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(Biphenyl-2,2′-diyl)[1,3-bis(diphenylphosphanyl)-propane-κ^2P,P']platinum(II)

D. Paul Rillema,[a]* Curtis Moore[b] and Ali Jehan[a]

[a]Department of Chemistry, Wichita State University, Wichita, KS 67260, USA, and [b]Crystallographic Laboratory, University of California, San Diego, LaJolla, CA 92093, USA. *Correspondence e-mail: paul.rillema@wichita.edu

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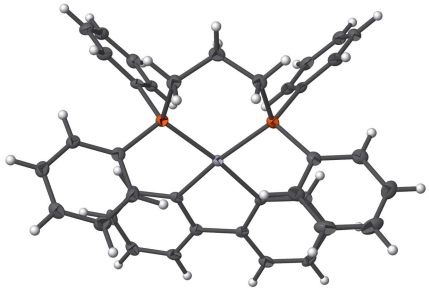
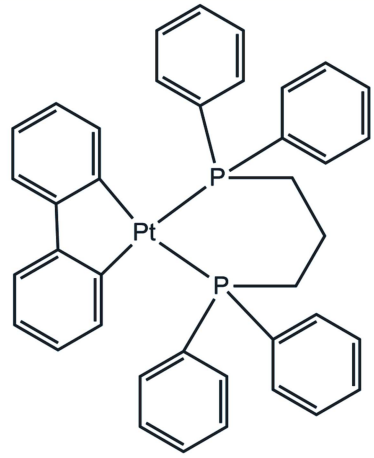
Structural data: full structural data are available from iucrdata.iucr.org

The C_2P_2 donor set in the title compound, $[Pt(C_{12}H_8)(C_{27}H_{26}P_2)]$, defines a distorted planar coordination environment about the Pt^{II} atom with small deviations from planarity. The bidentate nature of the biphenyl dianionic ligand results in a C—Pt—C bond angle of 79.94 (16)° and a P—Pt—P bond angle of 93.40 (4)°. The average Pt—C bond length is 2.083 (3) Å [range 2.081 (4)–2.085 (4) Å]; the average Pt—P bond length is 2.308 (8) Å [range 2.3030 (11)–2.3136 (11) Å].

3D view



Chemical scheme



Structure description

We are interested in preparing Pt^{II} complexes containing the biphenyl dianion (bph^{2-}) and bidentate ligands due to their excited state properties (Rillema *et al.*, 2015) and determining their structures as a guide to design better photochromophores. The molecular structures of Pt(bph)(diimine) complexes revealed the bph^{2-} and the diimine ligands were not in the same plane as expected for square-planar Pt^{II} complexes, but were in an *X* or bowed configuration (Rillema *et al.*, 2013*a*,*b*). Extensive π–π stacking was found for $Pt(bph)(CO)_2$ (Chen *et al.*, 1995) but little π–π interaction is expected for the title compound (Fig. 1) due to its three-dimensional structure.

In the title compound, the C_2P_2 donor set approximates an isosceles trapezoid with a short distance defined by the C1—C2 distance of 2.676 (6) Å and the long distance defined by the P1—P2 distance of 3.360 (2) Å. The average length of the sides (C—P distance) is 3.198 (13) Å [range 3.188 (4)–3.207 (4) Å]. For the title compound, the average Pt—C bond length, the Pt—P bond length, the C—Pt—C bond angle and the P—Pt—P bond angle can be compared with a similar platinum(II) complex having a methyl group linking the two P atoms, *viz.* (2,2′-bi-*o*-phenylene-diyl)(bis(diphenylphosphanyl)methane)platinum(II) (DePriest *et al.*, 2000) and a compound with two phenyl groups in place of the biphenyl dianionic ligand, *viz.* bis(4-bromo-2-dimethylaminophenyl)[1,3-

