Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Bis{1-[2-(diphenylphosphino)ethyl]-3-ethylimidazol-2-ylidene}palladium(II) bis(hexafluoridophosphate) acetonitrile 2.85-solvate

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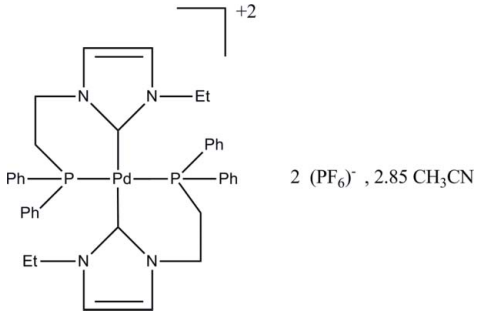
Received 16 March 2010; accepted 9 April 2010

Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.006 Å; some non-H atoms missing; disorder in solvent or counterion; $R$ factor = 0.047; $wR$ factor = 0.129; data-to-parameter ratio = 18.5.

In the structure of the title compound, $[Pd(C_{19}H_{21}N_2P)_2](PF_6)_2\cdot2.85CH_3CN$, the two six-membered NHC-phosphane chelate rings form a distorted square-planar coordination geometry around the $Pd^{II}$ atom, which lies 0.212 (1) Å above the coordination plane. The sum of the bond angles at $Pd^{II}$ is 358.3°, with C—Pd—P bite angles of 84.03 (10) and 83.54 (9)°. The structure includes three acetonitrile solvent molecules, one with partial site occupation and one with severe disorder, which was eventually excluded from the refinement.

## Related literature

For the structures of related $Pd^{II}$ complexes, see: Chiu *et al.* (2005); Lee *et al.* (2004*a*,*b*); Navarro *et al.* (2004); Tsoureas *et al.* (2003). For refinement aspects, see: Spek (2009).




## Experimental

### Crystal data

$[Pd(C_{19}H_{21}N_2P)_2](PF_6)_2\cdot2.85C_2H_3N$
$M_r$ = 1130.45
Triclinic, $P\overline{1}$
$a$ = 11.114 (2) Å
$b$ = 11.343 (2) Å
$c$ = 20.243 (4) Å
$\alpha$ = 77.490 (4)°
$\beta$ = 83.580 (5)°
$\gamma$ = 85.301 (4)°
$V$ = 2471.4 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.59 mm$^{-1}$
$T$ = 120 K
0.42 × 0.20 × 0.20 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.790, $T_{max}$ = 0.891
20500 measured reflections
10802 independent reflections
9025 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
$S$ = 1.05
10802 reflections
584 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pd1—C31 | 2.031 (3) | Pd1—P1 | 2.3085 (9) |
| Pd1—C1 | 2.033 (3) | Pd1—P2 | 2.3100 (9) |
| C31—Pd1—C1 | 173.56 (13) | C31—Pd1—P2 | 83.54 (9) |
| C31—Pd1—P1 | 94.24 (9) | C1—Pd1—P2 | 96.46 (10) |
| C1—Pd1—P1 | 84.03 (10) | P1—Pd1—P2 | 164.44 (3) |

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2316).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m522 [ **doi:10.1107/S160053681001319X** ]

# Bis{1-[2-(diphenylphosphino)ethyl]-3-ethylimidazol-2-ylidene}palladium(II) bis(hexafluoridophosphate) acetonitrile 2.85-solvate

**A. A. Aziza, U. Flörke, H. Egold and G. Henkel**

## Comment

The two six-membered NHC-phosphane chelate rings form a distorted square-planar coordination geometry around the palladium(II) atom which lies 0.212 (1) Å above the coordination plane. The sum of bond angles at Pd is 358.3° with C1—Pd1—P1 and C31—Pd1—P2 bite angles of 84.03 (10)° and 83.54 (9)°, respectively. The trans C1—Pd1—C31 and P1—Pd1—P2 bond angles are 173.56 (13)° and 164.44 (3)° and thus deviate clearly from linearity. The Pd—C bond lengths (2.031 (3) and 2.033 (3) Å) are within the expected range and the Pd—P bond lengths of 2.3085 (9) and 2.3100 (9) Å also are comparable to those in other complexes containing Pd-NHC phosphane ligands (e.g. Chiu *et al.* (2005); Lee *et al.* (2004*a*,*b*); Navarro *et al.* (2004); Tsoureas *et al.* (2003)). There are no intermolecular contacts shorter than the van der Waals distances.

## Experimental

To a solution of 3-[2-(diphenylphosphino)ethyl]-1-ethylimidazolium-hexafluoridophosphate (195 mg, 0.46 mmol) in THF (10 ml) was added $KN(SiMe_3)_2$ (118 mg, 0.46 mmol + 30%) and the mixture was stirred at room temperature under $N_2$ for 30 min. Then $[Pd(COD)Cl_2]$ (66 mg, 0.230 mmol; COD = 1,5-cyclooctadiene) was added to the reaction mixture and the colour changed from pale yellow to yellow–orange. The reaction mixture was stirred for another 2 h and then the solvent was removed under vacuum. Yellow crystals were obtained from an acetonitrile solution by diethyl ether diffusion.

## Refinement

For the final refinement, data were cut off at θ = 27.1° in order to get 99% completeness. H atoms were clearly identified in difference Fourier syntheses, idealized and refined at calculated positions riding on the C atoms with isotropic displacement parameters $U_{iso}(H) = 1.2U(C_{eq})$ or $1.5U(-CH_3)$. All methyl H atoms were allowed to rotate but not to tip. There are three acetonitrile solvent molecules per asymmetric unit. Two of these could be refined easily, the N300 one with an occupation factor of 0.85 (1). It was, however, not possible to refine successfully the third heavily distorted acetonitrile molecule. After treatment of the data with the SQUEEZE facility of PLATON (Spek, 2009) refinement then proceeded smoothly.

## Figures

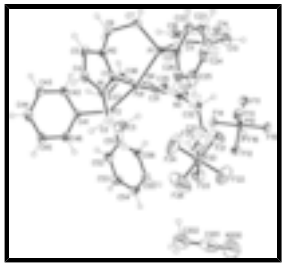

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. For clarity, the N300 solvent molecule with partial site occupation was omitted.

