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trans-(μ-5,5′-Diethynyl-2,2′-bipyridine)bis[phenylbis(triethylphosphine)platinum(II)]

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Key indicators

Single-crystal synchrotron study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.068
Data-to-parameter ratio = 25.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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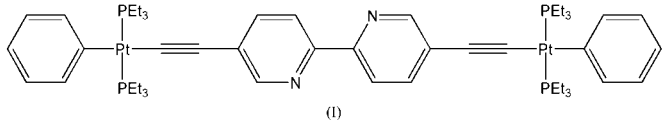
The title compound, $[Pt_2(C_6H_5)_2(C_{14}H_6N_2)(C_6H_{15}P)_4]$, is a dinuclear Pt^{II} di-yne complex that exhibits π-conjugation along the molecular backbone. It is used as a model complex for rigid-rod platinum poly-yne polymers of which it is a precursor. Such compounds are of interest because of the extended π-conjugation through the aromatic/heteroaromatic spacer group in the backbone. The asymmetric unit contains two half molecules of the title compound, each lying on a crystallographic centre of symmetry situated at the mid-point of the central C—C bond of the bipyridine unit.

Comment

In this paper, we report the structural characterization of the title compound, (I), which is a dinuclear platinum(II) di-yne species, *trans*-[(Ph)$(PEt_3)_2$Pt—C≡C—*R*—C≡C—Pt$(PEt_3)_2$-(Ph)] (*R* = 2,2′-bipyridine-5,5′-diyl). Such organoplatinum species form the building blocks for rigid-rod platinum poly-ynes of general formula *trans*-[Pt$(PX_3)_2$—C≡C—*R*—C≡C—] (*X* = tertiary phosphines and *R* = aromatic/heteroaromatic spacer group). Platinum(II) poly-ynes are of immense current interest due to π-electron conjugation along the rigid backbone of the organometallic polymer. These materials possess a wide variety of interesting properties useful for application in modern technology. For example, incorporating platinum into the polymer backbone introduces strong spin-orbit coupling and phosphorescence can be readily observed (Wittmann *et al.*, 1994; Beljonne *et al.*, 1996; Younus *et al.*, 1998; Chawdhury *et al.*, 1998, 1999). Platinum(II) poly-ynes provide model systems for the study of some of the basic photophysical properties that occur in conjugated organic and organometallic polymers (Khan, Al-Mandhary, Al-Suti, Hisahm *et al.*, 2002; Khan, Al-Mandhary, Al-Suti, Feeder *et al.*, 2002; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Mahon *et al.*, 2003; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Male *et al.*, 2003), are used in optoelectronic devices such as light emitting diodes (LEDs), lasers, photocells and field-effect transistors (FETs) (Wilson *et al.*, 2000; Wilson, Chawdhury *et al.*, 2001; Wilson, Dhoot *et al.*, 2001). Group 10 metal poly-ynes also show interesting alignment and liquid crystal properties, one-dimensional conductivity and non-linear optical (NLO) properties (Takahashi *et al.*, 1984; Wilson *et al.*, 2003).



(I)

Precursors to these species, such as the title compound, (I), are utilized as models in the study of the molecular and electronic

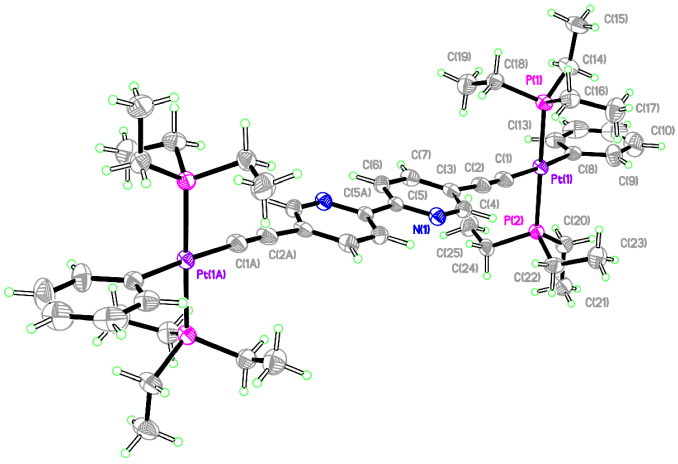


Figure 1
View of molecule 1 of (I) (50% probability displacement ellipsoids). The suffix *A* denotes symmetry position $1-x, 1-y, -z$.

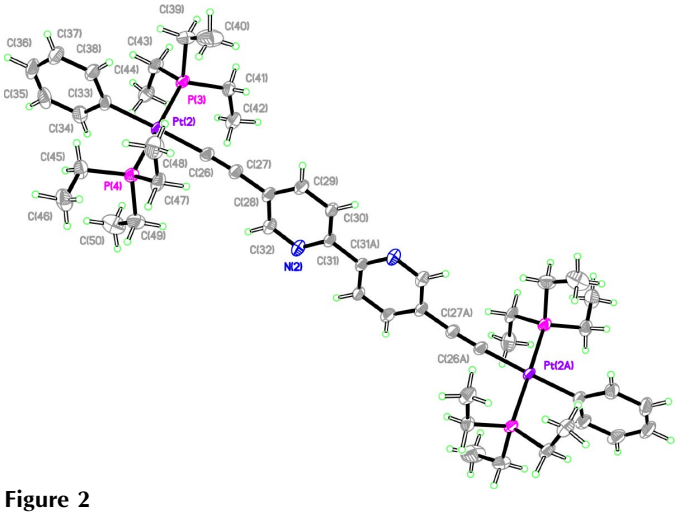


Figure 2
View of molecule 2 of (I) (50% probability displacement ellipsoids). The suffix *A* denotes symmetry position $1-x, 2-y, -z$.

properties and structure–property relationships in the metal poly-ynes.

