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# *catena*-Poly[[(benzyldiphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^2 O:O'$ -[(benzyldiphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^4 O,O':O',O''$ ]

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The structure of the title complex,  $[Ag_2(NO_3)_2(C_{19}H_{17}P)_2]_n$ , reveals a chain emanating from the coordination of one phosphine ligand to each silver(I) cation, as well as the bis-monodentate coordination of a bridging nitrato ligand (per Ag atom) and the bis-bidentate coordination of another bridging nitrato ligand (per Ag atom). The distorted four-coordinate Ag atoms are characterized by bonding angles that notably deviate from the ideal tetrahedral shape.



### Structure description

The solid-state molecular structure of the title compound was established using singlecrystal X-ray diffraction with data measured at 150 K. The complex crystallizes in the orthorhombic space group  $Pna2_1$  with Z = 4. The asymmetric unit contains two unique silver atoms, each with one benzyldiphenyl phosphine ligand coordinated with bond lengths Ag1-P1 = 2.3506 (19) and Ag2-P2 = 2.3612 (19) Å. As seen in Fig. 1, each of the four-coordinate silver atoms are heavily distorted with bond angles P1-Ag1-O4 [129.6 (2)°], O1-Ag1-O4 [88.5 (3)°], P2-Ag1-O2 [121.08 (15)°], P2-Ag2-O2 [121.08 (15)°], O2-Ag2-O6 [96.0 (3)°] and P2-Ag2-O6 [142.8 (3)°]. Two unique nitrato groups bridge alternating silver atoms to form a polymeric chain. One nitrato group bridges Ag1 and Ag2 *via* three oxygen atoms (O1 and O2 bind to Ag1, O2 and O3 binds to Ag2) in a bis-bidentate fashion. This results in a near co-planar bond angle of Ag1-O2-Ag2 = 170.3 (5)°. The second nitrato group connects Ag1 to another Ag2 atom in a bis-monodentate fashion using only two oxygen atoms (O4 bonds to Ag1 and O6 bonds to Ag2). Differences in the respective Ag-O bond lengths of the two different







The molecular structure of the asymmetric unit in the title compound showing displacement ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

nitrato groups are observed to fall within shorter [2.295 (7)-2.406 (7) Å] and longer [2.460 (6)–2.635 (7) Å] ranges.

The inorganic polymer packs in three dimensions as layers of one-dimensional ribbons when viewed along the b axis (Fig. 2); the chain has glide symmetry. Furthermore, the aromatic rings of the phosphine ligands then overlap in an adjacent layer to form a hydrophobic layer in between Ag-NO<sub>3</sub>-containing layers.

### Synthesis and crystallization

Benzyldiphenylphosphine (1 mmol) was dissolved in acetonitrile (10 ml). Silver nitrate (1 mmol) was dissolved in acetonitrile (10 ml). In order to obtain the given 1:1 molar ratio, the solutions were mixed. The resulting solution was heated to 353 K for approximately 2 h. The solution was removed from the heat and left to slowly cool. During the



Figure 2

Perspective views along the (a) a and (b) b axes of the molecular packing of the title compound.

Table 1	
Experimental details.	
Crystal data	
Chemical formula	$[Ag_2(NO_3)_2(C_{19}H_{17}P)_2]$
$M_{ m r}$	892.35
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	18.0126 (3), 10.6251 (2), 19.2397 (3)
$V(Å^3)$	3682.20 (11)
Z	4
Radiation type	Cu Ka
$\mu \text{ (mm}^{-1})$	9.75
Crystal size (mm)	$0.21\times0.15\times0.12$
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku OD, 2022)
$T_{\min}, T_{\max}$	0.665, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	53360, 7741, 7352
R <sub>int</sub>	0.068
$(\sin \theta / \lambda)_{\max} ( \text{\AA}^{-1} )$	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.044, 0.120, 1.05
No. of reflections	7741
No. of parameters	451
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\rm max},  \Delta \rho_{\rm min}  ({\rm e}  {\rm A}^{-3})$	2.51, -0.73
Absolute structure	Flack x determined using 3276 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.009(4)
<u> </u>	

Computer programs: CrysAlis PRO (Rigaku OD, 2022), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), and OLEX2 (Dolomanov et al., 2009).

process of the slow evaporation of the solvent, clear colorless crystals started to form.

### Refinement

Experimental details including crystal data, data collection and structure refinement details are summarized in Table 1. The highest calculated residual electron density peak is 2.51 e<sup>-</sup> Å<sup>-3</sup> and is located 0.99 Å from Ag2, which is attributed to the presence of the strong absorber (Ag), as well as imperfections in the absorption correction process.

### Acknowledgements

Financial assistance from the South African National Research Foundation (SA NRF), the University of Pretoria (UP) and the University of Johannesburg (UJ) is gratefully acknowledged.

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# full crystallographic data

## *IUCrData* (2022). 7, x220772 [https://doi.org/10.1107/S2414314622007726]

# *catena*-Poly[[(benzyldiphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^2 O:O'$ -[(benzyl-diphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^4 O, O':O', O''$ ]

# Kariska Potgieter, Frederick P. Malan and Reinout Meijboom

*catena*-Poly[[(benzyldiphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^2 O:O'$ -[(benzyldiphenylphosphine- $\kappa P$ )silver(I)]- $\mu$ -nitrato- $\kappa^4 O,O':O',O''$ ]

## Crystal data

 $[Ag_{2}(NO_{3})_{2}(C_{19}H_{17}P)_{2}]$   $M_{r} = 892.35$ Orthorhombic,  $Pna2_{1}$  a = 18.0126 (3) Å b = 10.6251 (2) Å c = 19.2397 (3) Å V = 3682.20 (11) Å<sup>3</sup> Z = 4F(000) = 1792

## Data collection

XtaLAB Synergy R, DW system, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm<sup>-1</sup> ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)

## Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.044$  $wR(F^2) = 0.120$ S = 1.057741 reflections 451 parameters 1 restraint Primary atom site location: dual Hydrogen site location: inferred from neighbouring sites  $D_x = 1.610 \text{ Mg m}^{-3}$ Cu K $\alpha$  radiation,  $\lambda = 1.54184 \text{ Å}$ Cell parameters from 34740 reflections  $\theta = 4.6-78.2^{\circ}$  $\mu = 9.75 \text{ mm}^{-1}$ T = 150 KBlock, colourless  $0.21 \times 0.14 \times 0.12 \text{ mm}$ 

 $T_{\min} = 0.665, T_{\max} = 1.000$ 53360 measured reflections 7741 independent reflections 7352 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.068$  $\theta_{\max} = 79.5^{\circ}, \theta_{\min} = 4.6^{\circ}$  $h = -18 \rightarrow 22$  $k = -13 \rightarrow 13$  $l = -24 \rightarrow 24$ 

H-atom parameters constrained  $w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0747P)^{2} + 4.1236P]$ where  $P = (F_{o}^{2} + 2F_{c}^{2})/3$   $(\Delta/\sigma)_{max} < 0.001$   $\Delta\rho_{max} = 2.51 \text{ e } \text{Å}^{-3}$   $\Delta\rho_{min} = -0.73 \text{ e } \text{Å}^{-3}$ Absolute structure: Flack *x* determined using 3276 quotients  $[(I^{+})-(I^{-})]/[(I^{+})+(I^{-})]$  (Parsons *et al.*, 2013) Absolute structure parameter: -0.009 (4)

### Special details

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

Refinement. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms.