**Bis{1-[2-(diphenylphosphino)ethyl]-3-ethyl-imidazol-2-ylidene}palladium(II) bis(hexafluoridophosphate) acetonitrile 2.85-solvate**

*Crystal data*

| | |
|---|---|
| $[Pd(C_{19}H_{21}N_2P)_2](PF_6)_2 \cdot 2.85C_2H_3N$ | $Z = 2$ |
| $M_r = 1130.45$ | $F(000) = 1150$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.519$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 11.114$ (2) Å | Cell parameters from 1002 reflections |
| $b = 11.343$ (2) Å | $\theta = 2.3$–$28.1°$ |
| $c = 20.243$ (4) Å | $\mu = 0.59$ mm$^{-1}$ |
| $\alpha = 77.490$ (4)° | $T = 120$ K |
| $\beta = 83.580$ (5)° | Prism, pale-yellow |
| $\gamma = 85.301$ (4)° | 0.42 × 0.20 × 0.20 mm |
| $V = 2471.4$ (8) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 10802 independent reflections |
| Radiation source: sealed tube | 9025 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.032$ |
| φ and ω scans | $\theta_{max} = 27.1°$, $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $h = -14 \rightarrow 14$ |
| $T_{min} = 0.790$, $T_{max} = 0.891$ | $k = -14 \rightarrow 14$ |
| 20500 measured reflections | $l = -24 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | Hydrogen site location: difference Fourier map |
| $wR(F^2) = 0.129$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 3.077P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 10802 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 584 parameters | $\Delta\rho_{max} = 0.90$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.56$ e Å$^{-3}$ |

*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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor wR and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pd1 | 0.14297 (2) | 0.58147 (2) | 0.214403 (12) | 0.01778 (8) | |
| P1 | 0.10291 (8) | 0.69609 (8) | 0.29654 (4) | 0.02250 (19) | |
| P2 | 0.14709 (8) | 0.50588 (8) | 0.11694 (4) | 0.02037 (18) | |
| N1 | −0.0082 (3) | 0.3656 (3) | 0.29190 (14) | 0.0242 (6) | |
| N2 | −0.1052 (3) | 0.5386 (3) | 0.28212 (14) | 0.0233 (6) | |
| N3 | 0.3767 (3) | 0.7229 (2) | 0.16884 (14) | 0.0216 (6) | |
| N4 | 0.2425 (2) | 0.7651 (2) | 0.09788 (14) | 0.0215 (6) | |
| C1 | 0.0041 (3) | 0.4847 (3) | 0.26744 (16) | 0.0220 (7) | |
| C2 | 0.0877 (4) | 0.2695 (3) | 0.28886 (19) | 0.0318 (8) | |
| H2A | 0.1630 | 0.3058 | 0.2653 | 0.038* | |
| H2B | 0.0633 | 0.2136 | 0.2621 | 0.038* | |
| C3 | 0.1126 (4) | 0.1990 (4) | 0.3589 (2) | 0.0424 (10) | |
| H3A | 0.1764 | 0.1354 | 0.3547 | 0.064* | |
| H3B | 0.0384 | 0.1622 | 0.3822 | 0.064* | |
| H3C | 0.1390 | 0.2537 | 0.3851 | 0.064* | |
| C4 | −0.1260 (3) | 0.3454 (3) | 0.32047 (17) | 0.0280 (8) | |
| H4A | −0.1578 | 0.2692 | 0.3406 | 0.034* | |
| C5 | −0.1863 (3) | 0.4538 (3) | 0.31420 (17) | 0.0256 (7) | |
| H5A | −0.2691 | 0.4692 | 0.3290 | 0.031* | |
| C6 | −0.1331 (3) | 0.6692 (3) | 0.26246 (18) | 0.0267 (7) | |
| H6A | −0.2208 | 0.6868 | 0.2738 | 0.032* | |
| H6B | −0.1152 | 0.6955 | 0.2126 | 0.032* | |
| C7 | −0.0607 (3) | 0.7417 (3) | 0.2980 (2) | 0.0299 (8) | |
| H7A | −0.0954 | 0.7329 | 0.3459 | 0.036* | |
| H7B | −0.0703 | 0.8284 | 0.2759 | 0.036* | |
| C11 | 0.1811 (3) | 0.8350 (3) | 0.2794 (2) | 0.0301 (8) | |
| C12 | 0.2725 (4) | 0.8492 (4) | 0.3179 (2) | 0.0412 (10) | |
| H12A | 0.2886 | 0.7895 | 0.3572 | 0.049* | |
| C13 | 0.3400 (5) | 0.9504 (5) | 0.2990 (3) | 0.0581 (14) | |
| H13A | 0.4010 | 0.9612 | 0.3261 | 0.070* | |
| C14 | 0.3197 (5) | 1.0347 (4) | 0.2416 (3) | 0.0620 (16) | |
| H14A | 0.3678 | 1.1030 | 0.2285 | 0.074* | |
| C15 | 0.2303 (4) | 1.0217 (4) | 0.2027 (3) | 0.0551 (14) | |
| H15A | 0.2168 | 1.0810 | 0.1628 | 0.066* | |
| C16 | 0.1588 (4) | 0.9219 (3) | 0.2213 (2) | 0.0396 (10) | |
| H16A | 0.0960 | 0.9135 | 0.1948 | 0.047* | |
| C21 | 0.1273 (3) | 0.6228 (3) | 0.38290 (17) | 0.0273 (7) | |
| C22 | 0.0872 (4) | 0.6806 (4) | 0.4361 (2) | 0.0399 (10) | |