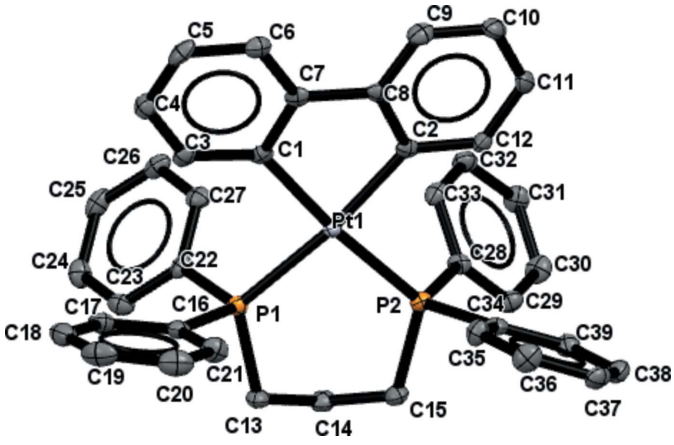


Figure 1
The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

bis(diphenylphosphanyl)propane-*P*:*P*]platinum(II), (Amijs *et al.*, 2005). The average Pt—C bond lengths are similar for the series: 2.084 (3), 2.05 (1) and 2.065 (4) Å, respectively. The average Pt—P bond lengths in the series are also similar: 2.314 (4), 2.305 (8) and 2.2998 (11) Å, respectively. However, the C—Pt—C and P—Pt—P bond angles are markedly affected by removing the bond between the two phenyl rings of biphenyl and substituting methyl for the propyl linkage of the bidentate diphosphine ligand. Replacement of the propyl group with the methyl group results in an 20% decrease in the average P—Pt—P angle of 92 (3)° [range 93.40 (4) to 89.69 (6)°] to 73.10 (9)°. The C—Pt—C angle increases 10% from an average of 80.4 (7)° [range 79.94 (16) to 80.9 (4)°] to 89.69 (6)° after replacement of the bidentate biphenyl ligand with two phenyl groups. In the crystal packing, apart from van der Waals forces (Fig. 2), other noticeable intermolecular interactions are not present.

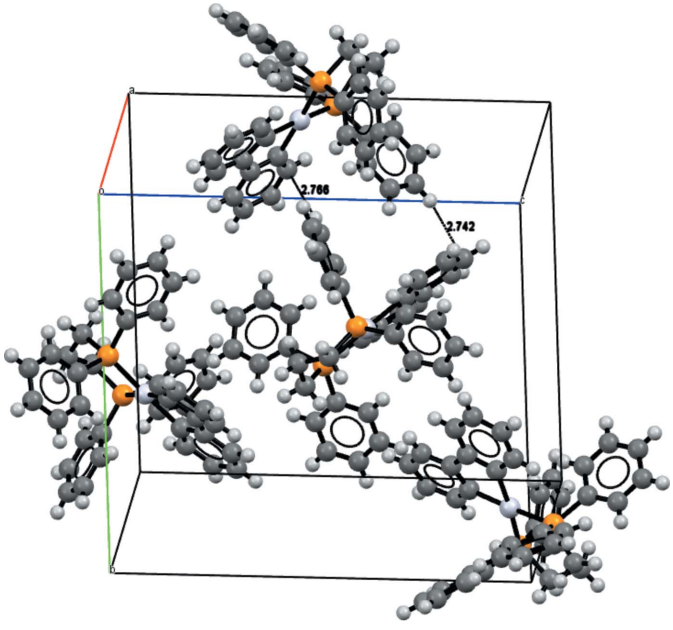


Figure 2
Packing diagram showing C—H···C interactions within van der Waals radii for H and C.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Pt(C_{12}H_8)(C_{27}H_{26}P_2)]$
M_r	759.69
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	10.4487 (8), 16.8817 (13), 17.3829 (14)
V (Å^3)	3066.2 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.71
Crystal size (mm)	0.16 × 0.14 × 0.13
Data collection	
Diffractometer	Bruker X8 APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.061, 0.092
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34318, 5614, 5472
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.016, 0.035, 1.04
No. of reflections	5614
No. of parameters	379
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.32
Absolute structure	Flack x determined using 2339 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.015 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Synthesis and crystallization

The compound was synthesized according to previously published procedures (DePriest *et al.*, 2000) with substitution of 1,3-bis(diphenylphosphanyl)propane for 1,1-bis(diphenylphosphanyl)methane. X-ray quality crystals were obtained by recrystallization from methylene chloride.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