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
Ag1	0.20763 (3)	0.67285 (6)	0.57043 (3)	0.04561 (16)
Ag2	0.49695 (3)	0.61627 (5)	0.44110 (5)	0.04420 (16)
P1	0.20175 (9)	0.65229 (16)	0.69195 (10)	0.0293 (3)
P2	0.52210 (9)	0.42137 (17)	0.38704 (10)	0.0337 (4)
01	0.1529 (4)	0.5950 (6)	0.4664 (3)	0.0513 (14)
O3	0.0623 (3)	0.6720 (6)	0.4045 (3)	0.0487 (14)
O2	0.0958 (4)	0.7638 (5)	0.4994 (3)	0.0461 (13)
N1	0.1028 (4)	0.6746 (6)	0.4568 (3)	0.0374 (13)
C26	0.4647 (3)	0.2889 (7)	0.4155 (4)	0.0321 (13)
N2	0.3496 (4)	0.7223 (7)	0.4926 (4)	0.0487 (17)
05	0.3505 (5)	0.6175 (7)	0.5180 (4)	0.067 (2)
O4	0.2935 (4)	0.7904 (7)	0.5001 (5)	0.068 (2)
O6	0.4046 (4)	0.7612 (7)	0.4599 (6)	0.092 (3)
C1	0.2459 (4)	0.5121 (6)	0.7253 (4)	0.0372 (15)
C14	0.0614 (3)	0.5503 (8)	0.6926 (4)	0.0365 (15)
C31	0.4020 (4)	0.3152 (7)	0.4557 (4)	0.0384 (15)
H31	0.3917	0.3989	0.4701	0.046*
C27	0.4797 (4)	0.1673 (7)	0.3947 (4)	0.0355 (14)
H27	0.5217	0.1503	0.3665	0.043*
C19	0.0502 (4)	0.4320 (8)	0.7222 (5)	0.0465 (19)
H19	0.0705	0.4135	0.7666	0.056*
C37	0.6669 (5)	0.2182 (9)	0.5650 (6)	0.0526 (19)
H37	0.6626	0.1396	0.5883	0.063*
C9	0.3472 (5)	0.9341 (9)	0.7401 (5)	0.054 (2)
H9	0.3865	0.9766	0.7170	0.065*
C11	0.2715 (5)	0.9051 (8)	0.8408 (5)	0.0471 (18)
H11	0.2592	0.9286	0.8871	0.057*
C28	0.4326 (4)	0.0685 (7)	0.4153 (4)	0.0395 (16)
H28	0.4436	-0.0157	0.4023	0.047*
C35	0.7050 (5)	0.4361 (9)	0.5645 (6)	0.052 (2)
H35	0.7282	0.5052	0.5871	0.062*
C13	0.1073 (4)	0.6497 (7)	0.7280 (4)	0.0360 (14)
H13A	0.1096	0.6322	0.7785	0.043*
H13B	0.0837	0.7330	0.7215	0.043*
C33	0.6447 (4)	0.3482 (7)	0.4637 (4)	0.0355 (15)
C10	0.3299 (6)	0.9636 (8)	0.8070 (6)	0.055 (2)
H10	0.3583	1.0253	0.8308	0.066*
C7	0.2484 (4)	0.7797 (7)	0.7387 (4)	0.0337 (14)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(A^2)$ 

