Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2,5-Diphenylpent-4-yn-1-en-3-ylidene)-triphenylphosphorane

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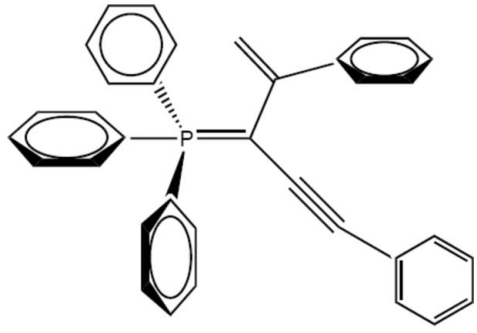
Received 20 November 2007; accepted 22 November 2007

Key indicators: single-crystal X-ray study; T = 383 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.133; data-to-parameter ratio = 10.8.

The title compound, $C_{45}H_{27}P$, was obtained as a product of the reaction of triphenylmethylenephosphorane with one molar equivalent of 1,4-diphenylbutadiyne in toluene. The compound was very stable under ambient conditions, but rapidly decomposed in solution when exposed to the air. The P atom is tetracoordinated in an approximately tetrahedral geometry. The length of the C≡C triple bond [1.206 (2) Å] is in the normal range.

Related literature

Related crystal structures of α,β-unsaturated-C,P ylides have been reported, see: Koollenz *et al.* (1996).



Experimental

Crystal data

$C_{35}H_{27}P$
M_r = 478.54
Triclinic, $P\overline{1}$
a = 11.439 (2) Å
b = 11.609 (2) Å
c = 11.913 (2) Å
α = 116.00 (3)°
β = 97.24 (3)°
γ = 108.47 (3)°
V = 1281.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 383 (2) K
0.27 × 0.25 × 0.22 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.966, T_{max} = 0.972
9166 measured reflections
4661 independent reflections
4077 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.133
S = 1.06
4661 reflections
433 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—C19	1.7294 (15)	P1—C1	1.8178 (19)
P1—C13	1.8104 (15)	C20—C21	1.206 (2)
P1—C7	1.8132 (18)	C28—C29	1.343 (2)
C19—P1—C13	108.20 (7)	C13—P1—C1	107.73 (7)
C19—P1—C7	117.53 (8)	C7—P1—C1	106.29 (8)
C13—P1—C7	105.18 (7)	C21—C20—C19	179.42 (18)
C19—P1—C1	111.39 (7)	C20—C21—C22	164.32 (18)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the NSFC (Nos. 20572062 and 20372042) and by the Doctoral Program of the MOE (Nos. 20050422010 and 20050422011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2053).

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Koollenz, G., Penn, G., Theuer, R., Fabian, W. M. F., Abd El-Nabi, H. A., Xiong, Z., Peters, K., Peters, E.-M. & von Schnering, H. G. (1996). *Tetrahedron*, **52**, 15, 5427–5440.
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supplementary materials

Acta Cryst. (2008). E**64**, o68 [**doi:10.1107/S1600536807062034**]

(2,5-Diphenylpent-4-yn-1-en-3-ylidene)triphenylphosphorane

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Comment

In the title molecule (Fig.1) the phosphorane atom is coordinated in a tetragonal pyramid by three C atoms of phenyl groups and one sp_2-C atom. The length of the C—C triple bond is in the range of classic one, and the carbon atoms linked to the C—C triple bond lie in nearly a line.

