[1,2-Bis(diphenylphosphanyl)ethane-κ2P,P]-chlorido(isonicotinamide-κN)palladium(II) nitrate acetonitrile monosolvate

Rafael A. Adrian, Bradley J. Lageman and Hadi D. Arman

Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio TX 78209, USA, and Department of Chemistry, The University of Texas at San Antonio, San Antonio TX 78249, USA. *Correspondence e-mail: adrian@uiwtx.edu

The Pd(II) central atom in the title complex, [PdCl(C26H24P2)(C6H6N2O)]NO3·CH3CN or [PdCl(dppe)(INAM)]NO3·CH3CN, where dppe is 1,2-bis(diphenylphosphanyl)ethane and INAM is isonicotinamide, exists in a slightly distorted square-planar environment defined by the two P atoms of the dppe ligand, a chloride ligand and the N atom of the isonicotinamide pyridyl ring. The crystal packing in the structure is held together by hydrogen bonds between the amide of the INAM ligand and the nitrate ions that complete the outer coordination sphere. A molecule of acetonitrile is also found in the asymmetric unit of the title complex.

Structure description

Palladium complexes containing 1,2-bis(diphenylphosphanyl)ethane as a ligand have received much attention over the last decade because of their application in catalysis (Naghipour et al., 2021; Thapa et al., 2019). Recently, some of the focus has shifted to exploring their cytotoxicity (Cullinane et al., 2018; Kuijpers & Blom, 2021) and biological activity (Al-Janabi et al., 2021). In our research group, we have been exploring the synthesis of palladium(II) and copper(II) complexes containing various ancillary ligands and isonicotinamide as active ligand; isonicotinamide has proven to be an effective antimitabolite due to its ability to enhance Sirt1 deacetylase activity, which reduces tumor growth (Li et al., 2009). With that in mind, herein, we report the synthesis and structure of the title palladium(II) dppe complex.

The asymmetric unit of the title compound, depicted in Fig. 1, consists of a Pd(II) ion in a distorted square-planar coordination environment defined by the two phosphorus atoms...
Synthesis and crystallization

To synthesize the title compound, [1,2-bis(diphenylphosphanyl)ethane]dichloridopalladium(II) (0.100 g, 0.174 mmol) was suspended in 40 ml of acetonitrile and stirred for 15 min. Solid AgNO₃ (0.030 g, 0.18 mmol) was added to the suspension and heated with stirring at 303 K for 2 h. After removing AgCl by filtration, using a 0.45 mm PTFE syringe filter, the resulting pale yellow solution was used to grow crystals by vapor diffusion with diethyl ether at 278 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Figure 1

The structures of the molecular entities of the title compound with displacement ellipsoids drawn at the 50% probability level; H atoms are omitted for clarity.

Figure 2

Perspective view of the packing structure of the title salt along the crystallographic a-axis; H atoms are omitted for clarity.

Figure 3

Capped sticks representation of the title compound showing the hydrogen-bond interactions (pink).
Acknowledgements
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Table 3
Experimental details.

| Crystal data          | [PdCl(C8H4P2)(C6H6N2O)]NO3\(-\)C3H8N |
|-----------------------|--------------------------------------|
| Chemical formula      | [PdCl(C8H4P2)(C6H6N2O)]NO3\(-\)C3H8N |
| Mw                    | 765.43                               |
| Crystal system, space group | Orthorhombic, P2\(_1\)2\(_1\)2\(_1\) |
| Temperature (K)       | 98                                   |
| a, b, c (Å)           | 10.3343 (2), 14.8655 (4), 21.7942 (4) |
| V (Å\(^3\))           | 3348.12 (13)                         |
| Radiation type        | Mo K                                  |
| μ (mm\(^{-1}\))       | 0.77                                  |
| Crystal size (mm)     | 0.30 × 0.10 × 0.03                   |

Data collection
Diffractometer        XtaLAB AFC12 (RCD3): Kappa single
Absorption correction  Multi-scan (CrysAlis PRO; Rigaku OD, 2019)

T\(_{\text{min}}, T_{\text{max}}\) 0.909, 1.000
No. of measured, independent and observed [I > 2σ(I)] reflections 36768, 6511, 5056
R\(_{\text{int}}\) 0.054
(sin θ/λ)\(_{\text{max}}\) (Å\(^{-1}\)) 0.616

Refinement
R[F\(^2\) > 2σ(F\(^2\))], wR(F\(^2\)), S 0.027, 0.045, 0.97
No. of reflections 6511
No. of parameters 416
H-atom treatment H-atom parameters constrained
Absolute structure Flack x determined using 1879 quotients [(I\(^+\)–I\(^–\))/[(I\(^+\)+I\(^–\)] (Parsons et al., 2013)

Absolute structure parameter −0.028 (12)

Computer programs: CrysAlis PRO (Rigaku OD, 2019), olex2.solve (Bourhis et al., 2015), SHELXL2014/7 (Sheldrick, 2015), and OLEX2 (Dolomanov et al., 2009).