C120.2310 (5)0.8122 (8)0.8074 (4)0.0419*H120.19170.77070.83090.049*C340.6760 (4)0.4487 (8)0.4988 (4)0.0402 (16)H340.67740.52880.47680.048*C150.0299 (5)0.5748 (11)0.6288 (5)0.054 (2)H150.03660.65540.60840.065*C380.6402 (4)0.2314 (9)0.4981 (5)0.0477 (19)H380.61860.16120.47510.057*C360.6994 (5)0.3173 (10)0.5976 (5)0.057 (2)H360.71860.30700.64320.069*C180.0101 (5)0.3420 (10)0.6875 (8)0.062 (3)H180.00250.26190.70820.074*C300.3549 (4)0.2173 (9)0.4743 (5)0.0460 (18)H300.31160.23470.50080.055*C60.2349 (5)0.681 (8)0.7926 (5)0.051 (2)H60.20100.50800.82330.061*C290.3703 (4)0.0948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.055*C80.3063 (5)0.8403 (8)0.7055 (5)0.4643 (9)H80.31860.81840.65900.56*C230.4662 (7)0.4667 (12)0.1562 (6)0.072 (3)H20.30460.48320.63580.066*C240.50100.4527 (9)0.6817 (6)0.074 (4) <th></th> <th></th> <th></th> <th></th> <th></th>					
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C15 $0.0299 (5)$ $0.5748 (11)$ $0.6288 (5)$ $0.054 (2)$ H15 $0.0366$ $0.6554$ $0.6084$ $0.065^*$ C38 $0.6402 (4)$ $0.2314 (9)$ $0.4981 (5)$ $0.0477 (19)$ H38 $0.6186$ $0.1612$ $0.4751$ $0.057^*$ C36 $0.6994 (5)$ $0.3173 (10)$ $0.5976 (5)$ $0.069^*$ C18 $0.0101 (5)$ $0.3420 (10)$ $0.6875 (8)$ $0.062 (3)$ H18 $0.0025$ $0.2619$ $0.7082$ $0.074^*$ C30 $0.3549 (4)$ $0.2137 (9)$ $0.4743 (5)$ $0.0661 (8)$ H30 $0.3116$ $0.2347$ $0.5008$ $0.055^*$ C6 $0.2349 (5)$ $0.4681 (8)$ $0.7926 (5)$ $0.051 (2)$ H6 $0.2010$ $0.5080$ $0.8233$ $0.061^*$ C29 $0.3703 (4)$ $0.0948 (8)$ $0.4548 (4)$ $0.0440 (18)$ H29 $0.3380$ $0.0286$ $0.4685$ $0.055^*$ C8 $0.3063 (5)$ $0.8403 (8)$ $0.7055 (5)$ $0.0463 (19)$ H8 $0.3186$ $0.8184$ $0.6590$ $0.056^*$ C23 $0.4602 (7)$ $0.4657 (12)$ $0.1562 (6)$ $0.072 (3)$ H23 $0.4468$ $0.4801$ $0.1091$ $0.086^*$ C24 $0.2970 (5)$ $0.4527 (9)$ $0.6317 (6)$ $0.074 (3)$ H2 $0.3046$ $0.4527 (9)$ $0.6317 (6)$ $0.074 (4)$ H22 $0.3699$ $0.5445$ $0.1967$ $0.88^*$ C25 $0.4526 (8)$ $0.3052 (9)$ $0.771 (9)$ $0$	H34	0.6774	0.5288	0.4768	0.048*
H15 $0.0366$ $0.6554$ $0.6084$ $0.065^{sh}$ C38 $0.6402$ (4) $0.2314$ (9) $0.4981$ (5) $0.0477$ (19)H38 $0.6186$ $0.1612$ $0.4751$ $0.057^{*h}$ C36 $0.6994$ (5) $0.3173$ (10) $0.5976$ (5) $0.057^{*h}$ H36 $0.7186$ $0.3070$ $0.6432$ $0.069^{*h}$ C18 $0.0101$ (5) $0.3420$ (10) $0.6875$ (8) $0.062$ (3)H18 $0.0025$ $0.2619$ $0.7082$ $0.074^{*h}$ C30 $0.3549$ (4) $0.2173$ (9) $0.4743$ (5) $0.0460$ (18)H30 $0.3116$ $0.2347$ $0.5008$ $0.055^{*h}$ C6 $0.2349$ (5) $0.4681$ (8) $0.7926$ (5) $0.051$ (2)H6 $0.2010$ $0.5080$ $0.8233$ $0.061^{*h}$ C29 $0.3703$ (4) $0.9948$ (8) $0.4548$ (4) $0.0440$ (18)H29 $0.3380$ $0.0286$ $0.4685$ $0.055^{*h}$ C8 $0.3063$ (5) $0.8403$ (8) $0.7055$ (5) $0.0463$ (19)H8 $0.3186$ $0.4801$ $0.1091$ $0.086^{*h}$ C20 $0.5020$ (4) $0.4527$ (9) $0.6817$ (6) $0.072$ (3)H24 $0.3099$ $0.5445$ $0.1967$ $0.088^{*h}$ C22 $0.5270$ (7) $0.4627$ (7) $0.3912$ (4) $0.0366$ (14)H24 $0.3699$ $0.5445$ $0.1967$ $0.088^{*h}$ C22 $0.5270$ (7) $0.4527$ (9) $0.6817$ (6) $0.774$ (3)H24 $0.3690$ $0.5445$ $0.1$	C15	0.0299 (5)	0.5748 (11)	0.6288 (5)	0.054 (2)
C38 $0.6402$ (4) $0.2314$ (9) $0.4981$ (5) $0.0477$ (19)H38 $0.6186$ $0.1612$ $0.4751$ $0.057*$ C36 $0.6994$ (5) $0.3173$ (10) $0.5976$ (5) $0.057$ (2)H36 $0.7186$ $0.3070$ $0.6432$ $0.066*$ C18 $0.0101$ (5) $0.3420$ (10) $0.6875$ (8) $0.062$ (3)H18 $0.0025$ $0.2619$ $0.7082$ $0.074*$ C30 $0.3549$ (4) $0.2173$ (9) $0.4743$ (5) $0.066$ (18)H30 $0.3116$ $0.2347$ $0.5008$ $0.055*$ C6 $0.2349$ (5) $0.4681$ (8) $0.7926$ (5) $0.051$ (2)H6 $0.2010$ $0.5080$ $0.8233$ $0.061*$ C29 $0.3703$ (4) $0.0948$ (8) $0.4548$ (4) $0.0440$ (18)H29 $0.3380$ $0.0286$ $0.4685$ $0.055*$ C8 $0.3063$ (5) $0.8403$ (8) $0.7055$ (5) $0.0463$ (19)H8 $0.3186$ $0.8184$ $0.6590$ $0.056*$ C23 $0.4602$ (7) $0.4667$ (12) $0.1562$ (6) $0.072$ (3)H23 $0.4468$ $0.4801$ $0.1091$ $0.086*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088*$ C32 $0.5102$ (4) $0.3733$ $0.1374$ $0.088*$ C32 $0.5102$ (17) $0.3912$ (4) $0.3066$ (14)H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ C32 $0.5$	H15	0.0366	0.6554	0.6084	0.065*
H380.61860.16120.47510.057*C360.6994 (5)0.3173 (10)0.5976 (5)0.057 (2)H360.71860.30700.64320.069*C180.0101 (5)0.3420 (10)0.6875 (8)0.062 (3)H180.00250.26190.70820.074*C300.3549 (4)0.2173 (9)0.4743 (5)0.0460 (18)H300.31160.23470.50080.055*C60.2349 (5)0.4681 (8)0.7926 (5)0.051 (2)H60.20100.50800.82330.061*C290.3703 (4)0.0948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.053*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48320.63580.066*C240.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.074 (3)H240.36990.54450.19670.088*C220.570 (7)0.4042 (15)0.1374 (0)0.087*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*C320.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.31090.073*	C38	0.6402 (4)	0.2314 (9)	0.4981 (5)	0.0477 (19)
C36 $0.6994$ (5) $0.3173$ (10) $0.5976$ (5) $0.057$ (2)H36 $0.7186$ $0.3070$ $0.6432$ $0.069^*$ C18 $0.0101$ (5) $0.3420$ (10) $0.6875$ (8) $0.062$ (3)H18 $0.0025$ $0.2619$ $0.7082$ $0.074^*$ C30 $0.3549$ (4) $0.2173$ (9) $0.4743$ (5) $0.0460$ (18)H30 $0.3116$ $0.2347$ $0.5008$ $0.055^*$ C6 $0.2349$ (5) $0.4681$ (8) $0.7926$ (5) $0.061^*$ C29 $0.3703$ (4) $0.0948$ (8) $0.4548$ (4) $0.0440$ (18)H29 $0.3380$ $0.0286$ $0.4685$ $0.055^*$ C8 $0.3063$ (5) $0.8403$ (8) $0.7055$ (5) $0.0463$ (19)H8 $0.3186$ $0.8184$ $0.6590$ $0.0556^*$ C23 $0.4602$ (7) $0.4667$ (12) $0.1562$ (6) $0.072$ (3)H23 $0.4468$ $0.4801$ $0.1091$ $0.086^*$ C24 $0.5020$ (4) $0.4327$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066^*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.888^*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32A $0.608$ $0.2803$ $0.3673$ $0.044^*$ C25 $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H2 $0.3540$ $0.3380$ $0.3673$ $0.04$	H38	0.6186	0.1612	0.4751	0.057*
H360.71860.30700.64320.069*C180.0101 (5)0.3420 (10)0.6875 (8)0.062 (3)H180.00250.26190.70820.074*C300.3549 (4)0.2173 (9)0.4743 (5)0.0460 (18)H300.31160.23470.50080.055*C60.2349 (5)0.4681 (8)0.7926 (5)0.051 (2)H60.20100.50800.82330.061*C290.3703 (4)0.0948 (8)0.4484 (4)0.0440 (18)H290.33800.02860.46850.053*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48320.63580.066*C240.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.0	C36	0.6994 (5)	0.3173 (10)	0.5976 (5)	0.057 (2)
C180.0101 (5)0.3420 (10)0.6875 (8)0.062 (3)H180.00250.26190.70820.074*C300.3549 (4)0.2173 (9)0.4743 (5)0.0460 (18)H300.31160.23470.50080.055*C60.2349 (5)0.4681 (8)0.7926 (5)0.051 (2)H60.20100.50800.82330.061*C290.3703 (4)0.9948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.53*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48010.10910.086*C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*C350.43540.78570.101*C40.3264 (8)0.3052 (9)0.7701 (9)0.884 (4)C40.35400.23450.78570.101*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2) <tr< td=""><td>H36</td><td>0.7186</td><td>0.3070</td><td>0.6432</td><td>0.069*</td></tr<>	H36	0.7186	0.3070	0.6432	0.069*