Experimental

To the solution of triphenylmethylenephosphorane(1.41 g, 5.11 mmol) in 30 ml of toluene was added 1,4-diphenyl-butadiyne(1.05 g, 5.20 mmol) at room temperature, a deep red solution formed rapidly. After stirring for at least 24 h the reaction solution was filtrated. The solid residue was dried and extracted with pentane and diethyl ether, respectively. Purple red crystals were obtained suitable for X-ray diffraction analysis. (yield:1.59 g, 65.1%, d.p.: 87 °C)

Refinement

All H atoms were positioned geometrically. All the H atoms are refined using a riding model with C—H = 0.92–1.02 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

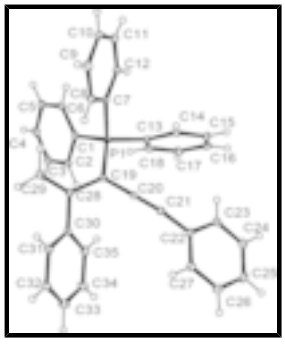


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

(2,5-Diphenylpent-4-yn-1-en-3-ylidene)triphenylphosphorane

Crystal data

$C_{35}H_{27}P$	$Z = 2$
$M_r = 478.54$	$F_{000} = 504$
Triclinic, $P\overline{1}$	$D_x = 1.240$ Mg m^{-3}
$a = 11.439$ (2) Å	Mo $K\alpha$ radiation

	λ = 0.71073 Å
b = 11.609 (2) Å	Cell parameters from 5612 reflections
c = 11.913 (2) Å	θ = 2.2–23.2º
α = 116.00 (3)º	μ = 0.13 mm^{-1}
β = 97.24 (3)º	T = 383 (2) K
γ = 108.47 (3)º	Cubic, purple red
V = 1281.9 (4) Å^3	0.27 × 0.25 × 0.22 mm

Data collection

Bruker SMART diffractometer	4661 independent reflections
Radiation source: fine-focus sealed tube	4077 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 383(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −14→14
T_{min} = 0.966, T_{max} = 0.972	k = −13→14
9166 measured reflections	l = −14→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.133	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.002
4661 reflections	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
433 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.68533 (3)	0.36252 (4)	0.11133 (3)	0.01164 (15)
C1	0.56521 (14)	0.24722 (17)	−0.05062 (14)	0.0144 (3)
C2	0.47129 (15)	0.11909 (18)	−0.07668 (15)	0.0164 (3)
C3	0.38692 (16)	0.02065 (19)	−0.20295 (16)	0.0187 (4)
C4	0.39421 (15)	0.04989 (18)	−0.30372 (15)	0.0193 (4)
C5	0.48380 (16)	0.1796 (2)	−0.27692 (16)	0.0206 (4)
C6	0.56947 (15)	0.27875 (19)	−0.15066 (15)	0.0168 (3)
C7	0.76840 (14)	0.52987 (17)	0.12146 (14)	0.0147 (3)
C8	0.74427 (15)	0.64557 (19)	0.19848 (16)	0.0188 (4)
C9	0.80051 (17)	0.7702 (2)	0.19820 (18)	0.0242 (4)
C10	0.88218 (17)	0.7816 (2)	0.12299 (18)	0.0243 (4)
C11	0.90960 (16)	0.6678 (2)	0.04955 (16)	0.0223 (4)
C12	0.85367 (15)	0.54293 (18)	0.04849 (15)	0.0163 (3)
C13	0.80689 (14)	0.29439 (18)	0.11596 (14)	0.0142 (3)
C14	0.92794 (15)	0.38344 (19)	0.21428 (15)	0.0163 (3)
C15	1.01613 (16)	0.3280 (2)	0.22863 (16)	0.0197 (4)
C16	0.98606 (16)	0.1863 (2)	0.14545 (17)	0.0222 (4)
C17	0.86805 (17)	0.0994 (2)	0.04615 (17)	0.0224 (4)
C18	0.77842 (16)	0.15322 (18)	0.03089 (16)	0.0191 (4)
C19	0.61694 (14)	0.36449 (17)	0.23325 (14)	0.0135 (3)
C20	0.68991 (14)	0.36051 (16)	0.33433 (14)	0.0132 (3)
C21	0.75197 (14)	0.35583 (17)	0.42069 (14)	0.0156 (3)
C22	0.80550 (14)	0.30986 (17)	0.49926 (14)	0.0153 (3)
C23	0.90307 (15)	0.26281 (19)	0.47269 (16)	0.0199 (4)
C24	0.94525 (16)	0.2043 (2)	0.53938 (17)	0.0232 (4)
C25	0.89336 (17)	0.1928 (2)	0.63495 (16)	0.0233 (4)
C26	0.80095 (17)	0.24431 (19)	0.66597 (16)	0.0211 (4)
C27	0.75698 (15)	0.30231 (18)	0.59963 (15)	0.0182 (3)
C28	0.48816 (14)	0.36477 (17)	0.22947 (14)	0.0142 (3)
C29	0.42860 (16)	0.4080 (2)	0.16165 (16)	0.0205 (4)
C30	0.41673 (14)	0.30236 (17)	0.30066 (14)	0.0143 (3)
C31	0.34931 (15)	0.36725 (18)	0.37822 (15)	0.0167 (3)
C32	0.27977 (15)	0.30599 (19)	0.44037 (16)	0.0199 (4)
C33	0.27776 (17)	0.1813 (2)	0.42805 (17)	0.0234 (4)
C34	0.34548 (17)	0.1160 (2)	0.35238 (18)	0.0233 (4)
C35	0.41519 (15)	0.17774 (18)	0.29087 (15)	0.0185 (3)
H21	0.3514 (19)	0.457 (2)	0.3947 (19)	0.024 (5)*
H5	0.630 (2)	0.366 (2)	−0.1330 (17)	0.017 (4)*
H1	0.4642 (19)	0.099 (2)	−0.0043 (18)	0.021 (5)*
H14	0.844 (2)	0.003 (3)	−0.013 (2)	0.042 (6)*
H2	0.328 (2)	−0.064 (2)	−0.2167 (19)	0.025 (5)*
H6	0.691 (2)	0.639 (2)	0.2514 (19)	0.023 (5)*
H23	0.229 (2)	0.134 (2)	0.4727 (19)	0.027 (5)*
H11	0.9484 (19)	0.480 (2)	0.2726 (19)	0.021 (5)*
H3	0.338 (2)	−0.017 (2)	−0.390 (2)	0.023 (5)*