The asymmetric unit of the triclinic unit cell of (I) contains two structurally similar half molecules of the title compound, each sitting on a centre of symmetry corresponding to the midpoint of the central C—C bond of the bipyridine ligand. The bipyridine ligands are orientated in the *trans* configuration with respect to the N atoms, as would be expected to minimize H···H contacts. The same configuration is observed in the trimethylsilyl-substituted derivative (Khan *et al.*, 2004); the bond parameters are also similar to those found in this derivative. The platinum centres exhibit the expected square-planar geometry and the bond parameters are similar to those reported in related platinum di-yne complexes (Khan, Al-Mandhary, Al-Suti, Hisahm *et al.*, 2002; Khan, Al-Mandhary, Al-Suti, Feeder *et al.*, 2002; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Mahon *et al.*, 2003; Khan, Al-Mandhary, Al-Suti, Raithby, Ahrens, Male *et al.*, 2003). The platinum square plane makes dihedral angles of 79.3 (1)° with the adjacent pyridine ring [73.4 (1)° in molecule 2], and 88.6 (1)° with the terminal phenyl ring [83.1 (1)° in molecule 2]. The two pyridine rings in each independent molecule are precisely coplanar by crystallographic symmetry. There are no significant short intermolecular contacts within the structure.

Experimental

The title compound was synthesized according to the procedure of Khan, Al-Mandhary, Al-Suti, Hisahm *et al.* (2002). To a stirred solution of *trans*-[$(PEt_3)_2$(Ph)PtCl] (0.543 g, 1.0 mmol) and 5,5′-bisethynyl-2,2′-bipyridine (0.102 g, 0.50 mmol) in CH_2Cl_2/$^iPr_2NH$ (50 ml, 1:1 *v*/*v*) under nitrogen was added a catalytic amount (approximately 5 mg) of CuI. The yellow solution was stirred at room temperature for 15 h, after which all volatile components were removed under reduced pressure. The residue was dissolved in CH_2Cl_2 and passed through a silica column, eluting with hexane–CH_2Cl_2 (1:1 *v*/*v*). Removal of the solvents *in vacuo* gave the title complex as a pale-yellow solid (0.43 g, 70%). Further purification was accomplished by triturating the complex in methanol.

Crystal data

$[Pt_2(C_6H_5)_2(C_{14}H_6N_2)(C_6H_{15}P)_4]$
M_r = 1219.19
Triclinic, $P\overline{1}$
a = 9.2651 (7) Å
b = 16.6840 (14) Å
c = 16.8258 (14) Å
α = 92.130 (2)°
β = 90.032 (2)°
γ = 94.958 (2)°
V = 2589.4 (4) Å^3
Z = 2
D_x = 1.564 Mg m^{-3}
Synchrotron radiation, λ = 0.6941 Å
Cell parameters from 25942 reflections
θ = 21.7–29.3°
μ = 5.55 mm^{-1}
T = 150 (2) K
Block, yellow
0.02 × 0.01 × 0.01 mm

Data collection

Bruker AXS SMART 1K CCD diffractometer
Narrow frame ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.895, T_{max} = 0.946
25942 measured reflections
13587 independent reflections
11103 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 29.3°
$h = -12 \rightarrow 12$
$k = -23 \rightarrow 23$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.068
S = 1.00
13587 reflections
535 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}

Aromatic, methylene and methyl H atoms were constrained as riding atoms, fixed to the parent atoms with distances of 0.95, 0.99 and 0.98 Å, respectively. The isotropic displacement parameters were fixed to 120% of those of the parent atoms for aromatic and methylene H atoms and 150% for methyl H atoms. The high residual electron density peaks were located close to the positions of the two unique Pt atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Synchrotron radiation, $\lambda = 0.6941$ Å
Cell parameters from 25942 reflections
$\theta = 21.7$–29.3°
$\mu = 5.55$ mm^{-1}
$T = 150$ K
Block, yellow
0.02 × 0.01 × 0.01 mm

