7427 (7)	-0.1780 (3)	0.1673 (4)	0.0626 (15)
H29A	0.6688	-0.2027	0.1890	0.075*
C30	0.8047 (9)	-0.2073 (3)	0.1041 (4)	0.0710 (18)
H30A	0.7712	-0.2517	0.0821	0.085*
C31	0.9150 (8)	-0.1712 (3)	0.0740 (4)	0.0646 (16)
H31A	0.9572	-0.1915	0.0318	0.078*
C32	0.9650 (7)	-0.1052 (3)	0.1049 (4)	0.0532 (13)
H32A	1.0417	-0.0815	0.0843	0.064*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.03953 (11)	0.06034 (14)	0.04452 (12)	-0.00352 (9)	0.01742 (8)	-0.00830 (8)
P1	0.0296 (6)	0.0527 (7)	0.0398 (6)	-0.0021 (5)	0.0129 (5)	-0.0041 (5)
N1	0.070 (3)	0.065 (3)	0.051 (3)	0.012 (2)	0.028 (2)	-0.003 (2)
N2	0.055 (3)	0.055 (3)	0.066 (3)	0.008 (2)	0.026 (2)	0.003 (2)
C1	0.039 (3)	0.057 (3)	0.055 (3)	-0.007 (2)	0.023 (2)	-0.007 (2)
C2	0.057 (3)	0.049 (3)	0.049 (3)	0.003 (2)	0.019 (2)	-0.001 (2)
C3	0.045 (3)	0.056 (3)	0.081 (4)	0.005 (2)	0.022 (3)	0.009 (3)
C4	0.056 (3)	0.054 (3)	0.061 (3)	0.000 (3)	0.009 (3)	0.003 (3)
C5	0.058 (3)	0.043 (3)	0.046 (3)	0.008 (2)	0.015 (2)	0.006 (2)
C6	0.052 (3)	0.037 (2)	0.040 (2)	0.008 (2)	0.014 (2)	0.0074 (18)
C7	0.050 (3)	0.042 (3)	0.046 (3)	0.009 (2)	0.019 (2)	0.006 (2)
C8	0.055 (3)	0.042 (2)	0.042 (3)	0.007 (2)	0.020 (2)	0.0054 (19)
C9	0.051 (3)	0.056 (3)	0.050 (3)	0.001 (2)	0.016 (2)	-0.001 (2)
C10	0.063 (3)	0.044 (3)	0.043 (3)	0.004 (2)	0.012 (2)	0.001 (2)
C11	0.061 (3)	0.042 (3)	0.043 (3)	0.013 (2)	0.016 (2)	0.004 (2)
C12	0.067 (4)	0.062 (3)	0.057 (3)	0.001 (3)	0.007 (3)	-0.007 (3)
C13	0.084 (5)	0.063 (4)	0.051 (3)	0.004 (3)	0.004 (3)	-0.013 (3)
C14	0.094 (5)	0.063 (4)	0.047 (3)	0.020 (3)	0.020 (3)	-0.004 (3)
C15	0.028 (2)	0.054 (3)	0.053 (3)	-0.0031 (19)	0.015 (2)	-0.001 (2)
C16	0.045 (3)	0.057 (3)	0.086 (4)	-0.006 (3)	0.005 (3)	-0.004 (3)
C17	0.066 (4)	0.048 (3)	0.135 (7)	-0.002 (3)	0.014 (4)	0.010 (4)
C18	0.079 (5)	0.077 (5)	0.097 (6)	-0.002 (4)	-0.002 (4)	0.037 (4)
C19	0.068 (4)	0.090 (5)	0.059 (4)	0.015 (4)	-0.001 (3)	0.010 (3)
C20	0.053 (3)	0.062 (3)	0.049 (3)	0.006 (3)	0.006 (2)	-0.002 (2)
C21	0.032 (2)	0.050 (3)	0.039 (2)	-0.0022 (19)	0.0126 (18)	-0.0030 (19)
C22	0.038 (3)	0.071 (4)	0.058 (3)	0.006 (2)	0.015 (2)	0.011 (3)
C23	0.035 (3)	0.075 (4)	0.080 (4)	0.010 (3)	0.008 (3)	0.003 (3)
C24	0.031 (3)	0.082 (4)	0.082 (4)	-0.003 (3)	0.020 (3)	-0.013 (3)

C25	0.048 (3)	0.079 (4)	0.062 (4)	-0.011 (3)	0.029 (3)	-0.003 (3)
C26	0.037 (2)	0.070 (3)	0.042 (3)	0.002 (2)	0.014 (2)	0.001 (2)
C27	0.038 (2)	0.053 (3)	0.039 (2)	-0.001 (2)	0.008 (2)	0.002 (2)
C28	0.041 (3)	0.063 (3)	0.050 (3)	-0.005 (2)	0.017 (2)	0.000 (2)
C29	0.050 (3)	0.064 (4)	0.073 (4)	-0.010 (3)	0.014 (3)	0.004 (3)
C30	0.081 (5)	0.053 (3)	0.070 (4)	-0.004 (3)	0.002 (4)	-0.005 (3)
C31	0.084 (5)	0.058 (3)	0.054 (3)	0.008 (3)	0.021 (3)	-0.006 (3)
C32	0.056 (3)	0.054 (3)	0.055 (3)	0.004 (2)	0.025 (3)	0.003 (2)

Geometric parameters (Å, °)