H10	0.871 (2)	0.462 (3)	−0.004 (2)	0.030 (5)*
H16	0.9390 (19)	0.268 (2)	0.4059 (19)	0.021 (5)*
H24	0.348 (2)	0.034 (3)	0.343 (2)	0.032 (6)*
H19	0.768 (2)	0.240 (2)	0.735 (2)	0.028 (5)*
H27	0.475 (2)	0.451 (2)	0.1141 (19)	0.025 (5)*
H4	0.487 (2)	0.202 (2)	−0.345 (2)	0.028 (5)*
H15	0.698 (2)	0.092 (2)	−0.0382 (19)	0.021 (5)*
H18	0.921 (2)	0.153 (2)	0.682 (2)	0.029 (5)*
H13	1.050 (2)	0.147 (2)	0.1566 (19)	0.027 (5)*
H12	1.095 (2)	0.388 (2)	0.295 (2)	0.025 (5)*
H22	0.234 (2)	0.355 (2)	0.496 (2)	0.028 (5)*
H25	0.461 (2)	0.133 (3)	0.238 (2)	0.034 (6)*
H7	0.787 (2)	0.853 (3)	0.255 (2)	0.042 (6)*
H20	0.693 (2)	0.338 (2)	0.621 (2)	0.031 (5)*
H17	1.009 (2)	0.167 (2)	0.513 (2)	0.032 (6)*
H8	0.924 (2)	0.870 (3)	0.125 (2)	0.032 (6)*
H9	0.966 (2)	0.670 (3)	0.001 (2)	0.033 (6)*
H26	0.339 (2)	0.390 (2)	0.1535 (18)	0.022 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0118 (2)	0.0110 (3)	0.0152 (2)	0.00594 (17)	0.00547 (16)	0.00793 (17)
C1	0.0143 (7)	0.0151 (9)	0.0155 (7)	0.0084 (6)	0.0046 (6)	0.0077 (6)
C2	0.0179 (7)	0.0137 (9)	0.0211 (8)	0.0078 (6)	0.0067 (6)	0.0106 (6)
C3	0.0175 (7)	0.0137 (9)	0.0246 (8)	0.0072 (7)	0.0055 (6)	0.0092 (7)
C4	0.0178 (8)	0.0172 (9)	0.0186 (8)	0.0085 (7)	0.0038 (6)	0.0054 (7)
C5	0.0194 (8)	0.0279 (11)	0.0186 (8)	0.0114 (7)	0.0076 (6)	0.0136 (7)
C6	0.0149 (7)	0.0145 (9)	0.0229 (8)	0.0053 (7)	0.0066 (6)	0.0115 (7)
C7	0.0128 (7)	0.0152 (9)	0.0180 (7)	0.0061 (6)	0.0030 (6)	0.0101 (6)
C8	0.0160 (7)	0.0181 (10)	0.0266 (8)	0.0090 (7)	0.0082 (7)	0.0131 (7)
C9	0.0214 (8)	0.0144 (10)	0.0413 (10)	0.0104 (7)	0.0079 (7)	0.0161 (8)
C10	0.0196 (8)	0.0217 (11)	0.0393 (10)	0.0057 (7)	0.0050 (7)	0.0248 (8)
C11	0.0189 (8)	0.0272 (11)	0.0235 (8)	0.0068 (7)	0.0059 (7)	0.0173 (7)
C12	0.0159 (7)	0.0156 (9)	0.0182 (7)	0.0049 (6)	0.0052 (6)	0.0105 (6)
C13	0.0157 (7)	0.0175 (9)	0.0184 (7)	0.0108 (7)	0.0101 (6)	0.0125 (6)
C14	0.0171 (7)	0.0167 (9)	0.0202 (7)	0.0086 (7)	0.0095 (6)	0.0113 (7)
C15	0.0170 (8)	0.0278 (10)	0.0238 (8)	0.0128 (7)	0.0096 (7)	0.0175 (7)
C16	0.0237 (8)	0.0287 (11)	0.0337 (9)	0.0196 (8)	0.0181 (7)	0.0231 (8)
C17	0.0291 (9)	0.0138 (10)	0.0349 (9)	0.0138 (7)	0.0185 (7)	0.0153 (7)
C18	0.0179 (8)	0.0154 (9)	0.0238 (8)	0.0075 (7)	0.0086 (7)	0.0089 (7)
C19	0.0144 (7)	0.0145 (9)	0.0164 (7)	0.0076 (6)	0.0072 (6)	0.0100 (6)
C20	0.0139 (7)	0.0100 (8)	0.0165 (7)	0.0055 (6)	0.0075 (6)	0.0064 (6)
C21	0.0157 (7)	0.0170 (9)	0.0169 (7)	0.0083 (6)	0.0076 (6)	0.0092 (6)
C22	0.0144 (7)	0.0110 (8)	0.0164 (7)	0.0031 (6)	0.0014 (6)	0.0061 (6)
C23	0.0180 (8)	0.0241 (10)	0.0217 (8)	0.0095 (7)	0.0077 (6)	0.0140 (7)
C24	0.0187 (8)	0.0281 (11)	0.0282 (9)	0.0135 (8)	0.0066 (7)	0.0162 (7)
C25	0.0245 (8)	0.0242 (11)	0.0233 (8)	0.0100 (8)	0.0018 (7)	0.0152 (7)