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Crystal data

$[Pt(C_{12}H_8)(C_{27}H_{26}P_2)]$
M_r = 759.69
Orthorhombic, $P2_12_12_1$
a = 10.4487 (8) Å
b = 16.8817 (13) Å
c = 17.3829 (14) Å
V = 3066.2 (4) Å^3
Z = 4
F(000) = 1504
D_x = 1.646 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9939 reflections
θ = 2.3–25.4°
μ = 4.71 mm^{-1}
T = 100 K
Block, yellow
0.16 × 0.14 × 0.13 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: sealed tube, fine-focus
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.061, T_{max} = 0.092
34318 measured reflections
5614 independent reflections
5472 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.4°, θ_{min} = 1.7°
h = −12→12
k = −20→20
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.035
S = 1.04
5614 reflections
379 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0167P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack x determined using 2339 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.015 (3)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.43259 (2)	0.45678 (2)	0.59054 (2)	0.01281 (5)
P1	0.63061 (10)	0.50521 (7)	0.55401 (7)	0.0150 (2)
P2	0.32547 (10)	0.52666 (6)	0.49673 (6)	0.0147 (2)
C1	0.5101 (4)	0.3901 (2)	0.6801 (2)	0.0135 (9)
C2	0.2673 (4)	0.4035 (2)	0.6328 (2)	0.0142 (9)
C3	0.6388 (4)	0.3790 (3)	0.7007 (3)	0.0183 (10)
H3	0.7035	0.4000	0.6682	0.022*
C4	0.6753 (4)	0.3386 (2)	0.7667 (3)	0.0195 (10)
H4	0.7635	0.3331	0.7788	0.023*
C5	0.5839 (4)	0.3064 (2)	0.8146 (2)	0.0211 (10)
H5	0.6085	0.2801	0.8606	0.025*
C6	0.4554 (4)	0.3126 (2)	0.7949 (2)	0.0192 (10)
H6	0.3920	0.2894	0.8269	0.023*
C7	0.4185 (4)	0.3531 (2)	0.7278 (2)	0.0154 (9)
C8	0.2855 (4)	0.3584 (2)	0.7003 (2)	0.0152 (9)
C9	0.1838 (4)	0.3177 (3)	0.7346 (3)	0.0204 (10)
H9	0.1977	0.2892	0.7810	0.024*
C10	0.0630 (4)	0.3183 (2)	0.7018 (2)	0.0215 (10)
H10	−0.0054	0.2899	0.7250	0.026*
C11	0.0432 (4)	0.3609 (2)	0.6348 (3)	0.0193 (10)
H11	−0.0388	0.3609	0.6111	0.023*
C12	0.1438 (4)	0.4041 (2)	0.6018 (3)	0.0168 (10)
H12	0.1275	0.4347	0.5570	0.020*
C13	0.6409 (4)	0.5878 (3)	0.4846 (3)	0.0196 (11)
H13A	0.6266	0.6382	0.5124	0.024*
H13B	0.7286	0.5894	0.4630	0.024*
C14	0.5459 (4)	0.5826 (2)	0.4185 (3)	0.0212 (10)
H14A	0.5455	0.5280	0.3979	0.025*
H14B	0.5733	0.6187	0.3767	0.025*
C15	0.4107 (4)	0.6049 (2)	0.4443 (3)	0.0197 (10)
H15A	0.3600	0.6194	0.3983	0.024*
H15B	0.4160	0.6524	0.4776	0.024*
C16	0.7210 (4)	0.5468 (3)	0.6349 (2)	0.0174 (9)
C17	0.8461 (4)	0.5268 (2)	0.6541 (3)	0.0205 (10)
H17	0.8945	0.4937	0.6209	0.025*
C18	0.9004 (4)	0.5550 (3)	0.7215 (3)	0.0267 (11)
H18	0.9853	0.5403	0.7348	0.032*
C19	0.8315 (5)	0.6046 (3)	0.7697 (3)	0.0303 (12)
H19	0.8685	0.6234	0.8161	0.036*
C20	0.7076 (5)	0.6268 (3)	0.7495 (3)	0.0285 (11)
H20	0.6608	0.6623	0.7813	0.034*
C21	0.6528 (4)	0.5972 (3)	0.6831 (3)	0.0228 (11)
H21	0.5675	0.6115	0.6702	0.027*
C22	0.7279 (4)	0.4291 (2)	0.5079 (2)	0.0158 (9)
C23	0.8501 (4)	0.4447 (3)	0.4783 (2)	0.0191 (10)