| | | | | |
|---|---|---|---|---|
| H22A | 0.0465 | 0.7585 | 0.4270 | 0.048* |
| C23 | 0.1068 (5) | 0.6240 (6) | 0.5024 (2) | 0.0529 (13) |
| H23A | 0.0802 | 0.6635 | 0.5387 | 0.063* |
| C24 | 0.1641 (5) | 0.5121 (5) | 0.5151 (2) | 0.0538 (13) |
| H24A | 0.1756 | 0.4733 | 0.5606 | 0.065* |
| C25 | 0.2059 (5) | 0.4536 (5) | 0.4633 (2) | 0.0493 (12) |
| H25A | 0.2468 | 0.3758 | 0.4731 | 0.059* |
| C26 | 0.1879 (4) | 0.5092 (4) | 0.39648 (19) | 0.0352 (9) |
| H26A | 0.2167 | 0.4697 | 0.3604 | 0.042* |
| C31 | 0.2673 (3) | 0.6927 (3) | 0.15747 (16) | 0.0200 (6) |
| C32 | 0.4479 (3) | 0.6611 (3) | 0.22448 (18) | 0.0294 (8) |
| H32A | 0.3963 | 0.6051 | 0.2581 | 0.035* |
| H32B | 0.4742 | 0.7216 | 0.2477 | 0.035* |
| C33 | 0.5575 (3) | 0.5912 (3) | 0.1988 (2) | 0.0334 (8) |
| H33A | 0.6026 | 0.5504 | 0.2371 | 0.050* |
| H33B | 0.6096 | 0.6468 | 0.1664 | 0.050* |
| H33C | 0.5315 | 0.5308 | 0.1761 | 0.050* |
| C34 | 0.4190 (3) | 0.8157 (3) | 0.11711 (18) | 0.0263 (7) |
| H34A | 0.4934 | 0.8534 | 0.1139 | 0.032* |
| C35 | 0.3350 (3) | 0.8424 (3) | 0.07238 (18) | 0.0257 (7) |
| H35A | 0.3384 | 0.9023 | 0.0315 | 0.031* |
| C36 | 0.1317 (3) | 0.7596 (3) | 0.06651 (18) | 0.0252 (7) |
| H36A | 0.1286 | 0.8249 | 0.0253 | 0.030* |
| H36B | 0.0605 | 0.7732 | 0.0986 | 0.030* |
| C37 | 0.1246 (4) | 0.6381 (3) | 0.04706 (17) | 0.0281 (8) |
| H37A | 0.1869 | 0.6319 | 0.0088 | 0.034* |
| H37B | 0.0443 | 0.6354 | 0.0308 | 0.034* |
| C41 | 0.0274 (3) | 0.4071 (3) | 0.11525 (17) | 0.0230 (7) |
| C42 | −0.0919 (3) | 0.4487 (3) | 0.13059 (17) | 0.0267 (7) |
| H42A | −0.1088 | 0.5300 | 0.1356 | 0.032* |
| C43 | −0.1864 (3) | 0.3721 (4) | 0.13863 (19) | 0.0322 (8) |
| H43A | −0.2674 | 0.4003 | 0.1499 | 0.039* |
| C44 | −0.1616 (4) | 0.2546 (4) | 0.13016 (19) | 0.0352 (9) |
| H44A | −0.2257 | 0.2016 | 0.1365 | 0.042* |
| C45 | −0.0438 (4) | 0.2132 (3) | 0.1125 (2) | 0.0353 (9) |
| H45A | −0.0276 | 0.1330 | 0.1056 | 0.042* |
| C46 | 0.0501 (4) | 0.2903 (3) | 0.10514 (19) | 0.0287 (8) |
| H46A | 0.1307 | 0.2624 | 0.0930 | 0.034* |
| C51 | 0.2878 (3) | 0.4266 (3) | 0.09389 (17) | 0.0238 (7) |
| C52 | 0.3191 (4) | 0.4080 (4) | 0.0279 (2) | 0.0356 (9) |
| H52A | 0.2669 | 0.4395 | −0.0067 | 0.043* |
| C53 | 0.4262 (4) | 0.3436 (4) | 0.0130 (2) | 0.0443 (10) |
| H53A | 0.4468 | 0.3311 | −0.0319 | 0.053* |
| C54 | 0.5031 (4) | 0.2975 (4) | 0.0622 (2) | 0.0396 (10) |
| H54A | 0.5763 | 0.2534 | 0.0513 | 0.047* |
| C55 | 0.4740 (4) | 0.3153 (3) | 0.1277 (2) | 0.0335 (8) |
| H55A | 0.5274 | 0.2843 | 0.1617 | 0.040* |
| C56 | 0.3655 (3) | 0.3792 (3) | 0.14365 (18) | 0.0262 (7) |
| H56A | 0.3448 | 0.3903 | 0.1888 | 0.031* |