H18 $0.0025$ $0.2619$ $0.7082$ $0.074^*$ C30 $0.3549$ (4) $0.2173$ (9) $0.4743$ (5) $0.0460$ (18)H30 $0.3116$ $0.2347$ $0.5008$ $0.055^*$ C6 $0.2349$ (5) $0.4681$ (8) $0.7926$ (5) $0.051$ (2)H6 $0.2010$ $0.5080$ $0.8233$ $0.061^*$ C29 $0.3703$ (4) $0.0948$ (8) $0.4548$ (4) $0.0440$ (18)H29 $0.3380$ $0.0286$ $0.4685$ $0.053^*$ C3 $0.4602$ (7) $0.4667$ (12) $0.1552$ (6) $0.072$ (3)H8 $0.3186$ $0.8184$ $0.6590$ $0.056^*$ C23 $0.4602$ (7) $0.4667$ (12) $0.1562$ (6) $0.072$ (3)H23 $0.4468$ $0.4801$ $0.1091$ $0.086^*$ C20 $0.5020$ (4) $0.4340$ (7) $0.2941$ (4) $0.4046$ (17)C2 $0.2970$ (5) $0.4527$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066^*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088^*$ C32 $0.5100$ $0.4220$ $0.3662$ $0.044^*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32A $0.6208$ $0.2803$ $0.3673$ $0.044^*$ C32 $0.6180$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H32A $0.6208$ $0.2803$ $0.3662$ $0.044^*$ <td>C18</td> <td>0.0101 (5)</td> <td>0.3420 (10)</td> <td>0.6875 (8)</td> <td>0.062 (3)</td>	C18	0.0101 (5)	0.3420 (10)	0.6875 (8)	0.062 (3)
C30 $0.3549 (4)$ $0.2173 (9)$ $0.4743 (5)$ $0.0460 (18)$ H30 $0.3116$ $0.2347$ $0.5008$ $0.055*$ C6 $0.2349 (5)$ $0.4681 (8)$ $0.7926 (5)$ $0.051 (2)$ H6 $0.2010$ $0.5080$ $0.8233$ $0.061*$ C29 $0.3703 (4)$ $0.0948 (8)$ $0.4548 (4)$ $0.0440 (18)$ H29 $0.3380$ $0.0286$ $0.4685$ $0.053*$ C8 $0.3063 (5)$ $0.8403 (8)$ $0.7055 (5)$ $0.0463 (19)$ H8 $0.3186$ $0.8184$ $0.6590$ $0.056*$ C23 $0.4602 (7)$ $0.4667 (12)$ $0.1562 (6)$ $0.072 (3)$ H23 $0.4468$ $0.4801$ $0.1091$ $0.086*$ C20 $0.5502 (4)$ $0.4340 (7)$ $0.2941 (4)$ $0.0406 (17)$ C2 $0.2970 (5)$ $0.4527 (9)$ $0.6817 (6)$ $0.055 (2)$ H2 $0.3046$ $0.4832$ $0.6338$ $0.066*$ C24 $0.4162 (8)$ $0.5068 (11)$ $0.2077 (6)$ $0.074 (4)$ H24 $0.3699$ $0.5445$ $0.1967$ $0.88*$ C22 $0.5270 (7)$ $0.4042 (15)$ $0.1374$ $0.089*$ C32 $0.6180 (4)$ $0.3627 (7)$ $0.3912 (4)$ $0.0366 (14)$ H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044*$ C25 $0.4356 (6)$ $0.4945 (10)$ $0.2755 (5)$ $0.061 (2)$ H25 $0.4054$ $0.2345$ $0.7857$ $0.101*$ <	H18	0.0025	0.2619	0.7082	0.074*
H300.31160.23470.50080.055*C60.2349 (5)0.4681 (8)0.7926 (5)0.051 (2)H60.20100.50800.82330.061*C290.3703 (4)0.0948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.053*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48010.10910.086*C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C220.570 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H20.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H20.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H20.5450.78570.101*C2 <td>C30</td> <td>0.3549 (4)</td> <td>0.2173 (9)</td> <td>0.4743 (5)</td> <td>0.0460 (18)</td>	C30	0.3549 (4)	0.2173 (9)	0.4743 (5)	0.0460 (18)
C6 $0.2349 (5)$ $0.4681 (8)$ $0.7926 (5)$ $0.051 (2)$ H6 $0.2010$ $0.5080$ $0.8233$ $0.061*$ C29 $0.3703 (4)$ $0.0948 (8)$ $0.4548 (4)$ $0.0440 (18)$ H29 $0.3380$ $0.0286$ $0.4685$ $0.053*$ C8 $0.3063 (5)$ $0.8403 (8)$ $0.7055 (5)$ $0.0463 (19)$ H8 $0.3186$ $0.8184$ $0.6590$ $0.056*$ C23 $0.4602 (7)$ $0.4667 (12)$ $0.1562 (6)$ $0.072 (3)$ H23 $0.4468$ $0.4801$ $0.1091$ $0.086*$ C20 $0.5020 (4)$ $0.4320 (7)$ $0.2941 (4)$ $0.0406 (17)$ C2 $0.2970 (5)$ $0.4527 (9)$ $0.6817 (6)$ $0.055 (2)$ H2 $0.3046$ $0.4832$ $0.6358$ $0.066*$ C24 $0.4162 (8)$ $0.5068 (11)$ $0.2077 (6)$ $0.074 (3)$ H24 $0.3699$ $0.5445$ $0.1967$ $0.88*$ C22 $0.5270 (7)$ $0.4042 (15)$ $0.1732 (6)$ $0.074 (4)$ H22 $0.583$ $0.3733$ $0.3673$ $0.044*$ C32 $0.6180 (4)$ $0.3267 (7)$ $0.3912 (4)$ $0.0366 (14)$ H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ C25 $0.4366 (6)$ $0.4945 (10)$ $0.2755 (5)$ $0.061 (2)$ H25 $0.4054$ $0.5280$ $0.3109$ $0.73*$ C4 $0.3264 (8)$ $0.3052 (9)$ $0.7701 (9)$ $0.084 (4)$ H4 $0.3540$ $0.2345$ $0.7857$ $0.101*$ <	H30	0.3116	0.2347	0.5008	0.055*
H60.20100.50800.82330.061*C290.3703 (4)0.0948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.053*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48010.10910.086*C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.067* (3)L240.36990.54450.19670.088*C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H240.36990.54450.19670.088*C320.6180 (4)0.3627 (7)0.3912 (4)0.3666 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*H32B0.65100.42200.36620.044*H40.35400.23450.78570.101*C210.5468 (5)0.3811 (1)0.2420 (5)0.056 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.884 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3811 (11)0.2220 (5)0.056 (2)H21 <td>C6</td> <td>0.2349 (5)</td> <td>0.4681 (8)</td> <td>0.7926 (5)</td> <td>0.051(2)</td>	C6	0.2349 (5)	0.4681 (8)	0.7926 (5)	0.051(2)
C290.3703 (4)0.0948 (8)0.4548 (4)0.0440 (18)H290.33800.02860.46850.053*C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48010.10910.086*C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.	H6	0.2010	0.5080	0.8233	0.061*
$129$ $0.3380$ $0.0286$ $0.4685$ $0.053^*$ $C8$ $0.3063 (5)$ $0.8403 (8)$ $0.7055 (5)$ $0.0463 (19)$ $18$ $0.3186$ $0.8184$ $0.6590$ $0.056^*$ $C23$ $0.4602 (7)$ $0.4667 (12)$ $0.1562 (6)$ $0.072 (3)$ $123$ $0.4468$ $0.4801$ $0.1091$ $0.086^*$ $C20$ $0.5020 (4)$ $0.4340 (7)$ $0.2941 (4)$ $0.0406 (17)$ $C2$ $0.2970 (5)$ $0.4527 (9)$ $0.6817 (6)$ $0.055 (2)$ $142$ $0.3046$ $0.4832$ $0.6358$ $0.066^*$ $C24$ $0.4162 (8)$ $0.5068 (11)$ $0.2077 (6)$ $0.074 (3)$ $124$ $0.3699$ $0.5445$ $0.1967$ $0.088^*$ $C22$ $0.5270 (7)$ $0.4042 (15)$ $0.1732 (6)$ $0.074 (4)$ $122$ $0.5583$ $0.3733$ $0.1374$ $0.089^*$ $C32$ $0.6180 (4)$ $0.3627 (7)$ $0.3912 (4)$ $0.0366 (14)$ $132A$ $0.6208$ $0.2803$ $0.3673$ $0.044^*$ $C25$ $0.4366 (6)$ $0.4945 (10)$ $0.2755 (5)$ $0.061 (2)$ $125$ $0.4054$ $0.5280$ $0.3109$ $0.073^*$ $C4$ $0.3264 (8)$ $0.3052 (9)$ $0.7701 (9)$ $0.084 (4)$ $144$ $0.3540$ $0.2345$ $0.7857$ $0.101^*$ $C25$ $0.4366 (5)$ $0.3452$ $0.2534$ $0.067^*$ $C17$ $-0.0197 (6)$ $0.3671 (14)$ $0.6222 (7)$ $0.075 (4)$ $144$ $0.3540$ $0.30$	C29	0.3703 (4)	0.0948 (8)	0.4548 (4)	0.0440 (18)
11.511.511.511.511.6C80.3063 (5)0.8403 (8)0.7055 (5)0.0463 (19)H80.31860.81840.65900.056*C230.4602 (7)0.4667 (12)0.1562 (6)0.072 (3)H230.44680.48010.10910.086*C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H30.37130.30960.67510.097*	H29	0 3380	0.0286	0 4685	0.053*