Data collection

Bruker AXS SMART 1K CCD diffractometer
Radiation source: Daresbury SRS, Station 9.8
Silicon 111 monochromator
ω rotation with narrow frames scans
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)
$T_{min} = 0.895$, $T_{max} = 0.946$
25942 measured reflections
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$R_{int} = 0.024$
$\theta_{max} = 29.3°$, $\theta_{min} = 1.7°$
$h = -12 \rightarrow 12$
$k = -23 \rightarrow 23$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.068$
$S = 1.00$
13587 reflections
535 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
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 1.63$ e Å^{-3}
$\Delta\rho_{min} = -1.86$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	−0.056171 (12)	0.219787 (7)	0.268849 (7)	0.02461 (4)
C1	0.0782 (4)	0.2933 (2)	0.2043 (2)	0.0328 (8)
C2	0.1591 (4)	0.3341 (2)	0.1640 (2)	0.0335 (8)
C3	0.2565 (3)	0.37971 (19)	0.1128 (2)	0.0275 (7)
C4	0.3556 (4)	0.4404 (2)	0.1445 (2)	0.0299 (7)
H4A	0.3561	0.4498	0.2005	0.036*
C5	0.4487 (3)	0.47315 (18)	0.02252 (19)	0.0234 (6)
N1	0.4496 (3)	0.48608 (17)	0.10188 (17)	0.0278 (6)
C6	0.3565 (3)	0.4135 (2)	−0.0147 (2)	0.0288 (7)
H6A	0.3592	0.4049	−0.0708	0.035*
C7	0.2603 (4)	0.3665 (2)	0.0307 (2)	0.0308 (7)
H7A	0.1969	0.3252	0.0058	0.037*
C8	−0.1940 (3)	0.1404 (2)	0.3286 (2)	0.0282 (7)
C9	−0.1909 (5)	0.1335 (3)	0.4111 (2)	0.0459 (10)
H9A	−0.1245	0.1684	0.4419	0.055*
C10	−0.2828 (6)	0.0764 (3)	0.4496 (3)	0.0652 (15)
H10A	−0.2781	0.0731	0.5058	0.078*
C11	−0.3796 (5)	0.0253 (3)	0.4065 (4)	0.0647 (15)
H11A	−0.4417	−0.0137	0.4325	0.078*
C12	−0.3856 (4)	0.0311 (3)	0.3263 (3)	0.0539 (12)
H12A	−0.4523	−0.0044	0.2962	0.065*
C13	−0.2961 (4)	0.0878 (2)	0.2879 (2)	0.0360 (8)
H13A	−0.3043	0.0911	0.2319	0.043*
P1	0.11175 (9)	0.12746 (5)	0.25446 (5)	0.02818 (18)
C14	0.0654 (4)	0.0264 (2)	0.2895 (3)	0.0411 (9)
H14A	0.0255	0.0313	0.3439	0.049*
H14B	−0.0123	−0.0002	0.2549	0.049*
C15	0.1892 (5)	−0.0279 (3)	0.2915 (3)	0.0506 (11)
H15A	0.1496	−0.0840	0.2955	0.076*
H15B	0.2515	−0.0124	0.3376	0.076*
H15C	0.2462	−0.0223	0.2427	0.076*
C16	0.2827 (4)	0.1622 (3)	0.3029 (2)	0.0390 (8)
H16A	0.3552	0.1236	0.2894	0.047*
H16B	0.3181	0.2149	0.2818	0.047*
C17	0.2708 (5)	0.1708 (3)	0.3926 (3)	0.0560 (12)
H17A	0.3658	0.1895	0.4152	0.084*
H17B	0.2379	0.1186	0.4140	0.084*
H17C	0.2010	0.2100	0.4064	0.084*
C18	0.1658 (4)	0.1120 (2)	0.1522 (2)	0.0347 (8)

H18A	0.2194	0.1619	0.1343	0.042*
H18B	0.2327	0.0688	0.1494	0.042*
C19	0.0395 (4)	0.0892 (3)	0.0957 (3)	0.0486 (10)
H19A	0.0762	0.0813	0.0416	0.073*
H19B	−0.0258	0.1325	0.0966	0.073*
H19C	−0.0135	0.0393	0.1123	0.073*
P2	−0.20890 (9)	0.31932 (5)	0.28326 (5)	0.02622 (17)
C20	−0.3695 (4)	0.2985 (2)	0.3437 (2)	0.0345 (8)
H20A	−0.4257	0.2503	0.3201	0.041*
H20B	−0.3377	0.2847	0.3973	0.041*
C21	−0.4704 (5)	0.3651 (3)	0.3535 (3)	0.0542 (12)
H21A	−0.5479	0.3488	0.3907	0.081*
H21B	−0.5127	0.3751	0.3018	0.081*
H21C	−0.4158	0.4143	0.3743	0.081*
C22	−0.1162 (4)	0.4095 (2)	0.3288 (2)	0.0369 (8)
H22A	−0.0381	0.4302	0.2929	0.044*
H22B	−0.1856	0.4513	0.3350	0.044*
C23	−0.0512 (5)	0.3957 (3)	0.4094 (2)	0.0474 (10)
H23A	0.0012	0.4457	0.4299	0.071*
H23B	0.0159	0.3536	0.4039	0.071*
H23C	−0.1288	0.3789	0.4463	0.071*
C24	−0.2759 (4)	0.3526 (2)	0.1890 (2)	0.0358 (8)
H24A	−0.3323	0.3996	0.1994	0.043*
H24B	−0.1925	0.3700	0.1551	0.043*
Pt2	1.032188 (11)	0.724753 (7)	0.232281 (7)	0.02203 (4)
C25	−0.3718 (5)	0.2862 (3)	0.1442 (3)	0.0526 (11)
H25A	−0.4019	0.3060	0.0931	0.079*
H25B	−0.4578	0.2712	0.1760	0.079*
H25C	−0.3172	0.2391	0.1347	0.079*
C26	0.8978 (3)	0.7826 (2)	0.1645 (2)	0.0270 (7)
C27	0.8145 (3)	0.8179 (2)	0.1275 (2)	0.0282 (7)
C28	0.7191 (3)	0.8674 (2)	0.0884 (2)	0.0267 (7)
C29	0.6389 (3)	0.8430 (2)	0.0203 (2)	0.0303 (7)
H29A	0.6436	0.7901	−0.0020	0.036*
C30	0.5535 (3)	0.8948 (2)	−0.0145 (2)	0.0265 (6)
H30A	0.4999	0.8781	−0.0613	0.032*
C31	0.5454 (3)	0.97124 (19)	0.01828 (19)	0.0230 (6)
N2	0.6194 (3)	0.99657 (18)	0.08523 (18)	0.0312 (6)
C32	0.7027 (4)	0.9459 (2)	0.1183 (2)	0.0317 (7)
H32A	0.7546	0.9639	0.1653	0.038*
C33	1.1639 (3)	0.6651 (2)	0.30475 (19)	0.0295 (7)
C34	1.2448 (4)	0.7037 (3)	0.3676 (2)	0.0368 (8)
H34A	1.2425	0.7601	0.3763	0.044*
C35	1.3285 (4)	0.6618 (3)	0.4177 (2)	0.0469 (11)
H35A	1.3819	0.6899	0.4598	0.056*
C36	1.3346 (4)	0.5799 (3)	0.4068 (3)	0.0515 (12)
H36A	1.3916	0.5515	0.4412	0.062*
C37	1.2575 (4)	0.5400 (3)	0.3457 (3)	0.0456 (10)