C26	0.0253 (8)	0.0200 (10)	0.0176 (8)	0.0069 (7)	0.0070 (6)	0.0110 (7)
C27	0.0186 (7)	0.0171 (9)	0.0195 (7)	0.0082 (7)	0.0078 (6)	0.0087 (6)
C28	0.0147 (7)	0.0127 (8)	0.0172 (7)	0.0077 (6)	0.0062 (6)	0.0074 (6)
C29	0.0180 (8)	0.0257 (10)	0.0266 (8)	0.0133 (7)	0.0099 (6)	0.0165 (7)
C30	0.0108 (7)	0.0135 (8)	0.0167 (7)	0.0054 (6)	0.0034 (6)	0.0063 (6)
C31	0.0157 (7)	0.0153 (9)	0.0205 (7)	0.0088 (7)	0.0061 (6)	0.0086 (6)
C32	0.0185 (8)	0.0191 (9)	0.0244 (8)	0.0095 (7)	0.0109 (7)	0.0107 (7)
C33	0.0237 (8)	0.0243 (10)	0.0286 (9)	0.0098 (7)	0.0144 (7)	0.0171 (7)
C34	0.0268 (9)	0.0169 (10)	0.0340 (9)	0.0115 (8)	0.0148 (7)	0.0161 (8)
C35	0.0193 (8)	0.0151 (9)	0.0224 (8)	0.0092 (7)	0.0091 (6)	0.0086 (6)