C23 $0.3186$ $0.8184$ $0.6590$ $0.056^*$ C23 $0.4602$ (7) $0.4667$ (12) $0.1562$ (6) $0.072$ (3)H23 $0.4468$ $0.4801$ $0.1091$ $0.086^*$ C20 $0.5020$ (4) $0.4340$ (7) $0.2941$ (4) $0.0406$ (17)C2 $0.2970$ (5) $0.4527$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066^*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088^*$ C22 $0.5270$ (7) $0.4042$ (15) $0.1732$ (6) $0.074$ (4)H22 $0.5583$ $0.3733$ $0.1374$ $0.089*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044*$ C25 $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H25 $0.4054$ $0.5280$ $0.3109$ $0.073*$ C4 $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4)H4 $0.3540$ $0.2345$ $0.7857$ $0.101*$ C21 $0.5468$ (5) $0.3811$ (11) $0.22234$ $0.067*$ C17 $-0.0197$ (6) $0.3671$ (14) $0.6222$ (7) $0.075$ (4)H3 $0.3713$ $0.3096$ $0.6751$ $0.097*$ C16 $-0.0106$ (6) $0.4861$ (17) $0.5941$ (6) $0.079$ (4)	C8	0.3063 (5)	0.8403 (8)	0.7055 (5)	0.035 0.0463 (19)
Inc $0.5140$ $0.5164$ $0.050$ $0.050$ C23 $0.4602$ (7) $0.4667$ (12) $0.1562$ (6) $0.072$ (3)H23 $0.4468$ $0.4801$ $0.1091$ $0.086^*$ C20 $0.5020$ (4) $0.4340$ (7) $0.2941$ (4) $0.0406$ (17)C2 $0.2970$ (5) $0.4527$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066^*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088^*$ C22 $0.5270$ (7) $0.4042$ (15) $0.1732$ (6) $0.074$ (4)H22 $0.5583$ $0.3733$ $0.1374$ $0.089^*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32B $0.6510$ $0.4220$ $0.3662$ $0.044^*$ C25 $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H25 $0.4054$ $0.5280$ $0.3109$ $0.073^*$ C4 $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4)H4 $0.3540$ $0.2345$ $0.7857$ $0.101^*$ C21 $0.5468$ (5) $0.3881$ (11) $0.2420$ (5) $0.056$ (2)H21 $0.5915$ $0.3452$ $0.2524$ (7) $0.075$ (4)H17 $-0.0458$ $0.3038$ $0.5973$ $0.090^*$ C3 $0.3366$ (7) $0.3495$ (11) $0.7051$ (9) $0.081$ (4)H3 $0.3713$ $0.3096$ $0.6751$ $0.097^*$ <td>H8</td> <td>0.3186</td> <td>0.8184</td> <td>0.6590</td> <td>0.056*</td>	H8	0.3186	0.8184	0.6590	0.056*
C2D $0.1602$ (1) $0.1601$ (12) $0.1091$ $0.081(0)$ H23 $0.4468$ $0.4801$ $0.1091$ $0.086*$ C20 $0.5020$ (4) $0.4340$ (7) $0.2941$ (4) $0.0406$ (17)C2 $0.2970$ (5) $0.4527$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088*$ C22 $0.5270$ (7) $0.4042$ (15) $0.1732$ (6) $0.074$ (4)H22 $0.5583$ $0.3733$ $0.1374$ $0.089*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044*$ C25 $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H25 $0.4054$ $0.5280$ $0.3109$ $0.073*$ C4 $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4)H4 $0.3540$ $0.2345$ $0.2834$ $0.067*$ C17 $-0.0197$ (6) $0.3671$ (14) $0.6222$ (7) $0.075$ (4)H17 $-0.0458$ $0.3038$ $0.5973$ $0.909*$ C3 $0.3366$ (7) $0.3495$ (11) $0.7051$ (9) $0.081$ (4)H3 $0.3713$ $0.3096$ $0.6751$ $0.097*$ C16 $-0.0106$ (6) $0.4861$ (17) $0.5941$ (6) $0.075$ (4) <td>C23</td> <td>0.3100 0.4602(7)</td> <td>0.4667(12)</td> <td>0.1562 (6)</td> <td>0.020</td>	C23	0.3100 0.4602(7)	0.4667(12)	0.1562 (6)	0.020
Inters0.14030.14040.14340 (7)0.2941 (4)0.0406 (17)C200.5020 (4)0.4340 (7)0.2941 (4)0.0406 (17)C20.2970 (5)0.4527 (9)0.6817 (6)0.055 (2)H20.30460.48320.63580.066*C240.4162 (8)0.5068 (11)0.2077 (6)0.074 (3)H240.36990.54450.19670.088*C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.5062<	H23	0.4468	0.4801	0.1091	0.072 (3)
C20 $0.3020$ (Y) $0.4527$ (9) $0.6317$ (6) $0.0500$ (17)C2 $0.2970$ (5) $0.4527$ (9) $0.6817$ (6) $0.055$ (2)H2 $0.3046$ $0.4832$ $0.6358$ $0.066^*$ C24 $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3)H24 $0.3699$ $0.5445$ $0.1967$ $0.088^*$ C22 $0.5270$ (7) $0.4042$ (15) $0.1732$ (6) $0.074$ (4)H22 $0.5583$ $0.3733$ $0.1374$ $0.089^*$ C32 $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14)H32A $0.6208$ $0.2803$ $0.3673$ $0.044^*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044^*$ C25 $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2)H25 $0.4054$ $0.5280$ $0.3109$ $0.073^*$ C4 $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4)H4 $0.3540$ $0.2345$ $0.7857$ $0.101^*$ C21 $0.5468$ (5) $0.3881$ (11) $0.2420$ (5) $0.056$ (2)H21 $0.5915$ $0.3452$ $0.2534$ $0.067^*$ C17 $-0.0197$ (6) $0.3671$ (14) $0.6222$ (7) $0.075$ (4)H17 $-0.0458$ $0.3038$ $0.5973$ $0.999^*$ C3 $0.3366$ (7) $0.3495$ (11) $0.7051$ (9) $0.081$ (4)H3 $0.3713$ $0.3096$ $0.6751$ $0.097^*$ C16 $-0.0106$ (6) $0.4861$ (17) $0.5941$ (6) $0.0$	C20	0.5020 (4)	0.4340(7)	0.1091 0.2941 (4)	0.000
C2 $0.276(6)$ $0.4827(7)$ $0.6317(6)$ $0.035(2)$ H2 $0.3046$ $0.4832$ $0.6358$ $0.066*$ C24 $0.4162(8)$ $0.5068(11)$ $0.2077(6)$ $0.074(3)$ H24 $0.3699$ $0.5445$ $0.1967$ $0.088*$ C22 $0.5270(7)$ $0.4042(15)$ $0.1732(6)$ $0.074(4)$ H22 $0.5583$ $0.3733$ $0.1374$ $0.089*$ C32 $0.6180(4)$ $0.3627(7)$ $0.3912(4)$ $0.0366(14)$ H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044*$ C25 $0.4366(6)$ $0.4945(10)$ $0.2755(5)$ $0.061(2)$ H25 $0.4054$ $0.5280$ $0.3109$ $0.073*$ C4 $0.3264(8)$ $0.3052(9)$ $0.7701(9)$ $0.084(4)$ H4 $0.3540$ $0.2345$ $0.7857$ $0.101*$ C21 $0.5468(5)$ $0.3881(11)$ $0.2420(5)$ $0.056(2)$ H21 $0.5915$ $0.3452$ $0.2534$ $0.667*$ C17 $-0.0197(6)$ $0.3671(14)$ $0.6222(7)$ $0.075(4)$ H17 $-0.0458$ $0.3038$ $0.5973$ $0.090*$ C3 $0.3366(7)$ $0.3495(11)$ $0.7051(9)$ $0.081(4)$ H3 $0.3713$ $0.3096$ $0.6751$ $0.097*$ C16 $-0.0106(6)$ $0.4861(17)$ $0.5941(6)$ $0.075(4)$ H16 $-0.0326$ $0.5062$ $0.5506$ $0.095*$ C5 $0.2766(8)$ $0.3279$ <td>C20</td> <td>0.3020(4) 0.2970(5)</td> <td>0.4527(9)</td> <td>0.2941(4) 0.6817(6)</td> <td>0.0400(17)</td>	C20	0.3020(4) 0.2970(5)	0.4527(9)	0.2941(4) 0.6817(6)	0.0400(17)
112 $0.3040$ $0.4352$ $0.0338$ $0.000$ $C24$ $0.4162$ (8) $0.5068$ (11) $0.2077$ (6) $0.074$ (3) $H24$ $0.3699$ $0.5445$ $0.1967$ $0.088*$ $C22$ $0.5270$ (7) $0.4042$ (15) $0.1732$ (6) $0.074$ (4) $H22$ $0.5583$ $0.3733$ $0.1374$ $0.089*$ $C32$ $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14) $H32A$ $0.6208$ $0.2803$ $0.3673$ $0.044*$ $H32B$ $0.6510$ $0.4220$ $0.3662$ $0.044*$ $C25$ $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2) $H25$ $0.4054$ $0.5280$ $0.3109$ $0.073*$ $C4$ $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4) $H4$ $0.3540$ $0.2345$ $0.7857$ $0.101*$ $C21$ $0.5468$ (5) $0.3452$ $0.2534$ $0.067*$ $C17$ $-0.0197$ (6) $0.3671$ (14) $0.6222$ (7) $0.075$ (4) $H17$ $-0.0458$ $0.3038$ $0.5973$ $0.090*$ $C3$ $0.3366$ (7) $0.3495$ (11) $0.7051$ (9) $0.81$ (4) $H3$ $0.3713$ $0.3096$ $0.6751$ $0.097*$ $C16$ $-0.0106$ (6) $0.4861$ (17) $0.5941$ (6) $0.079$ (4) $H16$ $-0.0326$ $0.5062$ $0.5506$ $0.095*$ $C5$ $0.2696$ $0.3279$ $0.8589$ $0.090*$	С2 H2	0.2076 (5)	0.4832	0.6358	0.055 (2)