H37A	1.2607	0.4835	0.3378	0.055*
C38	1.1744 (4)	0.5820 (2)	0.2952 (2)	0.0353 (8)
H38A	1.1230	0.5533	0.2527	0.042*
P3	1.21085 (8)	0.73062 (5)	0.13842 (5)	0.02451 (17)
C39	1.2266 (4)	0.6336 (2)	0.0875 (2)	0.0389 (9)
H39A	1.3060	0.6399	0.0483	0.047*
H39B	1.2549	0.5953	0.1271	0.047*
C40	1.0923 (5)	0.5972 (3)	0.0450 (3)	0.0650 (14)
H40A	1.1060	0.5416	0.0277	0.098*
H40B	1.0742	0.6287	−0.0014	0.098*
H40C	1.0094	0.5975	0.0812	0.098*
C41	1.1923 (4)	0.7976 (2)	0.0561 (2)	0.0333 (8)
H41A	1.2740	0.7918	0.0191	0.040*
H41B	1.1018	0.7796	0.0269	0.040*
C42	1.1889 (4)	0.8867 (2)	0.0799 (2)	0.0385 (8)
H42A	1.1749	0.9173	0.0323	0.058*
H42B	1.2807	0.9065	0.1056	0.058*
H42C	1.1089	0.8935	0.1169	0.058*
C43	1.3961 (3)	0.7501 (2)	0.1757 (2)	0.0338 (8)
H43A	1.4183	0.7042	0.2079	0.041*
H43B	1.4623	0.7512	0.1295	0.041*
C44	1.4305 (4)	0.8267 (2)	0.2254 (2)	0.0396 (9)
H44A	1.5274	0.8267	0.2487	0.059*
H44B	1.3588	0.8300	0.2680	0.059*
H44C	1.4274	0.8733	0.1917	0.059*
P4	0.84663 (8)	0.71218 (5)	0.32216 (5)	0.02637 (17)
C45	0.8725 (4)	0.6497 (3)	0.4062 (2)	0.0354 (8)
H45A	0.9029	0.5973	0.3859	0.042*
H45B	0.9526	0.6759	0.4395	0.042*
C46	0.7398 (4)	0.6336 (3)	0.4590 (2)	0.0475 (11)
H46A	0.7637	0.5994	0.5024	0.071*
H46B	0.6601	0.6063	0.4273	0.071*
H46C	0.7103	0.6848	0.4812	0.071*
C47	0.6787 (3)	0.6703 (2)	0.2762 (2)	0.0333 (8)
H47A	0.5993	0.6737	0.3152	0.040*
H47B	0.6568	0.7032	0.2307	0.040*
C48	0.6822 (5)	0.5840 (3)	0.2472 (3)	0.0496 (10)
H48A	0.5958	0.5679	0.2149	0.074*
H48B	0.6841	0.5493	0.2929	0.074*
H48C	0.7691	0.5785	0.2149	0.074*
C49	0.7969 (4)	0.8093 (3)	0.3636 (2)	0.0415 (9)
H49A	0.7735	0.8434	0.3193	0.050*
H49B	0.7084	0.7999	0.3961	0.050*
C50	0.9137 (5)	0.8542 (3)	0.4143 (3)	0.0583 (12)
H50A	0.8847	0.9078	0.4293	0.087*
H50B	1.0044	0.8596	0.3843	0.087*
H50C	0.9280	0.8245	0.4625	0.087*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01776 (6)	0.02830 (7)	0.02832 (7)	0.00233 (4)	0.00581 (4)	0.00743 (5)
C1	0.0240 (15)	0.0351 (19)	0.041 (2)	0.0112 (13)	0.0085 (14)	0.0094 (15)
C2	0.0276 (16)	0.0296 (18)	0.045 (2)	0.0072 (13)	0.0094 (14)	0.0095 (15)
C3	0.0205 (14)	0.0255 (16)	0.0383 (19)	0.0063 (12)	0.0093 (13)	0.0118 (13)
C4	0.0306 (16)	0.0310 (18)	0.0287 (17)	0.0048 (13)	0.0070 (13)	0.0044 (13)
C5	0.0207 (14)	0.0231 (15)	0.0274 (16)	0.0050 (11)	0.0055 (11)	0.0062 (12)
N1	0.0241 (13)	0.0306 (15)	0.0291 (15)	0.0020 (11)	0.0042 (11)	0.0066 (11)
C6	0.0293 (16)	0.0288 (17)	0.0284 (17)	0.0016 (13)	0.0040 (13)	0.0034 (13)
C7	0.0250 (15)	0.0257 (17)	0.041 (2)	−0.0017 (13)	0.0037 (14)	0.0066 (14)
C8	0.0223 (14)	0.0296 (17)	0.0336 (18)	0.0059 (12)	0.0067 (13)	0.0033 (13)
C9	0.042 (2)	0.059 (3)	0.037 (2)	−0.0003 (19)	0.0080 (17)	0.0130 (19)
C10	0.068 (3)	0.076 (4)	0.053 (3)	0.005 (3)	0.029 (2)	0.028 (3)
C11	0.052 (3)	0.051 (3)	0.091 (4)	−0.005 (2)	0.038 (3)	0.018 (3)
C12	0.033 (2)	0.036 (2)	0.091 (4)	−0.0046 (17)	0.017 (2)	−0.001 (2)
C13	0.0265 (16)	0.0332 (19)	0.048 (2)	0.0030 (14)	0.0058 (15)	0.0004 (16)
P1	0.0195 (4)	0.0325 (5)	0.0336 (5)	0.0047 (3)	0.0069 (3)	0.0086 (4)
C14	0.0306 (18)	0.039 (2)	0.056 (3)	0.0089 (15)	0.0111 (17)	0.0190 (18)
C15	0.046 (2)	0.043 (2)	0.067 (3)	0.0178 (19)	0.015 (2)	0.019 (2)
C16	0.0248 (16)	0.049 (2)	0.044 (2)	0.0063 (15)	0.0023 (15)	0.0028 (17)
C17	0.047 (2)	0.078 (3)	0.043 (3)	0.006 (2)	−0.0042 (19)	−0.003 (2)
C18	0.0323 (17)	0.0358 (19)	0.037 (2)	0.0055 (14)	0.0094 (14)	0.0039 (15)
C19	0.040 (2)	0.062 (3)	0.043 (2)	0.008 (2)	0.0008 (18)	0.000 (2)
P2	0.0217 (4)	0.0297 (4)	0.0279 (4)	0.0044 (3)	0.0016 (3)	0.0039 (3)
C20	0.0258 (16)	0.042 (2)	0.0359 (19)	0.0055 (14)	0.0086 (14)	0.0046 (16)
C21	0.043 (2)	0.063 (3)	0.061 (3)	0.025 (2)	0.021 (2)	0.012 (2)
C22	0.0351 (18)	0.0288 (18)	0.047 (2)	0.0029 (14)	−0.0061 (16)	−0.0025 (15)
C23	0.042 (2)	0.056 (3)	0.043 (2)	−0.0017 (19)	−0.0080 (18)	−0.002 (2)
C24	0.0339 (18)	0.046 (2)	0.0302 (18)	0.0140 (16)	−0.0011 (14)	0.0070 (15)
Pt2	0.01533 (5)	0.02664 (7)	0.02528 (7)	0.00658 (4)	−0.00191 (4)	0.00544 (5)
C25	0.055 (3)	0.066 (3)	0.038 (2)	0.014 (2)	−0.0137 (19)	−0.008 (2)
C26	0.0188 (14)	0.0328 (17)	0.0306 (17)	0.0067 (12)	0.0015 (12)	0.0059 (13)
C27	0.0234 (15)	0.0324 (18)	0.0302 (17)	0.0075 (13)	0.0024 (12)	0.0085 (13)
C28	0.0175 (13)	0.0324 (17)	0.0319 (17)	0.0063 (12)	0.0027 (12)	0.0135 (13)
C29	0.0265 (15)	0.0297 (17)	0.0362 (19)	0.0087 (13)	0.0009 (13)	0.0082 (14)
C30	0.0235 (14)	0.0301 (17)	0.0271 (16)	0.0070 (12)	−0.0030 (12)	0.0045 (13)
C31	0.0161 (12)	0.0275 (16)	0.0263 (16)	0.0041 (11)	−0.0002 (11)	0.0077 (12)
N2	0.0280 (14)	0.0314 (15)	0.0351 (16)	0.0065 (11)	−0.0079 (12)	0.0054 (12)
C32	0.0256 (15)	0.0357 (19)	0.0346 (18)	0.0059 (13)	−0.0056 (13)	0.0060 (14)
C33	0.0192 (14)	0.047 (2)	0.0248 (16)	0.0104 (13)	0.0017 (12)	0.0117 (14)
C34	0.0233 (16)	0.055 (2)	0.0328 (19)	0.0051 (15)	0.0020 (13)	0.0094 (16)
C35	0.0223 (16)	0.090 (3)	0.029 (2)	0.0064 (18)	−0.0018 (14)	0.017 (2)
C36	0.0309 (19)	0.087 (4)	0.043 (2)	0.027 (2)	0.0070 (17)	0.035 (2)
C37	0.038 (2)	0.056 (3)	0.049 (2)	0.0227 (18)	0.0151 (18)	0.028 (2)
C38	0.0279 (16)	0.042 (2)	0.038 (2)	0.0118 (15)	0.0052 (14)	0.0163 (16)
P3	0.0196 (3)	0.0260 (4)	0.0291 (4)	0.0075 (3)	0.0006 (3)	0.0048 (3)