| | | | | | |
|---|---|---|---|---|---|
| P10 | 0.78890 (8) | 0.89315 (8) | 0.08279 (5) | 0.0250 (2) | |
| F11 | 0.7426 (2) | 1.03165 (19) | 0.07981 (13) | 0.0408 (6) | |
| F12 | 0.8351 (2) | 0.7545 (2) | 0.08694 (13) | 0.0425 (6) | |
| F13 | 0.6962 (2) | 0.8529 (2) | 0.14901 (11) | 0.0391 (5) | |
| F14 | 0.6869 (2) | 0.8796 (2) | 0.03586 (12) | 0.0380 (5) | |
| F15 | 0.8896 (2) | 0.9069 (2) | 0.13115 (12) | 0.0383 (5) | |
| F16 | 0.8808 (2) | 0.9332 (2) | 0.01755 (12) | 0.0446 (6) | |
| P20 | 0.49733 (11) | 0.28058 (11) | 0.35088 (6) | 0.0413 (3) | |
| F21 | 0.5132 (3) | 0.4160 (3) | 0.35538 (17) | 0.0684 (9) | |
| F22 | 0.6133 (3) | 0.2418 (3) | 0.38990 (17) | 0.0776 (10) | |
| F23 | 0.5813 (3) | 0.3003 (3) | 0.28115 (14) | 0.0584 (7) | |
| F24 | 0.3828 (3) | 0.3256 (5) | 0.31074 (19) | 0.1052 (15) | |
| F25 | 0.4106 (3) | 0.2649 (4) | 0.42035 (17) | 0.0807 (11) | |
| F26 | 0.4822 (5) | 0.1461 (4) | 0.3489 (3) | 0.134 (2) | |
| N200 | 0.8799 (7) | 0.0600 (8) | 0.3056 (6) | 0.149 (4) | |
| C201 | 0.7923 (8) | 0.0335 (5) | 0.2890 (4) | 0.083 (2) | |
| C202 | 0.6818 (7) | 0.0013 (7) | 0.2705 (4) | 0.095 (2) | |
| H20A | 0.6639 | −0.0804 | 0.2956 | 0.143* | |
| H20B | 0.6895 | 0.0032 | 0.2215 | 0.143* | |
| H20C | 0.6158 | 0.0589 | 0.2814 | 0.143* | |
| N300 | 0.6186 (8) | 0.7019 (8) | 0.3728 (4) | 0.115 (4) | 0.852 (11) |
| C301 | 0.5552 (7) | 0.6772 (10) | 0.4114 (4) | 0.094 (3) | 0.852 (11) |
| C302 | 0.4552 (18) | 0.6296 (16) | 0.4684 (10) | 0.226 (9)* | 0.852 (11) |
| H30A | 0.4254 | 0.6941 | 0.4924 | 0.340* | 0.852 (11) |
| H30B | 0.4888 | 0.5606 | 0.5004 | 0.340* | 0.852 (11) |
| H30C | 0.3880 | 0.6041 | 0.4483 | 0.340* | 0.852 (11) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.01780 (13) | 0.02025 (13) | 0.01547 (12) | −0.00351 (9) | −0.00124 (9) | −0.00340 (9) |
| P1 | 0.0217 (4) | 0.0254 (4) | 0.0219 (4) | −0.0036 (3) | −0.0001 (3) | −0.0083 (3) |
| P2 | 0.0215 (4) | 0.0236 (4) | 0.0166 (4) | −0.0023 (3) | −0.0028 (3) | −0.0046 (3) |
| N1 | 0.0255 (16) | 0.0276 (14) | 0.0201 (14) | −0.0059 (12) | −0.0026 (11) | −0.0044 (11) |
| N2 | 0.0201 (15) | 0.0308 (15) | 0.0194 (14) | −0.0036 (12) | −0.0037 (11) | −0.0046 (11) |
| N3 | 0.0177 (14) | 0.0252 (14) | 0.0219 (14) | −0.0021 (11) | −0.0013 (11) | −0.0048 (11) |
| N4 | 0.0154 (14) | 0.0252 (14) | 0.0220 (14) | −0.0003 (11) | −0.0003 (11) | −0.0018 (11) |
| C1 | 0.0240 (17) | 0.0262 (16) | 0.0161 (15) | −0.0055 (13) | −0.0041 (13) | −0.0026 (12) |
| C2 | 0.036 (2) | 0.0240 (17) | 0.033 (2) | −0.0044 (15) | 0.0054 (16) | −0.0044 (15) |
| C3 | 0.040 (2) | 0.040 (2) | 0.041 (2) | 0.0041 (18) | −0.0026 (19) | 0.0013 (18) |
| C4 | 0.0293 (19) | 0.0350 (19) | 0.0197 (16) | −0.0143 (15) | −0.0004 (14) | −0.0025 (14) |
| C5 | 0.0194 (17) | 0.0381 (19) | 0.0191 (16) | −0.0084 (14) | −0.0014 (13) | −0.0029 (14) |
| C6 | 0.0195 (17) | 0.0313 (18) | 0.0280 (18) | 0.0004 (14) | −0.0037 (14) | −0.0037 (14) |
| C7 | 0.0233 (19) | 0.0316 (18) | 0.037 (2) | 0.0020 (14) | 0.0004 (15) | −0.0144 (16) |
| C11 | 0.0280 (19) | 0.0268 (17) | 0.038 (2) | −0.0044 (15) | 0.0049 (16) | −0.0161 (15) |
| C12 | 0.039 (2) | 0.041 (2) | 0.049 (3) | −0.0104 (19) | −0.0021 (19) | −0.0183 (19) |
| C13 | 0.051 (3) | 0.045 (3) | 0.085 (4) | −0.019 (2) | −0.001 (3) | −0.025 (3) |
| C14 | 0.055 (3) | 0.029 (2) | 0.103 (5) | −0.016 (2) | 0.015 (3) | −0.020 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.042 (3) | 0.029 (2) | 0.085 (4) | 0.0002 (19) | 0.010 (3) | 0.000 (2) |
| C16 | 0.041 (2) | 0.0262 (18) | 0.048 (2) | −0.0008 (17) | 0.0039 (19) | −0.0055 (17) |
| C21 | 0.0233 (18) | 0.040 (2) | 0.0210 (17) | −0.0080 (15) | −0.0005 (14) | −0.0111 (15) |
| C22 | 0.031 (2) | 0.061 (3) | 0.032 (2) | −0.0025 (19) | −0.0003 (17) | −0.021 (2) |
| C23 | 0.046 (3) | 0.093 (4) | 0.025 (2) | −0.013 (3) | 0.0034 (19) | −0.025 (2) |
| C24 | 0.051 (3) | 0.088 (4) | 0.023 (2) | −0.019 (3) | −0.0053 (19) | −0.005 (2) |
| C25 | 0.054 (3) | 0.056 (3) | 0.037 (2) | −0.009 (2) | −0.014 (2) | 0.001 (2) |
| C26 | 0.038 (2) | 0.043 (2) | 0.0251 (19) | −0.0060 (18) | −0.0043 (16) | −0.0071 (16) |
| C31 | 0.0152 (15) | 0.0223 (15) | 0.0224 (16) | 0.0003 (12) | −0.0001 (12) | −0.0059 (13) |
| C32 | 0.029 (2) | 0.0331 (18) | 0.0267 (18) | −0.0038 (15) | −0.0117 (15) | −0.0027 (15) |
| C33 | 0.0221 (19) | 0.035 (2) | 0.041 (2) | −0.0003 (15) | −0.0095 (16) | −0.0027 (17) |
| C34 | 0.0209 (17) | 0.0271 (17) | 0.0292 (18) | −0.0048 (14) | 0.0022 (14) | −0.0031 (14) |
| C35 | 0.0190 (17) | 0.0252 (16) | 0.0294 (18) | −0.0053 (13) | 0.0014 (14) | 0.0013 (14) |
| C36 | 0.0231 (18) | 0.0273 (17) | 0.0237 (17) | −0.0033 (14) | −0.0059 (14) | 0.0006 (13) |
| C37 | 0.035 (2) | 0.0307 (18) | 0.0183 (16) | −0.0052 (15) | −0.0068 (14) | −0.0004 (14) |
| C41 | 0.0206 (17) | 0.0292 (17) | 0.0208 (16) | −0.0055 (13) | −0.0052 (13) | −0.0056 (13) |
| C42 | 0.0280 (19) | 0.0326 (18) | 0.0224 (17) | −0.0025 (15) | −0.0049 (14) | −0.0108 (14) |
| C43 | 0.0185 (18) | 0.050 (2) | 0.0310 (19) | −0.0053 (16) | −0.0038 (15) | −0.0132 (17) |
| C44 | 0.037 (2) | 0.040 (2) | 0.0292 (19) | −0.0187 (18) | −0.0048 (16) | −0.0021 (16) |
| C45 | 0.045 (2) | 0.0256 (18) | 0.036 (2) | −0.0063 (16) | −0.0165 (18) | −0.0016 (15) |
| C46 | 0.0286 (19) | 0.0278 (17) | 0.0307 (19) | 0.0002 (14) | −0.0114 (15) | −0.0046 (14) |
| C51 | 0.0209 (17) | 0.0302 (17) | 0.0222 (16) | −0.0044 (14) | −0.0019 (13) | −0.0090 (14) |
| C52 | 0.033 (2) | 0.050 (2) | 0.0253 (19) | 0.0013 (18) | −0.0042 (16) | −0.0124 (17) |
| C53 | 0.042 (3) | 0.058 (3) | 0.035 (2) | 0.004 (2) | 0.0067 (19) | −0.021 (2) |
| C54 | 0.023 (2) | 0.050 (2) | 0.047 (2) | 0.0045 (17) | 0.0025 (17) | −0.019 (2) |
| C55 | 0.0247 (19) | 0.036 (2) | 0.042 (2) | 0.0003 (15) | −0.0078 (16) | −0.0120 (17) |
| C56 | 0.0204 (17) | 0.0314 (18) | 0.0274 (18) | −0.0026 (14) | −0.0020 (14) | −0.0076 (14) |
| P10 | 0.0195 (4) | 0.0224 (4) | 0.0318 (5) | −0.0031 (3) | −0.0055 (4) | −0.0006 (4) |
| F11 | 0.0470 (15) | 0.0263 (11) | 0.0493 (14) | 0.0035 (10) | −0.0139 (12) | −0.0057 (10) |
| F12 | 0.0409 (14) | 0.0265 (11) | 0.0612 (16) | 0.0034 (10) | −0.0146 (12) | −0.0085 (11) |
| F13 | 0.0283 (12) | 0.0513 (14) | 0.0342 (12) | −0.0092 (10) | 0.0001 (10) | −0.0005 (10) |
| F14 | 0.0313 (12) | 0.0439 (13) | 0.0414 (13) | −0.0072 (10) | −0.0152 (10) | −0.0065 (10) |
| F15 | 0.0304 (12) | 0.0381 (12) | 0.0483 (14) | −0.0049 (10) | −0.0179 (10) | −0.0049 (10) |
| F16 | 0.0357 (14) | 0.0526 (15) | 0.0412 (14) | −0.0110 (11) | 0.0058 (11) | −0.0023 (11) |
| P20 | 0.0336 (6) | 0.0489 (6) | 0.0426 (6) | −0.0133 (5) | −0.0027 (5) | −0.0088 (5) |
| F21 | 0.079 (2) | 0.0559 (18) | 0.070 (2) | −0.0091 (16) | 0.0168 (17) | −0.0225 (16) |
| F22 | 0.060 (2) | 0.099 (3) | 0.061 (2) | 0.0021 (18) | −0.0164 (16) | 0.0151 (18) |
| F23 | 0.0574 (18) | 0.0743 (19) | 0.0451 (16) | −0.0043 (15) | 0.0051 (13) | −0.0207 (14) |
| F24 | 0.045 (2) | 0.204 (5) | 0.070 (2) | −0.003 (2) | −0.0208 (17) | −0.031 (3) |
| F25 | 0.064 (2) | 0.102 (3) | 0.064 (2) | −0.0207 (19) | 0.0251 (17) | 0.0010 (19) |
| F26 | 0.142 (4) | 0.080 (3) | 0.194 (5) | −0.070 (3) | 0.053 (4) | −0.070 (3) |
| N200 | 0.083 (5) | 0.134 (7) | 0.256 (12) | −0.020 (5) | −0.010 (6) | −0.094 (7) |
| C201 | 0.107 (6) | 0.046 (3) | 0.090 (5) | 0.000 (4) | 0.019 (4) | −0.018 (3) |
| C202 | 0.083 (5) | 0.089 (5) | 0.125 (7) | −0.010 (4) | 0.006 (5) | −0.053 (5) |
| N300 | 0.104 (6) | 0.121 (7) | 0.088 (5) | 0.024 (5) | 0.051 (5) | 0.008 (5) |
| C301 | 0.053 (5) | 0.179 (10) | 0.059 (5) | −0.013 (5) | 0.005 (4) | −0.047 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Pd1—C31 | 2.031 (3) | C32—C33 | 1.504 (5) |
| Pd1—C1 | 2.033 (3) | C32—H32A | 0.9900 |
| Pd1—P1 | 2.3085 (9) | C32—H32B | 0.9900 |
| Pd1—P2 | 2.3100 (9) | C33—H33A | 0.9800 |
| P1—C21 | 1.806 (4) | C33—H33B | 0.9800 |
| P1—C11 | 1.811 (4) | C33—H33C | 0.9800 |
| P1—C7 | 1.848 (4) | C34—C35 | 1.344 (5) |
| P2—C51 | 1.805 (4) | C34—H34A | 0.9500 |
| P2—C41 | 1.815 (3) | C35—H35A | 0.9500 |
| P2—C37 | 1.847 (3) | C36—C37 | 1.523 (5) |
| N1—C1 | 1.347 (4) | C36—H36A | 0.9900 |
| N1—C4 | 1.387 (5) | C36—H36B | 0.9900 |
| N1—C2 | 1.467 (5) | C37—H37A | 0.9900 |
| N2—C1 | 1.347 (5) | C37—H37B | 0.9900 |
| N2—C5 | 1.379 (4) | C41—C46 | 1.383 (5) |
| N2—C6 | 1.466 (4) | C41—C42 | 1.395 (5) |
| N3—C31 | 1.348 (4) | C42—C43 | 1.391 (5) |
| N3—C34 | 1.386 (4) | C42—H42A | 0.9500 |
| N3—C32 | 1.467 (4) | C43—C44 | 1.381 (6) |
| N4—C31 | 1.347 (4) | C43—H43A | 0.9500 |
| N4—C35 | 1.387 (4) | C44—C45 | 1.389 (6) |
| N4—C36 | 1.459 (4) | C44—H44A | 0.9500 |
| C2—C3 | 1.512 (6) | C45—C46 | 1.391 (5) |
| C2—H2A | 0.9900 | C45—H45A | 0.9500 |
| C2—H2B | 0.9900 | C46—H46A | 0.9500 |
| C3—H3A | 0.9800 | C51—C56 | 1.391 (5) |
| C3—H3B | 0.9800 | C51—C52 | 1.400 (5) |
| C3—H3C | 0.9800 | C52—C53 | 1.383 (6) |
| C4—C5 | 1.339 (5) | C52—H52A | 0.9500 |
| C4—H4A | 0.9500 | C53—C54 | 1.375 (6) |
| C5—H5A | 0.9500 | C53—H53A | 0.9500 |
| C6—C7 | 1.528 (5) | C54—C55 | 1.382 (6) |
| C6—H6A | 0.9900 | C54—H54A | 0.9500 |
| C6—H6B | 0.9900 | C55—C56 | 1.397 (5) |
| C7—H7A | 0.9900 | C55—H55A | 0.9500 |
| C7—H7B | 0.9900 | C56—H56A | 0.9500 |
| C11—C12 | 1.386 (6) | P10—F16 | 1.584 (2) |
| C11—C16 | 1.392 (6) | P10—F14 | 1.595 (2) |
| C12—C13 | 1.384 (6) | P10—F12 | 1.601 (2) |
| C12—H12A | 0.9500 | P10—F13 | 1.603 (2) |
| C13—C14 | 1.362 (8) | P10—F11 | 1.603 (2) |
| C13—H13A | 0.9500 | P10—F15 | 1.605 (2) |
| C14—C15 | 1.371 (8) | P20—F26 | 1.558 (4) |
| C14—H14A | 0.9500 | P20—F22 | 1.569 (3) |
| C15—C16 | 1.396 (6) | P20—F24 | 1.577 (4) |
| C15—H15A | 0.9500 | P20—F21 | 1.583 (3) |