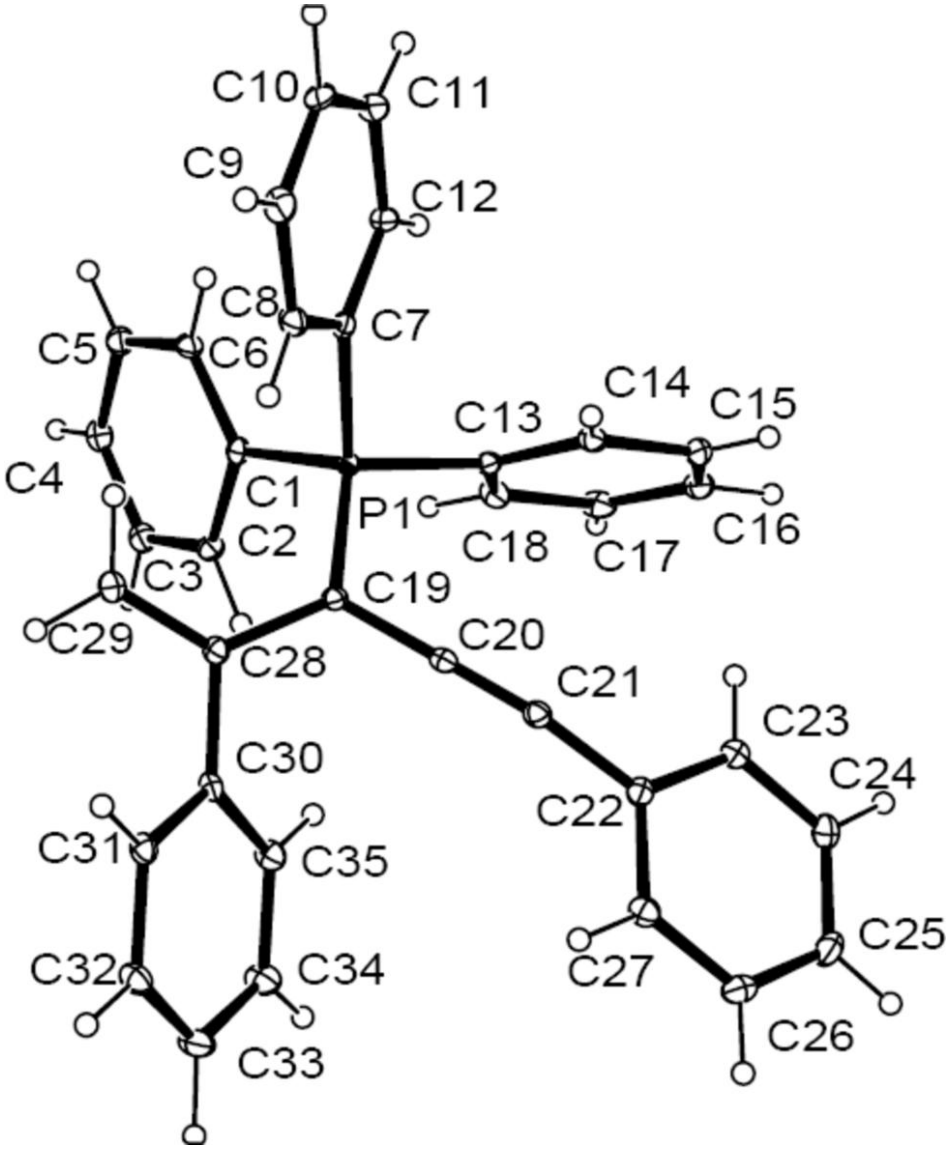
Geometric parameters (Å, °)