H23	0.8851	0.4965	0.4826	0.023*
C24	0.9200 (4)	0.3860 (3)	0.4430 (2)	0.0217 (10)
H24	1.0030	0.3972	0.4235	0.026*
C25	0.8689 (4)	0.3100 (3)	0.4359 (3)	0.0238 (11)
H25	0.9180	0.2692	0.4125	0.029*
C26	0.7477 (4)	0.2938 (3)	0.4626 (2)	0.0209 (10)
H26	0.7118	0.2426	0.4561	0.025*
C27	0.6780 (4)	0.3534 (3)	0.4995 (2)	0.0188 (10)
H27	0.5952	0.3419	0.5191	0.023*
C28	0.2667 (3)	0.4647 (2)	0.4184 (2)	0.0153 (8)
C29	0.2077 (4)	0.4952 (3)	0.3526 (2)	0.0200 (10)
H29	0.1991	0.5509	0.3469	0.024*
C30	0.1613 (4)	0.4452 (3)	0.2954 (3)	0.0233 (10)
H30	0.1201	0.4666	0.2514	0.028*
C31	0.1753 (4)	0.3638 (3)	0.3030 (3)	0.0204 (10)
H31	0.1421	0.3294	0.2646	0.024*
C32	0.2375 (4)	0.3327 (3)	0.3663 (3)	0.0200 (10)
H32	0.2492	0.2771	0.3705	0.024*
C33	0.2832 (4)	0.3826 (2)	0.4239 (2)	0.0175 (10)
H33	0.3257	0.3608	0.4673	0.021*
C34	0.1939 (4)	0.5878 (2)	0.5334 (3)	0.0166 (9)
C35	0.2107 (4)	0.6179 (3)	0.6078 (2)	0.0198 (10)
H35	0.2825	0.6016	0.6374	0.024*
C36	0.1244 (4)	0.6710 (3)	0.6389 (3)	0.0248 (11)
H36	0.1372	0.6906	0.6895	0.030*
C37	0.0195 (4)	0.6956 (2)	0.5968 (3)	0.0212 (10)
H37	−0.0392	0.7325	0.6182	0.025*
C38	0.0006 (4)	0.6661 (3)	0.5233 (3)	0.0218 (11)
H38	−0.0715	0.6828	0.4943	0.026*
C39	0.0867 (4)	0.6121 (2)	0.4918 (3)	0.0193 (10)
H39	0.0724	0.5918	0.4416	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01280 (7)	0.01190 (7)	0.01373 (8)	0.00037 (7)	0.00056 (7)	0.00096 (7)
P1	0.0148 (5)	0.0130 (6)	0.0171 (6)	0.0004 (5)	0.0019 (5)	0.0000 (5)
P2	0.0162 (5)	0.0129 (6)	0.0149 (6)	0.0007 (4)	−0.0001 (4)	0.0010 (4)
C1	0.019 (2)	0.010 (2)	0.012 (2)	0.0009 (18)	−0.0017 (17)	−0.0028 (18)
C2	0.018 (2)	0.010 (2)	0.015 (2)	0.0009 (17)	0.0043 (18)	−0.0026 (18)
C3	0.021 (2)	0.013 (2)	0.021 (3)	0.0029 (19)	0.000 (2)	−0.002 (2)
C4	0.020 (2)	0.020 (2)	0.018 (3)	0.0003 (19)	−0.006 (2)	−0.002 (2)
C5	0.031 (3)	0.019 (2)	0.013 (2)	0.010 (2)	−0.006 (2)	−0.0004 (18)
C6	0.024 (3)	0.015 (2)	0.018 (2)	0.0020 (19)	0.0061 (19)	0.0006 (18)
C7	0.021 (2)	0.0110 (19)	0.014 (2)	0.0001 (19)	0.001 (2)	−0.0041 (17)
C8	0.019 (2)	0.010 (2)	0.017 (2)	0.0003 (18)	0.0025 (19)	−0.0021 (18)
C9	0.025 (2)	0.020 (2)	0.017 (2)	0.0038 (19)	0.007 (2)	0.004 (2)
C10	0.018 (2)	0.018 (2)	0.028 (3)	−0.001 (2)	0.007 (2)	0.0040 (19)