124 $0.4102 (6)$ $0.5008 (11)$ $0.2077 (0)$ $0.074 (5)$ $1124$ $0.3699$ $0.5445$ $0.1967$ $0.088*$ $122$ $0.5270 (7)$ $0.4042 (15)$ $0.1732 (6)$ $0.074 (4)$ $1122$ $0.5583$ $0.3733$ $0.1374$ $0.089*$ $122$ $0.6180 (4)$ $0.3627 (7)$ $0.3912 (4)$ $0.0366 (14)$ $1132A$ $0.6208$ $0.2803$ $0.3673$ $0.044*$ $1132B$ $0.6510$ $0.4220$ $0.3662$ $0.044*$ $125$ $0.4366 (6)$ $0.4945 (10)$ $0.2755 (5)$ $0.061 (2)$ $125$ $0.4054$ $0.5280$ $0.3109$ $0.073*$ $124$ $0.3264 (8)$ $0.3052 (9)$ $0.7701 (9)$ $0.084 (4)$ $144$ $0.3540$ $0.2345$ $0.7857$ $0.101*$ $121$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $121$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $121$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $121$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $121$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $121$ $0.3366 (7)$ $0.3495 (11)$ $0.7051 (9)$ $0.81 (4)$ $133$ $0.3713$ $0.3096$ $0.6751$ $0.097*$ $146$ $-0.0106 (6)$ $0.4861 (17)$ $0.5941 (6)$ $0.079 (4)$ $116$ $-0.0326$ $0.5062$ $0.5506$ $0.095*$ $155$ $0.2696$ $0.3279$ $0.8589$ $0.090*$ <td>C24</td> <td>0.3040</td> <td>0.4052</td> <td>0.0558</td> <td>0.000</td>	C24	0.3040	0.4052	0.0558	0.000
11240.30990.34430.19070.0088C220.5270 (7)0.4042 (15)0.1732 (6)0.074 (4)H220.55830.37330.13740.089*C320.6180 (4)0.3627 (7)0.3912 (4)0.0366 (14)H32A0.62080.28030.36730.044*C250.4366 (6)0.49200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.884 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.81 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.32790.85890.900*	U24	0.4102 (8)	0.5008 (11)	0.2077 (0)	0.074 (3)
C22 $0.5270(7)$ $0.4042(15)$ $0.1732(0)$ $0.074(4)$ H22 $0.5583$ $0.3733$ $0.1374$ $0.089*$ C32 $0.6180(4)$ $0.3627(7)$ $0.3912(4)$ $0.0366(14)$ H32A $0.6208$ $0.2803$ $0.3673$ $0.044*$ H32B $0.6510$ $0.4220$ $0.3662$ $0.044*$ C25 $0.4366(6)$ $0.4945(10)$ $0.2755(5)$ $0.061(2)$ H25 $0.4054$ $0.5280$ $0.3109$ $0.073*$ C4 $0.3264(8)$ $0.3052(9)$ $0.7701(9)$ $0.084(4)$ H4 $0.3540$ $0.2345$ $0.7857$ $0.101*$ C21 $0.5468(5)$ $0.3452$ $0.2534$ $0.067*$ C17 $-0.0197(6)$ $0.3671(14)$ $0.6222(7)$ $0.075(4)$ H17 $-0.0458$ $0.3038$ $0.5973$ $0.090*$ C3 $0.3366(7)$ $0.3495(11)$ $0.7051(9)$ $0.081(4)$ H3 $0.3713$ $0.3096$ $0.6751$ $0.097*$ C16 $-0.0106(6)$ $0.4861(17)$ $0.5941(6)$ $0.079(4)$ H16 $-0.0326$ $0.5062$ $0.5506$ $0.095*$ C5 $0.2766(8)$ $0.3612(10)$ $0.8135(8)$ $0.075(4)$ H5 $0.2696$ $0.3279$ $0.8589$ $0.90*$	C22	0.5099	0.3443 0.4042 (15)	0.1737 (6)	0.033
1122 $0.3783$ $0.3733$ $0.1374$ $0.0367$ $C32$ $0.6180$ (4) $0.3627$ (7) $0.3912$ (4) $0.0366$ (14) $H32A$ $0.6208$ $0.2803$ $0.3673$ $0.044*$ $H32B$ $0.6510$ $0.4220$ $0.3662$ $0.044*$ $C25$ $0.4366$ (6) $0.4945$ (10) $0.2755$ (5) $0.061$ (2) $H25$ $0.4054$ $0.5280$ $0.3109$ $0.073*$ $C4$ $0.3264$ (8) $0.3052$ (9) $0.7701$ (9) $0.084$ (4) $H4$ $0.3540$ $0.2345$ $0.7857$ $0.101*$ $C21$ $0.5468$ (5) $0.3881$ (11) $0.2420$ (5) $0.056$ (2) $H21$ $0.5915$ $0.3452$ $0.2534$ $0.067*$ $C17$ $-0.0197$ (6) $0.3671$ (14) $0.6222$ (7) $0.075$ (4) $H17$ $-0.0458$ $0.3038$ $0.5973$ $0.090*$ $C3$ $0.3366$ (7) $0.3495$ (11) $0.7051$ (9) $0.081$ (4) $H3$ $0.3713$ $0.3096$ $0.6751$ $0.097*$ $C16$ $-0.0106$ (6) $0.4861$ (17) $0.5941$ (6) $0.079$ (4) $H16$ $-0.0326$ $0.5062$ $0.5506$ $0.095*$ $C5$ $0.2766$ (8) $0.3279$ $0.8589$ $0.900*$	U22	0.5270 (7)	0.4042 (13)	0.1732(0) 0.1374	0.074 (4)
C320.5180 (4)0.3627 (7)0.3912 (4)0.0360 (14)H32A0.62080.28030.36730.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	П22	0.5385	0.3733 0.3637(7)	0.1374 0.2012 (4)	$0.089^{\circ}$
H32A0.02080.28030.36750.044*H32B0.65100.42200.36620.044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.000*		0.0100 (4)	0.3027(7)	0.3912(4)	0.0300 (14)
H32B0.65100.42200.36620.0044*C250.4366 (6)0.4945 (10)0.2755 (5)0.061 (2)H250.40540.52800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.32790.85890.090*	П32А	0.0208	0.2803	0.3073	0.044
$C25$ $0.4366(6)$ $0.4943(10)$ $0.2735(5)$ $0.061(2)$ H25 $0.4054$ $0.5280$ $0.3109$ $0.073^*$ C4 $0.3264(8)$ $0.3052(9)$ $0.7701(9)$ $0.084(4)$ H4 $0.3540$ $0.2345$ $0.7857$ $0.101^*$ C21 $0.5468(5)$ $0.3881(11)$ $0.2420(5)$ $0.056(2)$ H21 $0.5915$ $0.3452$ $0.2534$ $0.067^*$ C17 $-0.0197(6)$ $0.3671(14)$ $0.6222(7)$ $0.075(4)$ H17 $-0.0458$ $0.3038$ $0.5973$ $0.090^*$ C3 $0.3366(7)$ $0.3495(11)$ $0.7051(9)$ $0.081(4)$ H3 $0.3713$ $0.3096$ $0.6751$ $0.097^*$ C16 $-0.0106(6)$ $0.4861(17)$ $0.5941(6)$ $0.079(4)$ H16 $-0.0326$ $0.5062$ $0.5506$ $0.095^*$ C5 $0.2766(8)$ $0.3279$ $0.8589$ $0.090^*$	H32B	0.0510	0.4220	0.3002	$0.044^{*}$
H250.40340.32800.31090.073*C40.3264 (8)0.3052 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	C25	0.4300 (0)	0.4943 (10)	0.2755 (5)	0.001 (2)
C40.3264 (8)0.3032 (9)0.7701 (9)0.084 (4)H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	H25	0.4054	0.5280	0.3109	$0.073^{*}$
H40.35400.23450.78570.101*C210.5468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	C4	0.3264 (8)	0.3052 (9)	0.7701 (9)	0.084 (4)
C210.3468 (5)0.3881 (11)0.2420 (5)0.056 (2)H210.59150.34520.25340.067*C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	H4	0.3540	0.2345	0.7857	$0.101^{*}$
H21 $0.5915$ $0.3452$ $0.2534$ $0.067^*$ C17 $-0.0197(6)$ $0.3671(14)$ $0.6222(7)$ $0.075(4)$ H17 $-0.0458$ $0.3038$ $0.5973$ $0.090^*$ C3 $0.3366(7)$ $0.3495(11)$ $0.7051(9)$ $0.081(4)$ H3 $0.3713$ $0.3096$ $0.6751$ $0.097^*$ C16 $-0.0106(6)$ $0.4861(17)$ $0.5941(6)$ $0.079(4)$ H16 $-0.0326$ $0.5062$ $0.5506$ $0.095^*$ C5 $0.2766(8)$ $0.3612(10)$ $0.8135(8)$ $0.075(4)$ H5 $0.2696$ $0.3279$ $0.8589$ $0.090^*$	C21	0.5468 (5)	0.3881 (11)	0.2420 (5)	0.056 (2)
C17-0.0197 (6)0.3671 (14)0.6222 (7)0.075 (4)H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	H2I	0.5915	0.3452	0.2534	0.06/*
H17-0.04580.30380.59730.090*C30.3366 (7)0.3495 (11)0.7051 (9)0.081 (4)H30.37130.30960.67510.097*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	C1/	-0.019/(6)	0.36/1 (14)	0.6222 (/)	0.075 (4)
C3       0.3366 (7)       0.3495 (11)       0.7051 (9)       0.081 (4)         H3       0.3713       0.3096       0.6751       0.097*         C16       -0.0106 (6)       0.4861 (17)       0.5941 (6)       0.079 (4)         H16       -0.0326       0.5062       0.5506       0.095*         C5       0.2766 (8)       0.3612 (10)       0.8135 (8)       0.075 (4)         H5       0.2696       0.3279       0.8589       0.090*	HI7	-0.0458	0.3038	0.5973	0.090*
H30.3/130.30960.6/510.09/*C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	C3	0.3366 (7)	0.3495 (11)	0.7051 (9)	0.081 (4)
C16-0.0106 (6)0.4861 (17)0.5941 (6)0.079 (4)H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	H3	0.3/13	0.3096	0.6751	0.097*
H16-0.03260.50620.55060.095*C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	C16	-0.0106 (6)	0.4861 (17)	0.5941 (6)	0.079 (4)
C50.2766 (8)0.3612 (10)0.8135 (8)0.075 (4)H50.26960.32790.85890.090*	HI6	-0.0326	0.5062	0.5506	0.095*
H5 0.2696 0.3279 0.8589 0.090*	05	0.2766 (8)	0.3612 (10)	0.8135 (8)	0.075 (4)
	Н5	0.2696	0.3279	0.8589	0.090*