P1—C19	1.7294 (15)	C17—C18	1.390 (2)
P1—C13	1.8104 (15)	C17—H14	0.95 (3)
P1—C7	1.8132 (18)	C18—H15	0.95 (2)
P1—C1	1.8178 (19)	C19—C20	1.403 (2)
C1—C6	1.394 (2)	C19—C28	1.4693 (19)
C1—C2	1.401 (2)	C20—C21	1.206 (2)
C2—C3	1.389 (2)	C21—C22	1.427 (2)
C2—H1	0.99 (2)	C22—C23	1.403 (2)
C3—C4	1.388 (2)	C22—C27	1.405 (2)
C3—H2	0.92 (2)	C23—C24	1.382 (2)
C4—C5	1.392 (3)	C23—H16	0.96 (2)
C4—H3	0.95 (2)	C24—C25	1.385 (3)
C5—C6	1.394 (3)	C24—H17	0.98 (2)
C5—H4	0.96 (2)	C25—C26	1.384 (2)
C6—H5	0.94 (2)	C25—H18	0.95 (2)
C7—C8	1.393 (2)	C26—C27	1.383 (2)
C7—C12	1.402 (2)	C26—H19	0.96 (2)
C8—C9	1.387 (3)	C27—H20	0.96 (2)
C8—H6	0.94 (2)	C28—C29	1.343 (2)
C9—C10	1.389 (3)	C28—C30	1.500 (2)
C9—H7	0.98 (2)	C29—H27	1.00 (2)
C10—C11	1.388 (3)	C29—H26	0.96 (2)
C10—H8	0.97 (3)	C30—C35	1.394 (2)
C11—C12	1.381 (3)	C30—C31	1.398 (2)
C11—H9	0.92 (2)	C31—C32	1.392 (2)
C12—H10	0.97 (2)	C31—H21	0.96 (2)
C13—C18	1.393 (2)	C32—C33	1.382 (3)
C13—C14	1.407 (2)	C32—H22	0.99 (2)
C14—C15	1.388 (2)	C33—C34	1.391 (2)
C14—H11	0.95 (2)	C33—H23	1.02 (2)
C15—C16	1.390 (3)	C34—C35	1.390 (2)
C15—H12	0.93 (2)	C34—H24	0.92 (2)
C16—C17	1.388 (3)	C35—H25	0.96 (2)
C16—H13	1.00 (2)		
C19—P1—C13	108.20 (7)	C16—C17—C18	120.08 (17)
C19—P1—C7	117.53 (8)	C16—C17—H14	123.3 (15)