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|---|---|---|---|
| C16—H16A | 0.9500 | P20—F23 | 1.586 (3) |
| C21—C22 | 1.391 (5) | P20—F25 | 1.598 (3) |
| C21—C26 | 1.392 (6) | N200—C201 | 1.147 (10) |
| C22—C23 | 1.390 (6) | C201—C202 | 1.421 (11) |
| C22—H22A | 0.9500 | C202—H20A | 0.9800 |
| C23—C24 | 1.359 (8) | C202—H20B | 0.9800 |
| C23—H23A | 0.9500 | C202—H20C | 0.9800 |
| C24—C25 | 1.378 (7) | N300—C301 | 1.000 (9) |
| C24—H24A | 0.9500 | C301—C302 | 1.549 (19) |
| C25—C26 | 1.391 (6) | C302—H30A | 0.9800 |
| C25—H25A | 0.9500 | C302—H30B | 0.9800 |
| C26—H26A | 0.9500 | C302—H30C | 0.9800 |
| C31—Pd1—C1 | 173.56 (13) | C33—C32—H32B | 109.4 |
| C31—Pd1—P1 | 94.24 (9) | H32A—C32—H32B | 108.0 |
| C1—Pd1—P1 | 84.03 (10) | C32—C33—H33A | 109.5 |
| C31—Pd1—P2 | 83.54 (9) | C32—C33—H33B | 109.5 |
| C1—Pd1—P2 | 96.46 (10) | H33A—C33—H33B | 109.5 |
| P1—Pd1—P2 | 164.44 (3) | C32—C33—H33C | 109.5 |
| C21—P1—C11 | 105.73 (18) | H33A—C33—H33C | 109.5 |
| C21—P1—C7 | 105.68 (18) | H33B—C33—H33C | 109.5 |
| C11—P1—C7 | 106.11 (17) | C35—C34—N3 | 107.0 (3) |
| C21—P1—Pd1 | 117.44 (13) | C35—C34—H34A | 126.5 |
| C11—P1—Pd1 | 115.02 (12) | N3—C34—H34A | 126.5 |
| C7—P1—Pd1 | 105.96 (12) | C34—C35—N4 | 106.4 (3) |
| C51—P2—C41 | 106.27 (16) | C34—C35—H35A | 126.8 |
| C51—P2—C37 | 107.06 (17) | N4—C35—H35A | 126.8 |
| C41—P2—C37 | 105.51 (16) | N4—C36—C37 | 111.9 (3) |
| C51—P2—Pd1 | 115.17 (11) | N4—C36—H36A | 109.2 |
| C41—P2—Pd1 | 115.95 (11) | C37—C36—H36A | 109.2 |
| C37—P2—Pd1 | 106.15 (12) | N4—C36—H36B | 109.2 |
| C1—N1—C4 | 110.3 (3) | C37—C36—H36B | 109.2 |
| C1—N1—C2 | 125.6 (3) | H36A—C36—H36B | 107.9 |
| C4—N1—C2 | 124.1 (3) | C36—C37—P2 | 114.2 (2) |
| C1—N2—C5 | 110.7 (3) | C36—C37—H37A | 108.7 |
| C1—N2—C6 | 123.4 (3) | P2—C37—H37A | 108.7 |
| C5—N2—C6 | 125.8 (3) | C36—C37—H37B | 108.7 |
| C31—N3—C34 | 110.5 (3) | P2—C37—H37B | 108.7 |
| C31—N3—C32 | 125.8 (3) | H37A—C37—H37B | 107.6 |
| C34—N3—C32 | 123.5 (3) | C46—C41—C42 | 119.2 (3) |
| C31—N4—C35 | 110.9 (3) | C46—C41—P2 | 123.0 (3) |
| C31—N4—C36 | 122.6 (3) | C42—C41—P2 | 117.6 (3) |
| C35—N4—C36 | 126.5 (3) | C43—C42—C41 | 120.5 (3) |
| N1—C1—N2 | 105.3 (3) | C43—C42—H42A | 119.8 |
| N1—C1—Pd1 | 133.2 (3) | C41—C42—H42A | 119.8 |
| N2—C1—Pd1 | 121.5 (2) | C44—C43—C42 | 119.5 (4) |
| N1—C2—C3 | 111.9 (3) | C44—C43—H43A | 120.2 |
| N1—C2—H2A | 109.2 | C42—C43—H43A | 120.2 |
| C3—C2—H2A | 109.2 | C43—C44—C45 | 120.7 (4) |
| N1—C2—H2B | 109.2 | C43—C44—H44A | 119.7 |