# data reports

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Agl	0.0474 (3)	0.0544 (3)	0.0350 (2)	-0.0033 (2)	0.0018 (2)	0.0002 (3)
Ag2	0.0444 (3)	0.0335 (3)	0.0547 (3)	-0.0016(2)	0.0037 (2)	-0.0057 (3)
P1	0.0242 (7)	0.0301 (8)	0.0335 (8)	0.0013 (6)	-0.0005 (6)	-0.0039(7)
P2	0.0254 (7)	0.0310 (8)	0.0448 (9)	-0.0035 (7)	0.0029 (7)	-0.0018(7)
01	0.059 (4)	0.049 (3)	0.045 (3)	0.016 (3)	0.001 (3)	-0.004(3)
03	0.041 (3)	0.058 (4)	0.048 (3)	0.002 (3)	-0.002(2)	-0.010(3)
O2	0.061 (3)	0.034 (3)	0.044 (3)	0.005 (2)	0.002 (2)	-0.003(2)
N1	0.037 (3)	0.034 (3)	0.041 (3)	0.004 (2)	0.002 (2)	0.006 (2)
C26	0.026 (3)	0.029 (3)	0.041 (4)	-0.002 (2)	-0.001 (3)	0.007 (3)
N2	0.038 (3)	0.038 (4)	0.069 (5)	-0.001(3)	0.020 (3)	-0.004 (3)
05	0.072 (5)	0.054 (4)	0.074 (5)	0.020 (3)	0.023 (4)	0.015 (3)
O4	0.060 (4)	0.050 (4)	0.092 (6)	0.016 (3)	0.035 (4)	0.017 (4)
06	0.068 (5)	0.045 (4)	0.163 (10)	-0.003(3)	0.071 (6)	0.003 (5)
C1	0.030 (3)	0.023 (3)	0.058 (4)	-0.001(2)	-0.012 (3)	-0.008 (3)
C14	0.022 (3)	0.052 (4)	0.036 (3)	-0.004(3)	0.004 (3)	-0.008(3)
C31	0.032 (3)	0.038 (4)	0.045 (4)	0.001 (3)	-0.001 (3)	0.002 (3)
C27	0.030 (3)	0.037 (4)	0.039 (4)	-0.006 (3)	0.000 (3)	0.006 (3)
C19	0.031 (3)	0.045 (4)	0.063 (5)	-0.002(3)	-0.004 (3)	-0.009 (4)
C37	0.044 (4)	0.058 (5)	0.055 (5)	0.010 (4)	0.005 (4)	0.011 (5)
C9	0.054 (5)	0.042 (4)	0.067 (6)	-0.020 (4)	-0.004 (4)	-0.003 (4)
C11	0.060 (5)	0.037 (4)	0.044 (4)	0.000 (4)	-0.011 (4)	-0.003 (3)
C28	0.039 (4)	0.034 (4)	0.046 (4)	-0.011 (3)	-0.010 (3)	0.005 (3)
C35	0.043 (4)	0.053 (5)	0.059 (5)	0.010 (4)	0.001 (4)	-0.019 (5)
C13	0.030 (3)	0.035 (4)	0.042 (4)	0.001 (3)	-0.001 (3)	-0.004 (3)
C33	0.023 (3)	0.037 (3)	0.047 (4)	-0.002 (3)	0.003 (3)	-0.002 (3)
C10	0.062 (5)	0.036 (4)	0.068 (6)	-0.011 (4)	-0.020 (5)	0.000 (4)
C7	0.034 (3)	0.026 (3)	0.041 (4)	0.002 (2)	-0.006 (3)	0.001 (3)
C12	0.046 (4)	0.043 (4)	0.035 (4)	-0.001 (3)	-0.009 (3)	-0.004 (3)
C34	0.031 (3)	0.038 (4)	0.052 (4)	0.005 (3)	-0.003 (3)	-0.002 (3)
C15	0.036 (4)	0.082 (6)	0.043 (4)	-0.018 (4)	0.002 (3)	-0.004 (5)
C38	0.036 (4)	0.044 (4)	0.063 (5)	-0.005 (3)	0.003 (3)	0.009 (4)
C36	0.051 (5)	0.077 (7)	0.044 (4)	0.028 (5)	0.003 (4)	0.002 (4)
C18	0.037 (4)	0.048 (5)	0.102 (9)	-0.008 (4)	0.000 (5)	-0.021 (6)
C30	0.027 (3)	0.059 (5)	0.052 (4)	-0.001 (3)	0.006 (3)	0.014 (4)
C6	0.055 (5)	0.032 (4)	0.066 (5)	-0.013 (3)	-0.026 (4)	0.007 (4)
C29	0.037 (4)	0.045 (4)	0.050 (5)	-0.011 (3)	-0.010 (3)	0.015 (3)
C8	0.045 (4)	0.037 (4)	0.057 (5)	-0.009 (3)	0.003 (4)	0.001 (4)
C23	0.078 (7)	0.079 (8)	0.059 (6)	-0.022 (6)	-0.022 (5)	0.029 (6)
C20	0.046 (4)	0.028 (4)	0.048 (4)	-0.019 (3)	-0.005 (3)	0.006 (3)
C2	0.038 (4)	0.048 (5)	0.079 (7)	0.011 (3)	-0.015 (4)	-0.021 (5)
C24	0.095 (8)	0.063 (6)	0.064 (7)	0.010 (6)	-0.020 (6)	0.016 (6)
C22	0.060 (6)	0.113 (10)	0.050 (6)	-0.028 (6)	0.014 (5)	-0.004 (6)
C32	0.030 (3)	0.035 (3)	0.045 (4)	-0.004 (3)	0.003 (3)	0.005 (3)
C25	0.077 (6)	0.050 (5)	0.054 (5)	0.014 (5)	-0.021 (5)	0.002 (4)
C4	0.088 (8)	0.030 (4)	0.135 (12)	0.019 (5)	-0.056 (8)	-0.012 (6)