C39	0.0360 (19)	0.036 (2)	0.046 (2)	0.0126 (15)	0.0051 (16)	−0.0046 (16)
C40	0.055 (3)	0.051 (3)	0.086 (4)	0.006 (2)	−0.003 (3)	−0.031 (3)
C41	0.0318 (17)	0.041 (2)	0.0284 (18)	0.0096 (15)	0.0007 (14)	0.0079 (15)
C42	0.0324 (18)	0.039 (2)	0.046 (2)	0.0063 (15)	−0.0006 (16)	0.0133 (17)
C43	0.0167 (14)	0.043 (2)	0.043 (2)	0.0081 (13)	−0.0003 (13)	0.0104 (16)
C44	0.0275 (17)	0.042 (2)	0.050 (2)	0.0054 (15)	−0.0065 (16)	0.0063 (17)
P4	0.0184 (4)	0.0327 (5)	0.0287 (4)	0.0048 (3)	0.0009 (3)	0.0036 (3)
C45	0.0218 (15)	0.054 (2)	0.0302 (18)	0.0009 (15)	−0.0013 (13)	0.0116 (16)
C46	0.0310 (19)	0.076 (3)	0.035 (2)	−0.0025 (19)	0.0045 (16)	0.016 (2)
C47	0.0161 (14)	0.045 (2)	0.040 (2)	0.0029 (13)	−0.0051 (13)	0.0150 (16)
C48	0.045 (2)	0.054 (3)	0.048 (3)	−0.0032 (19)	−0.0167 (19)	−0.001 (2)
C49	0.0351 (19)	0.047 (2)	0.043 (2)	0.0101 (17)	0.0104 (16)	0.0008 (18)
C50	0.057 (3)	0.054 (3)	0.060 (3)	−0.008 (2)	0.013 (2)	−0.009 (2)