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|---|---|---|---|
| C3—C2—H2B | 109.2 | C45—C44—H44A | 119.7 |
| H2A—C2—H2B | 107.9 | C44—C45—C46 | 119.3 (4) |
| C2—C3—H3A | 109.5 | C44—C45—H45A | 120.3 |
| C2—C3—H3B | 109.5 | C46—C45—H45A | 120.3 |
| H3A—C3—H3B | 109.5 | C41—C46—C45 | 120.8 (4) |
| C2—C3—H3C | 109.5 | C41—C46—H46A | 119.6 |
| H3A—C3—H3C | 109.5 | C45—C46—H46A | 119.6 |
| H3B—C3—H3C | 109.5 | C56—C51—C52 | 119.0 (3) |
| C5—C4—N1 | 106.9 (3) | C56—C51—P2 | 119.1 (3) |
| C5—C4—H4A | 126.6 | C52—C51—P2 | 121.9 (3) |
| N1—C4—H4A | 126.6 | C53—C52—C51 | 119.9 (4) |
| C4—C5—N2 | 106.9 (3) | C53—C52—H52A | 120.0 |
| C4—C5—H5A | 126.6 | C51—C52—H52A | 120.0 |
| N2—C5—H5A | 126.6 | C54—C53—C52 | 120.9 (4) |
| N2—C6—C7 | 112.6 (3) | C54—C53—H53A | 119.5 |
| N2—C6—H6A | 109.1 | C52—C53—H53A | 119.5 |
| C7—C6—H6A | 109.1 | C53—C54—C55 | 120.0 (4) |
| N2—C6—H6B | 109.1 | C53—C54—H54A | 120.0 |
| C7—C6—H6B | 109.1 | C55—C54—H54A | 120.0 |
| H6A—C6—H6B | 107.8 | C54—C55—C56 | 119.7 (4) |
| C6—C7—P1 | 114.3 (2) | C54—C55—H55A | 120.1 |
| C6—C7—H7A | 108.7 | C56—C55—H55A | 120.1 |
| P1—C7—H7A | 108.7 | C51—C56—C55 | 120.4 (3) |
| C6—C7—H7B | 108.7 | C51—C56—H56A | 119.8 |
| P1—C7—H7B | 108.7 | C55—C56—H56A | 119.8 |
| H7A—C7—H7B | 107.6 | F16—P10—F14 | 90.43 (14) |
| C12—C11—C16 | 119.9 (4) | F16—P10—F12 | 90.52 (14) |
| C12—C11—P1 | 121.1 (3) | F14—P10—F12 | 90.56 (13) |
| C16—C11—P1 | 118.5 (3) | F16—P10—F13 | 179.76 (15) |
| C13—C12—C11 | 119.8 (5) | F14—P10—F13 | 89.78 (13) |
| C13—C12—H12A | 120.1 | F12—P10—F13 | 89.59 (14) |
| C11—C12—H12A | 120.1 | F16—P10—F11 | 90.12 (14) |
| C14—C13—C12 | 120.4 (5) | F14—P10—F11 | 89.97 (13) |
| C14—C13—H13A | 119.8 | F12—P10—F11 | 179.17 (14) |
| C12—C13—H13A | 119.8 | F13—P10—F11 | 89.78 (14) |
| C13—C14—C15 | 120.4 (4) | F16—P10—F15 | 90.59 (14) |
| C13—C14—H14A | 119.8 | F14—P10—F15 | 178.91 (14) |
| C15—C14—H14A | 119.8 | F12—P10—F15 | 89.80 (13) |
| C14—C15—C16 | 120.5 (5) | F13—P10—F15 | 89.20 (13) |
| C14—C15—H15A | 119.8 | F11—P10—F15 | 89.66 (13) |
| C16—C15—H15A | 119.8 | F26—P20—F22 | 90.2 (3) |
| C11—C16—C15 | 118.9 (5) | F26—P20—F24 | 92.2 (3) |
| C11—C16—H16A | 120.5 | F22—P20—F24 | 177.4 (3) |
| C15—C16—H16A | 120.5 | F26—P20—F21 | 178.2 (3) |
| C22—C21—C26 | 119.7 (4) | F22—P20—F21 | 88.5 (2) |
| C22—C21—P1 | 120.1 (3) | F24—P20—F21 | 89.0 (2) |
| C26—C21—P1 | 120.2 (3) | F26—P20—F23 | 91.7 (2) |
| C23—C22—C21 | 119.9 (5) | F22—P20—F23 | 89.29 (18) |
| C23—C22—H22A | 120.1 | F24—P20—F23 | 89.78 (19) |