# data reports

C21	0.036 (4)	0.084 (7)	0.049 (5)	-0.008 (4)	0.001 (4)	0.003 (4)
C17	0.046 (5)	0.111 (10)	0.070 (7)	-0.025 (6)	0.002 (5)	-0.047 (7)
C3	0.069 (7)	0.050 (6)	0.125 (12)	0.029 (5)	-0.033 (7)	-0.022 (7)
C16	0.052 (5)	0.138 (13)	0.048 (5)	-0.043 (7)	-0.001 (4)	-0.021 (7)
C5	0.092 (8)	0.044 (5)	0.090 (9)	-0.019 (5)	-0.047 (7)	0.022 (6)

Geometric parameters (Å, °)

Ag1—P1	2.3506 (19)	C37—C38	1.381 (14)	
Ag1—O1	2.380 (6)	C37—C36	1.358 (15)	
Ag1—O4	2.406 (7)	C9—C10	1.360 (15)	
Ag2—P2	2.3612 (19)	C9—C8	1.407 (12)	
Ag2—O2 <sup>i</sup>	2.460 (6)	C11—C10	1.384 (14)	
Ag2—06	2.295 (7)	C11—C12	1.386 (12)	
P1—C1	1.806 (7)	C28—C29	1.384 (12)	
P1—C13	1.838 (8)	C35—C34	1.375 (14)	
Р1—С7	1.830(7)	C35—C36	1.417 (15)	
P2—C26	1.830(7)	C33—C34	1.383 (11)	
P2—C20	1.829 (9)	C33—C38	1.409 (11)	
Р2—С32	1.838 (7)	C33—C32	1.484 (11)	
O1—N1	1.251 (9)	C7—C12	1.400 (11)	
O3—N1	1.243 (9)	С7—С8	1.382 (11)	
O2—Ag2 <sup>ii</sup>	2.460 (6)	C15—C16	1.366 (15)	
O2—N1	1.260 (8)	C18—C17	1.39 (2)	
C26—C31	1.398 (10)	C30—C29	1.382 (13)	
C26—C27	1.379 (11)	C6—C5	1.420 (14)	
N2—O5	1.216 (10)	C23—C24	1.338 (19)	
N204	1.249 (10)	C23—C22	1.412 (19)	
N2—O6	1.245 (10)	C20—C25	1.389 (13)	
C1—C6	1.391 (13)	C20—C21	1.376 (13)	
C1—C2	1.396 (12)	C2—C3	1.383 (15)	
C14—C19	1.394 (12)	C24—C25	1.362 (15)	
C14—C13	1.504 (10)	C22—C21	1.381 (15)	
C14—C15	1.377 (12)	C4—C3	1.35 (2)	
C31—C30	1.389 (11)	C4—C5	1.36 (2)	
C27—C28	1.406 (10)	C17—C16	1.38 (2)	
C19—C18	1.372 (13)			
P1—Ag1—O1	141.80 (17)	C18—C19—C14	120.4 (10)	
P1—Ag1—O4	129.6 (2)	C36—C37—C38	120.1 (9)	
01—Ag1—O4	88.5 (3)	C10—C9—C8	119.4 (9)	
$P2 - Ag2 - O2^i$	121.08 (15)	C10—C11—C12	120.0 (9)	
O6—Ag2—P2	142.8 (3)	C29—C28—C27	119.6 (8)	
O6—Ag2—O2 <sup>i</sup>	96.0 (3)	C34—C35—C36	118.2 (9)	
C1—P1—Ag1	114.2 (3)	C14—C13—P1	110.4 (5)	
C1—P1—C13	105.1 (4)	C34—C33—C38	118.4 (8)	
C1—P1—C7	103.5 (3)	C34—C33—C32	120.6 (7)	
C13—P1—Ag1	114.8 (3)	C38—C33—C32	121.0 (7)	

C7—P1—Ag1	113.5 (2)	C9—C10—C11	121.1 (8)
C7—P1—C13	104.5 (3)	C12—C7—P1	122.9 (6)
C26—P2—Ag2	115.7 (2)	C8—C7—P1	117.6 (6)
C26—P2—C32	104.9 (3)	C8—C7—C12	119.3 (7)
C20—P2—Ag2	109.2 (3)	C11—C12—C7	119.7 (8)
C20—P2—C26	103.7 (3)	C35—C34—C33	121.8 (8)
C20—P2—C32	104.7 (4)	C16—C15—C14	121.7 (11)
C32—P2—Ag2	117.3 (3)	C37—C38—C33	120.5 (8)
N1—O1—Ag1	100.8 (5)	C37—C36—C35	120.9 (10)
N1—O2—Ag2 <sup>ii</sup>	99.5 (4)	C19—C18—C17	120.6 (12)
01—N1—O2	119.0 (7)	C29—C30—C31	120.9 (7)
O3—N1—O1	121.9 (7)	C1—C6—C5	117.2 (11)
O3—N1—O2	119.0 (6)	C30—C29—C28	120.1 (7)
C31—C26—P2	117.9 (5)	C7—C8—C9	120.4 (9)
C27—C26—P2	121.6 (5)	C24—C23—C22	118.9 (10)
C27—C26—C31	120.4 (6)	C25—C20—P2	117.0 (7)
O5—N2—O4	119.6 (7)	C21—C20—P2	124.8 (7)
O5—N2—O6	119.7 (7)	C21—C20—C25	118.3 (9)
O6—N2—O4	120.6 (8)	C3—C2—C1	120.2 (12)
N2—O4—Ag1	106.5 (5)	C23—C24—C25	121.3 (11)
N2—O6—Ag2	115.7 (6)	C21—C22—C23	120.0 (11)
C6C1P1	123.0 (6)	C33—C32—P2	112.4 (5)
C6—C1—C2	120.1 (8)	C24—C25—C20	121.3 (11)
C2-C1-P1	116.7 (7)	C3—C4—C5	120.4 (10)
C19—C14—C13	121.8 (7)	C20—C21—C22	120.2 (10)
C15—C14—C19	118.3 (8)	C16—C17—C18	118.8 (9)
C15—C14—C13	119.8 (8)	C4—C3—C2	120.5 (13)
C30—C31—C26	119.1 (7)	C15—C16—C17	120.1 (11)
C26—C27—C28	120.0 (7)	C4—C5—C6	121.6 (13)

Symmetry codes: (i) x+1/2, -y+3/2, z; (ii) x-1/2, -y+3/2, z.