C13—P1—C7	105.18 (7)	C18—C17—H14	116.6 (15)
C19—P1—C1	111.39 (7)	C17—C18—C13	119.88 (16)
C13—P1—C1	107.73 (7)	C17—C18—H15	118.6 (12)
C7—P1—C1	106.29 (8)	C13—C18—H15	121.5 (12)
C6—C1—C2	119.66 (15)	C20—C19—C28	121.62 (13)
C6—C1—P1	121.88 (13)	C20—C19—P1	115.92 (10)
C2—C1—P1	118.32 (12)	C28—C19—P1	122.42 (11)
C3—C2—C1	120.33 (15)	C21—C20—C19	179.42 (18)
C3—C2—H1	119.9 (12)	C20—C21—C22	164.32 (18)
C1—C2—H1	119.8 (12)	C23—C22—C27	118.19 (15)
C4—C3—C2	119.99 (17)	C23—C22—C21	120.51 (14)
C4—C3—H2	122.2 (12)	C27—C22—C21	121.19 (14)
C2—C3—H2	117.8 (12)	C24—C23—C22	120.55 (15)
C3—C4—C5	119.77 (16)	C24—C23—H16	119.4 (12)
C3—C4—H3	120.6 (13)	C22—C23—H16	120.1 (12)
C5—C4—H3	119.6 (13)	C23—C24—C25	120.65 (15)
C4—C5—C6	120.66 (16)	C23—C24—H17	117.8 (13)
C4—C5—H4	120.6 (13)	C25—C24—H17	121.4 (13)
C6—C5—H4	118.8 (13)	C26—C25—C24	119.34 (16)
C1—C6—C5	119.49 (16)	C26—C25—H18	118.5 (12)
C1—C6—H5	120.1 (11)	C24—C25—H18	122.1 (12)
C5—C6—H5	120.4 (11)	C27—C26—C25	120.76 (15)
C8—C7—C12	119.35 (16)	C27—C26—H19	120.4 (13)
C8—C7—P1	120.06 (12)	C25—C26—H19	118.8 (13)
C12—C7—P1	120.55 (13)	C26—C27—C22	120.41 (15)
C9—C8—C7	119.84 (15)	C26—C27—H20	121.1 (13)
C9—C8—H6	120.2 (13)	C22—C27—H20	118.5 (13)
C7—C8—H6	119.9 (13)	C29—C28—C19	125.09 (15)
C8—C9—C10	120.66 (16)	C29—C28—C30	118.87 (14)
C8—C9—H7	119.9 (15)	C19—C28—C30	115.91 (13)
C10—C9—H7	119.4 (15)	C28—C29—H27	120.4 (11)
C11—C10—C9	119.51 (18)	C28—C29—H26	118.9 (12)
C11—C10—H8	119.9 (13)	H27—C29—H26	120.5 (16)
C9—C10—H8	120.5 (12)	C35—C30—C31	118.12 (15)
C12—C11—C10	120.36 (16)	C35—C30—C28	120.97 (13)
C12—C11—H9	116.2 (15)	C31—C30—C28	120.91 (15)
C10—C11—H9	123.4 (15)	C32—C31—C30	120.45 (16)
C11—C12—C7	120.22 (16)	C32—C31—H21	116.8 (12)
C11—C12—H10	120.6 (14)	C30—C31—H21	122.6 (12)
C7—C12—H10	119.1 (14)	C33—C32—C31	120.64 (15)
C18—C13—C14	120.01 (15)	C33—C32—H22	120.8 (13)
C18—C13—P1	120.91 (12)	C31—C32—H22	118.5 (13)
C14—C13—P1	118.87 (12)	C32—C33—C34	119.68 (16)
C15—C14—C13	119.37 (16)	C32—C33—H23	122.9 (12)
C15—C14—H11	119.8 (12)	C34—C33—H23	117.5 (12)
C13—C14—H11	120.7 (12)	C35—C34—C33	119.51 (18)
C14—C15—C16	120.36 (16)	C35—C34—H24	118.0 (13)
C14—C15—H12	117.8 (13)	C33—C34—H24	122.4 (14)
C16—C15—H12	121.8 (13)	C34—C35—C30	121.56 (15)

C17—C16—C15	120.25 (15)	C34—C35—H25	119.7 (14)
C17—C16—H13	120.0 (12)	C30—C35—H25	118.7 (14)
C15—C16—H13	119.8 (13)		

Fig. 1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