Au1—C1	2.013 (5)	C16—C17	1.382 (9)
Au1—P1	2.2710 (13)	C16—H16A	0.9300
P1—C27	1.804 (5)	C17—C18	1.355 (11)
P1—C21	1.812 (5)	C17—H17A	0.9300
P1—C15	1.821 (5)	C18—C19	1.360 (10)
N1—C14	1.324 (8)	C18—H18A	0.9300
N1—C11	1.359 (7)	C19—C20	1.386 (8)
N2—C3	1.302 (8)	C19—H19A	0.9300
N2—C7	1.364 (7)	C20—H20A	0.9300
C1—C2	1.170 (7)	C21—C26	1.382 (7)
C2—C8	1.430 (7)	C21—C22	1.386 (7)
C3—C4	1.394 (9)	C22—C23	1.369 (8)
C3—H3A	0.9300	C22—H22A	0.9300
C4—C5	1.355 (8)	C23—C24	1.370 (9)
C4—H4A	0.9300	C23—H23A	0.9300
C5—C6	1.400 (7)	C24—C25	1.373 (9)
C5—H5A	0.9300	C24—H24A	0.9300
C6—C7	1.401 (7)	C25—C26	1.376 (7)
C6—C8	1.454 (7)	C25—H25A	0.9300
C7—C11	1.458 (8)	C26—H26A	0.9300
C8—C9	1.360 (7)	C27—C32	1.380 (7)
C9—C10	1.431 (7)	C27—C28	1.384 (7)
C9—H9A	0.9300	C28—C29	1.379 (8)
C10—C11	1.395 (8)	C28—H28A	0.9300
C10—C12	1.399 (8)	C29—C30	1.379 (9)
C12—C13	1.354 (9)	C29—H29A	0.9300
C12—H12A	0.9300	C30—C31	1.361 (9)
C13—C14	1.379 (10)	C30—H30A	0.9300
C13—H13A	0.9300	C31—C32	1.373 (8)
C14—H14A	0.9300	C31—H31A	0.9300
C15—C16	1.380 (8)	C32—H32A	0.9300
C15—C20	1.386 (7)		
C1—Au1—P1	173.59 (16)	C15—C16—H16A	120.0
C27—P1—C21	105.7 (2)	C17—C16—H16A	120.0
C27—P1—C15	105.1 (2)	C18—C17—C16	120.6 (6)
C21—P1—C15	106.1 (2)	C18—C17—H17A	119.7
C27—P1—Au1	117.42 (17)	C16—C17—H17A	119.7
C21—P1—Au1	112.66 (16)	C17—C18—C19	120.1 (6)

supplementary materials

C15—P1—Au1	108.97 (17)	C17—C18—H18A	119.9
C14—N1—C11	116.8 (6)	C19—C18—H18A	119.9
C3—N2—C7	117.8 (5)	C18—C19—C20	120.5 (7)
C2—C1—Au1	174.1 (5)	C18—C19—H19A	119.8
C1—C2—C8	176.3 (6)	C20—C19—H19A	119.8
N2—C3—C4	123.9 (6)	C15—C20—C19	119.7 (6)
N2—C3—H3A	118.0	C15—C20—H20A	120.2
C4—C3—H3A	118.0	C19—C20—H20A	120.2
C5—C4—C3	118.8 (6)	C26—C21—C22	118.6 (5)
C5—C4—H4A	120.6	C26—C21—P1	123.1 (4)
C3—C4—H4A	120.6	C22—C21—P1	118.3 (4)
C4—C5—C6	119.8 (5)	C23—C22—C21	121.0 (5)
C4—C5—H5A	120.1	C23—C22—H22A	119.5
C6—C5—H5A	120.1	C21—C22—H22A	119.5
C5—C6—C7	117.3 (5)	C22—C23—C24	119.9 (5)
C5—C6—C8	122.0 (5)	C22—C23—H23A	120.0
C7—C6—C8	120.8 (5)	C24—C23—H23A	120.0
N2—C7—C6	122.4 (5)	C23—C24—C25	120.0 (5)
N2—C7—C11	118.3 (5)	C23—C24—H24A	120.0
C6—C7—C11	119.3 (5)	C25—C24—H24A	120.0
C9—C8—C2	121.7 (5)	C24—C25—C26	120.3 (6)
C9—C8—C6	118.7 (5)	C24—C25—H25A	119.9
C2—C8—C6	119.6 (5)	C26—C25—H25A	119.9
C8—C9—C10	122.0 (5)	C25—C26—C21	120.3 (5)
C8—C9—H9A	119.0	C25—C26—H26A	119.8
C10—C9—H9A	119.0	C21—C26—H26A	119.8
C11—C10—C12	118.3 (5)	C32—C27—C28	118.5 (5)
C11—C10—C9	120.4 (5)	C32—C27—P1	122.4 (4)
C12—C10—C9	121.3 (6)	C28—C27—P1	119.0 (4)
N1—C11—C10	122.3 (5)	C29—C28—C27	121.2 (6)
N1—C11—C7	118.9 (5)	C29—C28—H28A	119.4
C10—C11—C7	118.8 (5)	C27—C28—H28A	119.4
C13—C12—C10	119.2 (7)	C30—C29—C28	119.2 (6)
C13—C12—H12A	120.4	C30—C29—H29A	120.4
C10—C12—H12A	120.4	C28—C29—H29A	120.4
C12—C13—C14	118.7 (6)	C31—C30—C29	120.0 (6)
C12—C13—H13A	120.6	C31—C30—H30A	120.0
C14—C13—H13A	120.6	C29—C30—H30A	120.0
N1—C14—C13	124.7 (6)	C30—C31—C32	121.0 (6)
N1—C14—H14A	117.7	C30—C31—H31A	119.5
C13—C14—H14A	117.7	C32—C31—H31A	119.5
C16—C15—C20	118.9 (5)	C31—C32—C27	120.1 (6)
C16—C15—P1	118.2 (4)	C31—C32—H32A	119.9
C20—C15—P1	122.8 (4)	C27—C32—H32A	119.9
C15—C16—C17	120.1 (6)		

Fig. 1