C11	0.012 (2)	0.016 (2)	0.030 (3)	0.0025 (18)	0.0025 (18)	0.000 (2)
C12	0.016 (2)	0.015 (2)	0.019 (3)	0.0033 (17)	−0.0005 (19)	0.003 (2)
C13	0.019 (2)	0.017 (2)	0.023 (3)	−0.0009 (19)	0.003 (2)	0.007 (2)
C14	0.024 (2)	0.019 (2)	0.021 (3)	0.0007 (18)	0.005 (2)	0.006 (2)
C15	0.022 (2)	0.017 (2)	0.020 (2)	−0.0008 (19)	−0.0014 (19)	0.0056 (18)
C16	0.019 (2)	0.013 (2)	0.020 (2)	−0.003 (2)	0.0027 (17)	0.002 (2)
C17	0.025 (2)	0.014 (3)	0.023 (3)	−0.0014 (19)	0.0022 (19)	−0.0012 (19)
C18	0.027 (2)	0.025 (3)	0.028 (3)	−0.008 (2)	−0.007 (2)	0.007 (2)
C19	0.049 (3)	0.022 (3)	0.019 (3)	−0.010 (2)	−0.008 (2)	−0.002 (2)
C20	0.042 (3)	0.023 (3)	0.021 (3)	−0.002 (2)	0.009 (2)	−0.003 (2)
C21	0.025 (2)	0.021 (3)	0.023 (3)	0.000 (2)	0.004 (2)	−0.004 (2)
C22	0.018 (2)	0.018 (2)	0.011 (2)	0.0044 (18)	−0.0027 (18)	0.0003 (18)
C23	0.023 (2)	0.018 (2)	0.017 (2)	−0.0049 (19)	−0.0002 (18)	−0.0005 (19)
C24	0.018 (2)	0.029 (3)	0.017 (2)	0.002 (2)	0.002 (2)	−0.0019 (19)
C25	0.027 (2)	0.026 (3)	0.019 (3)	0.012 (2)	−0.0025 (19)	−0.002 (2)
C26	0.029 (2)	0.016 (2)	0.017 (3)	0.004 (2)	−0.006 (2)	−0.0017 (19)
C27	0.022 (2)	0.020 (2)	0.015 (2)	−0.0008 (19)	−0.0013 (19)	0.0033 (19)
C28	0.0176 (18)	0.016 (2)	0.012 (2)	0.0003 (17)	0.0033 (16)	0.000 (2)
C29	0.027 (2)	0.016 (2)	0.018 (3)	0.002 (2)	0.001 (2)	−0.0005 (19)
C30	0.026 (2)	0.028 (3)	0.016 (2)	0.003 (2)	−0.0008 (18)	0.000 (2)
C31	0.023 (2)	0.021 (2)	0.017 (2)	0.002 (2)	0.0002 (19)	−0.006 (2)
C32	0.022 (2)	0.014 (2)	0.025 (3)	0.0009 (19)	0.002 (2)	−0.001 (2)
C33	0.018 (2)	0.021 (2)	0.015 (3)	0.0046 (18)	0.0026 (17)	0.0031 (19)
C34	0.018 (2)	0.013 (2)	0.019 (2)	−0.0028 (18)	0.0012 (19)	0.0040 (19)
C35	0.020 (2)	0.022 (2)	0.017 (3)	0.0032 (19)	−0.0039 (18)	−0.0029 (19)
C36	0.031 (3)	0.025 (3)	0.019 (3)	0.003 (2)	0.000 (2)	−0.005 (2)
C37	0.022 (2)	0.015 (2)	0.027 (3)	0.0048 (17)	0.005 (2)	0.000 (2)
C38	0.021 (2)	0.022 (3)	0.023 (3)	0.003 (2)	−0.002 (2)	0.006 (2)
C39	0.020 (2)	0.022 (2)	0.016 (2)	0.000 (2)	−0.0005 (19)	0.0032 (18)