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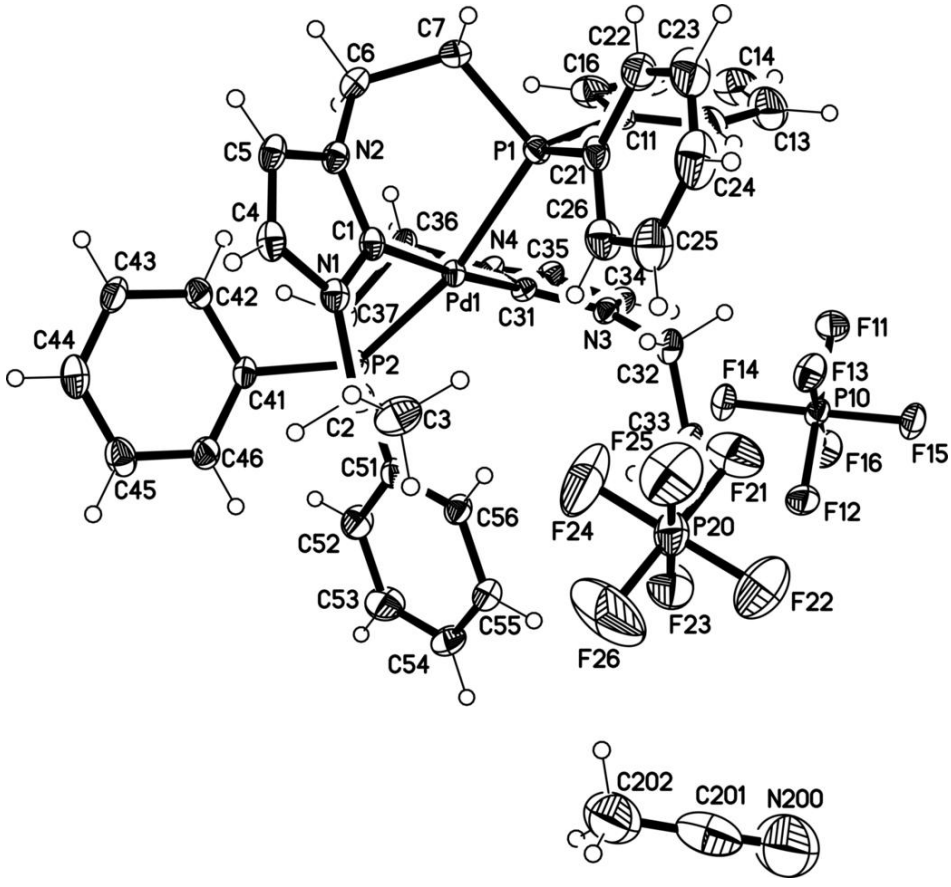
|---|---|---|---|
| C21—C22—H22A | 120.1 | F21—P20—F23 | 89.62 (17) |
| C24—C23—C22 | 119.8 (4) | F26—P20—F25 | 89.6 (2) |
| C24—C23—H23A | 120.1 | F22—P20—F25 | 91.9 (2) |
| C22—C23—H23A | 120.1 | F24—P20—F25 | 88.9 (2) |
| C23—C24—C25 | 121.4 (4) | F21—P20—F25 | 89.04 (19) |
| C23—C24—H24A | 119.3 | F23—P20—F25 | 178.2 (2) |
| C25—C24—H24A | 119.3 | N200—C201—C202 | 178.2 (9) |
| C24—C25—C26 | 119.5 (5) | C201—C202—H20A | 109.5 |
| C24—C25—H25A | 120.2 | C201—C202—H20B | 109.5 |
| C26—C25—H25A | 120.2 | H20A—C202—H20B | 109.5 |
| C25—C26—C21 | 119.6 (4) | C201—C202—H20C | 109.5 |
| C25—C26—H26A | 120.2 | H20A—C202—H20C | 109.5 |
| C21—C26—H26A | 120.2 | H20B—C202—H20C | 109.5 |
| N4—C31—N3 | 105.2 (3) | N300—C301—C302 | 175.1 (14) |
| N4—C31—Pd1 | 121.4 (2) | C301—C302—H30A | 109.5 |
| N3—C31—Pd1 | 133.0 (2) | C301—C302—H30B | 109.5 |
| N3—C32—C33 | 111.4 (3) | H30A—C302—H30B | 109.5 |
| N3—C32—H32A | 109.4 | C301—C302—H30C | 109.5 |
| C33—C32—H32A | 109.4 | H30A—C302—H30C | 109.5 |
| N3—C32—H32B | 109.4 | H30B—C302—H30C | 109.5 |
| C31—Pd1—P1—C21 | −121.77 (16) | Pd1—P1—C21—C26 | 11.0 (4) |
| C1—Pd1—P1—C21 | 64.46 (16) | C26—C21—C22—C23 | −0.6 (6) |
| P2—Pd1—P1—C21 | 157.10 (16) | P1—C21—C22—C23 | −179.7 (3) |
| C31—Pd1—P1—C11 | 3.65 (18) | C21—C22—C23—C24 | −0.6 (7) |
| C1—Pd1—P1—C11 | −170.13 (18) | C22—C23—C24—C25 | 1.4 (8) |
| P2—Pd1—P1—C11 | −77.49 (19) | C23—C24—C25—C26 | −0.9 (7) |
| C31—Pd1—P1—C7 | 120.51 (16) | C24—C25—C26—C21 | −0.3 (7) |
| C1—Pd1—P1—C7 | −53.27 (16) | C22—C21—C26—C25 | 1.0 (6) |
| P2—Pd1—P1—C7 | 39.38 (19) | P1—C21—C26—C25 | −179.9 (3) |
| C31—Pd1—P2—C51 | 67.33 (16) | C35—N4—C31—N3 | −1.1 (4) |
| C1—Pd1—P2—C51 | −119.15 (16) | C36—N4—C31—N3 | 178.9 (3) |
| P1—Pd1—P2—C51 | 149.91 (16) | C35—N4—C31—Pd1 | 173.0 (2) |
| C31—Pd1—P2—C41 | −167.71 (16) | C36—N4—C31—Pd1 | −7.0 (4) |
| C1—Pd1—P2—C41 | 5.81 (16) | C34—N3—C31—N4 | 1.2 (4) |
| P1—Pd1—P2—C41 | −85.13 (17) | C32—N3—C31—N4 | −173.9 (3) |
| C31—Pd1—P2—C37 | −50.94 (16) | C34—N3—C31—Pd1 | −171.9 (3) |
| C1—Pd1—P2—C37 | 122.58 (16) | C32—N3—C31—Pd1 | 13.0 (5) |
| P1—Pd1—P2—C37 | 31.64 (19) | P1—Pd1—C31—N4 | −107.3 (3) |
| C4—N1—C1—N2 | 1.3 (4) | P2—Pd1—C31—N4 | 57.2 (3) |
| C2—N1—C1—N2 | −179.1 (3) | P1—Pd1—C31—N3 | 64.8 (3) |
| C4—N1—C1—Pd1 | −175.5 (3) | P2—Pd1—C31—N3 | −130.6 (3) |
| C2—N1—C1—Pd1 | 4.1 (5) | C31—N3—C32—C33 | 108.9 (4) |
| C5—N2—C1—N1 | −1.3 (4) | C34—N3—C32—C33 | −65.6 (4) |
| C6—N2—C1—N1 | −178.1 (3) | C31—N3—C34—C35 | −0.8 (4) |
| C5—N2—C1—Pd1 | 175.9 (2) | C32—N3—C34—C35 | 174.4 (3) |
| C6—N2—C1—Pd1 | −0.9 (4) | N3—C34—C35—N4 | 0.1 (4) |
| P1—Pd1—C1—N1 | −130.2 (3) | C31—N4—C35—C34 | 0.6 (4) |
| P2—Pd1—C1—N1 | 65.4 (3) | C36—N4—C35—C34 | −179.4 (3) |
| P1—Pd1—C1—N2 | 53.4 (3) | C31—N4—C36—C37 | −63.7 (4) |