Geometric parameters (Å, º)

Pt1—C1	2.017 (4)	Pt2—P4	2.2914 (9)
Pt1—C8	2.051 (3)	C25—H25A	0.9800
Pt1—P2	2.2794 (8)	C25—H25B	0.9800
Pt1—P1	2.2889 (8)	C25—H25C	0.9800
C1—C2	1.197 (5)	C26—C27	1.199 (4)
C2—C3	1.438 (4)	C27—C28	1.436 (4)
C3—C7	1.391 (5)	C28—C29	1.393 (5)
C3—C4	1.397 (5)	C28—C32	1.405 (5)
C4—N1	1.334 (4)	C29—C30	1.368 (4)
C4—H4A	0.9500	C29—H29A	0.9500
C5—N1	1.344 (4)	C30—C31	1.380 (5)
C5—C6	1.386 (5)	C30—H30A	0.9500
C5—C5^{i}	1.478 (6)	C31—N2	1.354 (4)
C6—C7	1.385 (5)	C31—C31^{ii}	1.480 (5)
C6—H6A	0.9500	N2—C32	1.330 (4)
C7—H7A	0.9500	C32—H32A	0.9500
C8—C13	1.394 (5)	C33—C34	1.400 (5)
C8—C9	1.397 (5)	C33—C38	1.401 (5)
C9—C10	1.399 (6)	C34—C35	1.392 (5)
C9—H9A	0.9500	C34—H34A	0.9500
C10—C11	1.370 (8)	C35—C36	1.377 (7)
C10—H10A	0.9500	C35—H35A	0.9500
C11—C12	1.358 (7)	C36—C37	1.370 (6)
C11—H11A	0.9500	C36—H36A	0.9500
C12—C13	1.383 (6)	C37—C38	1.394 (5)
C12—H12A	0.9500	C37—H37A	0.9500
C13—H13A	0.9500	C38—H38A	0.9500
P1—C18	1.808 (4)	P3—C39	1.819 (4)
P1—C16	1.820 (4)	P3—C43	1.826 (3)
P1—C14	1.823 (4)	P3—C41	1.828 (3)
C14—C15	1.524 (5)	C39—C40	1.505 (6)
C14—H14A	0.9900	C39—H39A	0.9900

C14—H14B	0.9900	C39—H39B	0.9900
C15—H15A	0.9800	C40—H40A	0.9800
C15—H15B	0.9800	C40—H40B	0.9800
C15—H15C	0.9800	C40—H40C	0.9800
C16—C17	1.516 (6)	C41—C42	1.528 (5)
C16—H16A	0.9900	C41—H41A	0.9900
C16—H16B	0.9900	C41—H41B	0.9900
C17—H17A	0.9800	C42—H42A	0.9800
C17—H17B	0.9800	C42—H42B	0.9800
C17—H17C	0.9800	C42—H42C	0.9800
C18—C19	1.521 (5)	C43—C44	1.511 (5)
C18—H18A	0.9900	C43—H43A	0.9900
C18—H18B	0.9900	C43—H43B	0.9900
C19—H19A	0.9800	C44—H44A	0.9800
C19—H19B	0.9800	C44—H44B	0.9800
C19—H19C	0.9800	C44—H44C	0.9800
P2—C22	1.811 (4)	P4—C47	1.811 (3)
P2—C20	1.818 (3)	P4—C45	1.816 (4)
P2—C24	1.826 (3)	P4—C49	1.836 (4)
C20—C21	1.517 (5)	C45—C46	1.528 (5)
C20—H20A	0.9900	C45—H45A	0.9900
C20—H20B	0.9900	C45—H45B	0.9900
C21—H21A	0.9800	C46—H46A	0.9800
C21—H21B	0.9800	C46—H46B	0.9800
C21—H21C	0.9800	C46—H46C	0.9800
C22—C23	1.517 (5)	C47—C48	1.506 (6)
C22—H22A	0.9900	C47—H47A	0.9900
C22—H22B	0.9900	C47—H47B	0.9900
C23—H23A	0.9800	C48—H48A	0.9800
C23—H23B	0.9800	C48—H48B	0.9800
C23—H23C	0.9800	C48—H48C	0.9800
C24—C25	1.534 (6)	C49—C50	1.508 (6)
C24—H24A	0.9900	C49—H49A	0.9900
C24—H24B	0.9900	C49—H49B	0.9900
Pt2—C26	2.017 (3)	C50—H50A	0.9800
Pt2—C33	2.066 (3)	C50—H50B	0.9800
Pt2—P3	2.2869 (8)	C50—H50C	0.9800