Geometric parameters (Å, º)

Pt1—P1	2.3136 (11)	C17—C18	1.386 (6)
Pt1—P2	2.3030 (11)	C18—H18	0.9500
Pt1—C1	2.085 (4)	C18—C19	1.386 (6)
Pt1—C2	2.081 (4)	C19—H19	0.9500
P1—C13	1.848 (4)	C19—C20	1.392 (7)
P1—C16	1.834 (4)	C20—H20	0.9500
P1—C22	1.824 (4)	C20—C21	1.382 (6)
P2—C15	1.836 (4)	C21—H21	0.9500
P2—C28	1.824 (4)	C22—C23	1.402 (6)
P2—C34	1.834 (4)	C22—C27	1.388 (6)
C1—C3	1.404 (5)	C23—H23	0.9500
C1—C7	1.412 (6)	C23—C24	1.375 (6)
C2—C8	1.411 (6)	C24—H24	0.9500
C2—C12	1.399 (5)	C24—C25	1.395 (6)
C3—H3	0.9500	C25—H25	0.9500
C3—C4	1.387 (6)	C25—C26	1.375 (6)

C4—H4	0.9500	C26—H26	0.9500
C4—C5	1.380 (6)	C26—C27	1.398 (6)
C5—H5	0.9500	C27—H27	0.9500
C5—C6	1.390 (6)	C28—C29	1.397 (6)
C6—H6	0.9500	C28—C33	1.400 (6)
C6—C7	1.405 (6)	C29—H29	0.9500
C7—C8	1.471 (6)	C29—C30	1.392 (6)
C8—C9	1.400 (6)	C30—H30	0.9500
C9—H9	0.9500	C30—C31	1.388 (6)
C9—C10	1.385 (6)	C31—H31	0.9500
C10—H10	0.9500	C31—C32	1.381 (6)
C10—C11	1.385 (6)	C32—H32	0.9500
C11—H11	0.9500	C32—C33	1.394 (6)
C11—C12	1.401 (6)	C33—H33	0.9500
C12—H12	0.9500	C34—C35	1.400 (6)
C13—H13A	0.9900	C34—C39	1.395 (6)
C13—H13B	0.9900	C35—H35	0.9500
C13—C14	1.520 (6)	C35—C36	1.381 (6)
C14—H14A	0.9900	C36—H36	0.9500
C14—H14B	0.9900	C36—C37	1.381 (6)
C14—C15	1.529 (6)	C37—H37	0.9500
C15—H15A	0.9900	C37—C38	1.386 (7)
C15—H15B	0.9900	C38—H38	0.9500
C16—C17	1.391 (6)	C38—C39	1.393 (6)
C16—C21	1.391 (6)	C39—H39	0.9500
C17—H17	0.9500		

P2—Pt1—P1	93.40 (4)	C17—C16—P1	125.1 (3)
C1—Pt1—P1	92.76 (12)	C17—C16—C21	119.1 (4)
C1—Pt1—P2	173.79 (12)	C21—C16—P1	115.6 (3)
C2—Pt1—P1	172.62 (12)	C16—C17—H17	119.9
C2—Pt1—P2	93.91 (12)	C18—C17—C16	120.3 (4)
C2—Pt1—C1	79.94 (16)	C18—C17—H17	119.9
C13—P1—Pt1	119.88 (15)	C17—C18—H18	119.8
C16—P1—Pt1	112.65 (13)	C17—C18—C19	120.4 (4)
C16—P1—C13	100.5 (2)	C19—C18—H18	119.8
C22—P1—Pt1	111.73 (14)	C18—C19—H19	120.2
C22—P1—C13	102.2 (2)	C18—C19—C20	119.6 (4)
C22—P1—C16	108.64 (19)	C20—C19—H19	120.2
C15—P2—Pt1	118.98 (14)	C19—C20—H20	120.1
C28—P2—Pt1	113.49 (13)	C21—C20—C19	119.9 (4)
C28—P2—C15	101.83 (19)	C21—C20—H20	120.1
C28—P2—C34	109.30 (19)	C16—C21—H21	119.6
C34—P2—Pt1	113.99 (15)	C20—C21—C16	120.8 (4)
C34—P2—C15	97.55 (19)	C20—C21—H21	119.6
C3—C1—Pt1	129.4 (3)	C23—C22—P1	122.5 (3)
C3—C1—C7	116.1 (4)	C27—C22—P1	119.0 (3)
C7—C1—Pt1	114.4 (3)	C27—C22—C23	118.5 (4)