| | | | |
|---|---|---|---|
| P2—Pd1—C1—N2 | −110.9 (3) | C35—N4—C36—C37 | 116.4 (4) |
| C1—N1—C2—C3 | 120.2 (4) | N4—C36—C37—P2 | 52.2 (4) |
| C4—N1—C2—C3 | −60.2 (5) | C51—P2—C37—C36 | −113.4 (3) |
| C1—N1—C4—C5 | −0.8 (4) | C41—P2—C37—C36 | 133.7 (3) |
| C2—N1—C4—C5 | 179.6 (3) | Pd1—P2—C37—C36 | 10.2 (3) |
| N1—C4—C5—N2 | −0.1 (4) | C51—P2—C41—C46 | 6.3 (3) |
| C1—N2—C5—C4 | 0.9 (4) | C37—P2—C41—C46 | 119.8 (3) |
| C6—N2—C5—C4 | 177.6 (3) | Pd1—P2—C41—C46 | −123.1 (3) |
| C1—N2—C6—C7 | −65.3 (4) | C51—P2—C41—C42 | −179.2 (3) |
| C5—N2—C6—C7 | 118.4 (4) | C37—P2—C41—C42 | −65.8 (3) |
| N2—C6—C7—P1 | 46.9 (4) | Pd1—P2—C41—C42 | 51.4 (3) |
| C21—P1—C7—C6 | −109.5 (3) | C46—C41—C42—C43 | 2.8 (5) |
| C11—P1—C7—C6 | 138.5 (3) | P2—C41—C42—C43 | −171.8 (3) |
| Pd1—P1—C7—C6 | 15.8 (3) | C41—C42—C43—C44 | −1.1 (5) |
| C21—P1—C11—C12 | 20.4 (4) | C42—C43—C44—C45 | −1.2 (6) |
| C7—P1—C11—C12 | 132.4 (3) | C43—C44—C45—C46 | 1.6 (6) |
| Pd1—P1—C11—C12 | −110.9 (3) | C42—C41—C46—C45 | −2.4 (5) |
| C21—P1—C11—C16 | −167.6 (3) | P2—C41—C46—C45 | 172.0 (3) |
| C7—P1—C11—C16 | −55.7 (3) | C44—C45—C46—C41 | 0.2 (6) |
| Pd1—P1—C11—C16 | 61.1 (3) | C41—P2—C51—C56 | −107.9 (3) |
| C16—C11—C12—C13 | 0.8 (6) | C37—P2—C51—C56 | 139.7 (3) |
| P1—C11—C12—C13 | 172.6 (4) | Pd1—P2—C51—C56 | 21.9 (3) |
| C11—C12—C13—C14 | −1.8 (7) | C41—P2—C51—C52 | 69.9 (3) |
| C12—C13—C14—C15 | 1.4 (8) | C37—P2—C51—C52 | −42.5 (4) |
| C13—C14—C15—C16 | 0.0 (8) | Pd1—P2—C51—C52 | −160.2 (3) |
| C12—C11—C16—C15 | 0.6 (6) | C56—C51—C52—C53 | −0.2 (6) |
| P1—C11—C16—C15 | −171.4 (3) | P2—C51—C52—C53 | −178.1 (3) |
| C14—C15—C16—C11 | −1.0 (7) | C51—C52—C53—C54 | −0.2 (7) |
| C11—P1—C21—C22 | 60.2 (3) | C52—C53—C54—C55 | −0.1 (7) |
| C7—P1—C21—C22 | −52.0 (3) | C53—C54—C55—C56 | 0.7 (6) |
| Pd1—P1—C21—C22 | −169.9 (3) | C52—C51—C56—C55 | 0.8 (5) |
| C11—P1—C21—C26 | −118.9 (3) | P2—C51—C56—C55 | 178.8 (3) |
| C7—P1—C21—C26 | 128.9 (3) | C54—C55—C56—C51 | −1.1 (6) |

**Fig. 1**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