C1—Pt1—C8	176.58 (14)	C24—C25—H25A	109.5
C1—Pt1—P2	89.53 (9)	C24—C25—H25B	109.5
C8—Pt1—P2	92.15 (9)	H25A—C25—H25B	109.5
C1—Pt1—P1	86.75 (9)	C24—C25—H25C	109.5
C8—Pt1—P1	91.69 (9)	H25A—C25—H25C	109.5
P2—Pt1—P1	175.56 (3)	H25B—C25—H25C	109.5
C2—C1—Pt1	177.2 (3)	C27—C26—Pt2	176.8 (3)
C1—C2—C3	177.1 (4)	C26—C27—C28	174.1 (4)
C7—C3—C4	116.1 (3)	C29—C28—C32	115.9 (3)
C7—C3—C2	123.4 (3)	C29—C28—C27	124.0 (3)

C4—C3—C2	120.4 (3)	C32—C28—C27	120.1 (3)
N1—C4—C3	124.8 (3)	C30—C29—C28	120.3 (3)
N1—C4—H4A	117.6	C30—C29—H29A	119.8
C3—C4—H4A	117.6	C28—C29—H29A	119.8
N1—C5—C6	122.0 (3)	C29—C30—C31	119.9 (3)
N1—C5—C5^{i}	115.9 (4)	C29—C30—H30A	120.1
C6—C5—C5^{i}	122.1 (4)	C31—C30—H30A	120.1
C4—N1—C5	117.8 (3)	N2—C31—C30	121.5 (3)
C7—C6—C5	119.3 (3)	N2—C31—C31^{ii}	117.4 (4)
C7—C6—H6A	120.4	C30—C31—C31^{ii}	121.2 (4)
C5—C6—H6A	120.4	C32—N2—C31	118.1 (3)
C6—C7—C3	120.0 (3)	N2—C32—C28	124.3 (3)
C6—C7—H7A	120.0	N2—C32—H32A	117.8
C3—C7—H7A	120.0	C28—C32—H32A	117.8
C13—C8—C9	115.6 (3)	C34—C33—C38	115.6 (3)
C13—C8—Pt1	121.0 (3)	C34—C33—Pt2	122.9 (3)
C9—C8—Pt1	123.4 (3)	C38—C33—Pt2	121.6 (3)
C8—C9—C10	121.8 (4)	C35—C34—C33	122.0 (4)
C8—C9—H9A	119.1	C35—C34—H34A	119.0
C10—C9—H9A	119.1	C33—C34—H34A	119.0
C11—C10—C9	120.2 (5)	C36—C35—C34	120.6 (4)
C11—C10—H10A	119.9	C36—C35—H35A	119.7
C9—C10—H10A	119.9	C34—C35—H35A	119.7
C12—C11—C10	119.2 (4)	C37—C36—C35	119.2 (3)
C12—C11—H11A	120.4	C37—C36—H36A	120.4
C10—C11—H11A	120.4	C35—C36—H36A	120.4
C11—C12—C13	120.9 (4)	C36—C37—C38	120.2 (4)
C11—C12—H12A	119.6	C36—C37—H37A	119.9
C13—C12—H12A	119.6	C38—C37—H37A	119.9
C12—C13—C8	122.3 (4)	C37—C38—C33	122.5 (4)
C12—C13—H13A	118.9	C37—C38—H38A	118.8
C8—C13—H13A	118.9	C33—C38—H38A	118.8
C18—P1—C16	102.32 (17)	C39—P3—C43	99.16 (17)
C18—P1—C14	104.65 (19)	C39—P3—C41	102.75 (18)
C16—P1—C14	105.48 (19)	C43—P3—C41	106.87 (17)
C18—P1—Pt1	112.68 (12)	C39—P3—Pt2	112.23 (13)
C16—P1—Pt1	111.98 (13)	C43—P3—Pt2	116.15 (12)
C14—P1—Pt1	118.23 (12)	C41—P3—Pt2	117.39 (12)
C15—C14—P1	115.9 (3)	C40—C39—P3	115.7 (3)
C15—C14—H14A	108.3	C40—C39—H39A	108.4
P1—C14—H14A	108.3	P3—C39—H39A	108.4
C15—C14—H14B	108.3	C40—C39—H39B	108.4
P1—C14—H14B	108.3	P3—C39—H39B	108.4
H14A—C14—H14B	107.4	H39A—C39—H39B	107.4
C14—C15—H15A	109.5	C39—C40—H40A	109.5
C14—C15—H15B	109.5	C39—C40—H40B	109.5
H15A—C15—H15B	109.5	H40A—C40—H40B	109.5
C14—C15—H15C	109.5	C39—C40—H40C	109.5