C8—C2—Pt1	114.5 (3)	C22—C23—H23	119.6
C12—C2—Pt1	128.8 (3)	C24—C23—C22	120.8 (4)
C12—C2—C8	116.6 (4)	C24—C23—H23	119.6
C1—C3—H3	118.7	C23—C24—H24	120.0
C4—C3—C1	122.7 (4)	C23—C24—C25	119.9 (4)
C4—C3—H3	118.7	C25—C24—H24	120.0
C3—C4—H4	119.9	C24—C25—H25	119.8
C5—C4—C3	120.2 (4)	C26—C25—C24	120.4 (4)
C5—C4—H4	119.9	C26—C25—H25	119.8
C4—C5—H5	120.3	C25—C26—H26	120.3
C4—C5—C6	119.3 (4)	C25—C26—C27	119.5 (4)
C6—C5—H5	120.3	C27—C26—H26	120.3
C5—C6—H6	119.8	C22—C27—C26	121.0 (4)
C5—C6—C7	120.4 (4)	C22—C27—H27	119.5
C7—C6—H6	119.8	C26—C27—H27	119.5
C1—C7—C8	115.0 (4)	C29—C28—P2	123.2 (3)
C6—C7—C1	121.1 (4)	C29—C28—C33	118.4 (4)
C6—C7—C8	123.9 (4)	C33—C28—P2	118.4 (3)
C2—C8—C7	115.5 (4)	C28—C29—H29	119.5
C9—C8—C2	121.1 (4)	C30—C29—C28	120.9 (4)
C9—C8—C7	123.3 (4)	C30—C29—H29	119.5
C8—C9—H9	119.6	C29—C30—H30	120.1
C10—C9—C8	120.9 (4)	C31—C30—C29	119.8 (4)
C10—C9—H9	119.6	C31—C30—H30	120.1
C9—C10—H10	120.4	C30—C31—H31	120.0
C9—C10—C11	119.1 (4)	C32—C31—C30	120.1 (4)
C11—C10—H10	120.4	C32—C31—H31	120.0
C10—C11—H11	119.9	C31—C32—H32	119.9
C10—C11—C12	120.1 (4)	C31—C32—C33	120.3 (4)
C12—C11—H11	119.9	C33—C32—H32	119.9
C2—C12—C11	122.1 (4)	C28—C33—H33	119.8
C2—C12—H12	118.9	C32—C33—C28	120.5 (4)
C11—C12—H12	118.9	C32—C33—H33	119.8
P1—C13—H13A	108.7	C35—C34—P2	115.6 (3)
P1—C13—H13B	108.7	C39—C34—P2	125.9 (3)
H13A—C13—H13B	107.6	C39—C34—C35	118.2 (4)
C14—C13—P1	114.3 (3)	C34—C35—H35	119.5
C14—C13—H13A	108.7	C36—C35—C34	121.0 (4)
C14—C13—H13B	108.7	C36—C35—H35	119.5
C13—C14—H14A	109.3	C35—C36—H36	119.8
C13—C14—H14B	109.3	C35—C36—C37	120.4 (4)
C13—C14—C15	111.6 (4)	C37—C36—H36	119.8
H14A—C14—H14B	108.0	C36—C37—H37	120.2
C15—C14—H14A	109.3	C36—C37—C38	119.5 (4)
C15—C14—H14B	109.3	C38—C37—H37	120.2
P2—C15—H15A	108.6	C37—C38—H38	119.8
P2—C15—H15B	108.6	C37—C38—C39	120.4 (4)
C14—C15—P2	114.6 (3)	C39—C38—H38	119.8

C14—C15—H15A	108.6	C34—C39—H39	119.8
C14—C15—H15B	108.6	C38—C39—C34	120.4 (4)
H15A—C15—H15B	107.6	C38—C39—H39	119.8