H15A—C15—H15C	109.5	H40A—C40—H40C	109.5
H15B—C15—H15C	109.5	H40B—C40—H40C	109.5
C17—C16—P1	113.2 (3)	C42—C41—P3	115.4 (3)
C17—C16—H16A	108.9	C42—C41—H41A	108.4
P1—C16—H16A	108.9	P3—C41—H41A	108.4
C17—C16—H16B	108.9	C42—C41—H41B	108.4
P1—C16—H16B	108.9	P3—C41—H41B	108.4
H16A—C16—H16B	107.8	H41A—C41—H41B	107.5
C16—C17—H17A	109.5	C41—C42—H42A	109.5
C16—C17—H17B	109.5	C41—C42—H42B	109.5
H17A—C17—H17B	109.5	H42A—C42—H42B	109.5
C16—C17—H17C	109.5	C41—C42—H42C	109.5
H17A—C17—H17C	109.5	H42A—C42—H42C	109.5
H17B—C17—H17C	109.5	H42B—C42—H42C	109.5
C19—C18—P1	113.7 (3)	C44—C43—P3	116.9 (2)
C19—C18—H18A	108.8	C44—C43—H43A	108.1
P1—C18—H18A	108.8	P3—C43—H43A	108.1
C19—C18—H18B	108.8	C44—C43—H43B	108.1
P1—C18—H18B	108.8	P3—C43—H43B	108.1
H18A—C18—H18B	107.7	H43A—C43—H43B	107.3
C18—C19—H19A	109.5	C43—C44—H44A	109.5
C18—C19—H19B	109.5	C43—C44—H44B	109.5
H19A—C19—H19B	109.5	H44A—C44—H44B	109.5
C18—C19—H19C	109.5	C43—C44—H44C	109.5
H19A—C19—H19C	109.5	H44A—C44—H44C	109.5
H19B—C19—H19C	109.5	H44B—C44—H44C	109.5
C22—P2—C20	104.96 (19)	C47—P4—C45	105.07 (17)
C22—P2—C24	103.97 (18)	C47—P4—C49	102.16 (18)
C20—P2—C24	105.21 (17)	C45—P4—C49	106.49 (19)
C22—P2—Pt1	110.87 (12)	C47—P4—Pt2	112.00 (13)
C20—P2—Pt1	117.09 (12)	C45—P4—Pt2	116.65 (12)
C24—P2—Pt1	113.58 (12)	C49—P4—Pt2	113.16 (14)
C21—C20—P2	116.9 (3)	C46—C45—P4	115.3 (3)
C21—C20—H20A	108.1	C46—C45—H45A	108.5
P2—C20—H20A	108.1	P4—C45—H45A	108.5
C21—C20—H20B	108.1	C46—C45—H45B	108.5
P2—C20—H20B	108.1	P4—C45—H45B	108.5
H20A—C20—H20B	107.3	H45A—C45—H45B	107.5
C20—C21—H21A	109.5	C45—C46—H46A	109.5
C20—C21—H21B	109.5	C45—C46—H46B	109.5
H21A—C21—H21B	109.5	H46A—C46—H46B	109.5
C20—C21—H21C	109.5	C45—C46—H46C	109.5
H21A—C21—H21C	109.5	H46A—C46—H46C	109.5
H21B—C21—H21C	109.5	H46B—C46—H46C	109.5
C23—C22—P2	113.1 (3)	C48—C47—P4	113.5 (2)
C23—C22—H22A	109.0	C48—C47—H47A	108.9
P2—C22—H22A	109.0	P4—C47—H47A	108.9
C23—C22—H22B	109.0	C48—C47—H47B	108.9

P2—C22—H22B	109.0	P4—C47—H47B	108.9
H22A—C22—H22B	107.8	H47A—C47—H47B	107.7
C22—C23—H23A	109.5	C47—C48—H48A	109.5
C22—C23—H23B	109.5	C47—C48—H48B	109.5
H23A—C23—H23B	109.5	H48A—C48—H48B	109.5
C22—C23—H23C	109.5	C47—C48—H48C	109.5
H23A—C23—H23C	109.5	H48A—C48—H48C	109.5
H23B—C23—H23C	109.5	H48B—C48—H48C	109.5
C25—C24—P2	112.4 (3)	C50—C49—P4	113.8 (3)
C25—C24—H24A	109.1	C50—C49—H49A	108.8
P2—C24—H24A	109.1	P4—C49—H49A	108.8
C25—C24—H24B	109.1	C50—C49—H49B	108.8
P2—C24—H24B	109.1	P4—C49—H49B	108.8
H24A—C24—H24B	107.9	H49A—C49—H49B	107.7
C26—Pt2—C33	177.92 (12)	C49—C50—H50A	109.5
C26—Pt2—P3	92.89 (9)	C49—C50—H50B	109.5
C33—Pt2—P3	89.19 (9)	H50A—C50—H50B	109.5
C26—Pt2—P4	86.63 (9)	C49—C50—H50C	109.5
C33—Pt2—P4	91.28 (9)	H50A—C50—H50C	109.5
P3—Pt2—P4	176.53 (3)	H50B—C50—H50C	109.5

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