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full crystallographic data

*IUCrData* (2021). *IUCrData* (2021). 6, *211171*  [https://doi.org/10.1107/S2414314621011718]

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Crystal data

$[\text{PdCl(C}_{26}\text{H}_{24}\text{P}_{2})(\text{C}_{6}\text{H}_{6}\text{N}_{2}\text{O})\text{NO}_{3} \cdot \text{C}_{2}\text{H}_{3}\text{N}]$

$D_{i} = 1.518$ Mg m$^{-3}$

Orthorhombic, $P2_12_12_1$

$M_r = 765.43$

$a = 10.3343$ (2) Å

$b = 14.8655$ (4) Å

$c = 21.7942$ (4) Å

$V = 3348.12$ (13) Å$^3$

$Z = 4$

$F(000) = 1560$

Data collection

XtaLAB AFC12 (RCD3): Kappa single diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source

Mirror monochromator

$\omega$ scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2019)

$T_{\text{min}} = 0.909$, $T_{\text{max}} = 1.000$

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.045$

$S = 0.97$

6511 reflections

416 parameters

0 restraints

Primary atom site location: iterative

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 0.050P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.60$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -0.53$ e Å$^{-3}$

Absolute structure: Flack $x$ determined using 1879 quotients $[(I^+)-(I^-)]/[\langle I^+\rangle+\langle I^-\rangle]$ (Parsons et al., 2013)

Absolute structure parameter: $-0.028$ (12)

$\theta = 2.6$–$28.4^\circ$

$\mu = 0.77$ mm$^{-1}$

$T = 98$ K

Plank, clear colourless

$0.3 \times 0.1 \times 0.03$ mm

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$h = -12$–$12$

$k = -17$–$18$

$l = -21$–$26$

$R_{\text{int}} = 0.054$

$\Delta\rho_{\text{max}} = 0.60$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -0.53$ 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.

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

| Atom | x       | y       | z       | Uiso*/Ueq |
|------|---------|---------|---------|-----------|
| Pd1  | 0.67734 (2) | 0.50517 (2) | 0.74927 (2) | 0.01367 (7) |
| Cl1  | 0.68284 (10) | 0.35931 (7) | 0.79151 (5) | 0.0218 (3)  |
| P1   | 0.64267 (10) | 0.56282 (8) | 0.84262 (5) | 0.0151 (3)  |
| O1   | 0.9177 (2)   | 0.2660 (2)   | 0.49657 (13) | 0.0188 (8)  |
| N1   | 0.7138 (3)   | 0.4446 (2)   | 0.66393 (15) | 0.0130 (8)  |
| C1   | 0.6432 (4)   | 0.6856 (3)   | 0.83773 (18) | 0.0174 (10) |
| H1A  | 0.5924      | 0.7112      | 0.8720     | 0.021*      |
| H1B  | 0.7331      | 0.7082      | 0.8410     | 0.021*      |
| P2   | 0.64956 (9)  | 0.64655 (8)  | 0.71380 (5) | 0.0143 (3)  |
| O2   | 0.8163 (3)   | 0.0909 (2)   | 0.40345 (13)| 0.0285 (7)  |
| N2   | 0.7101 (3)   | 0.2228 (2)   | 0.48694 (15)| 0.0197 (9)  |
| H2C  | 0.7284      | 0.1859      | 0.4566     | 0.024*      |
| H2D  | 0.6298      | 0.2279      | 0.5000     | 0.024*      |
| C2   | 0.5844 (4)   | 0.7147 (3)   | 0.77645 (18)| 0.0168 (10) |
| H2A  | 0.6042      | 0.7790      | 0.7690     | 0.020*      |
| H2B  | 0.4892      | 0.7079      | 0.7780     | 0.020*      |
| O3   | 0.6447 (2)   | 0.1373 (2)   | 0.35577 (13)| 0.0347 (9)  |
| N3   | 0.7550 (3)   | 0.1013 (3)   | 0.35401 (17)| 0.0213 (9)  |
| C3   | 0.4854 (3)   | 0.5284 (3)   | 0.87202 (18)| 0.0172 (11) |
| O4   | 0.8039 (3)   | 0.07869 (19) | 0.30404 (13)| 0.0251 (7)  |
| N4   | 0.9979 (4)   | 0.5452 (3)   | 0.7596 (2)  | 0.0487 (12) |
| C4   | 0.4001 (3)   | 0.4843 (3)   | 0.83214 (19)| 0.0230 (11) |
| H4   | 0.4232      | 0.4750      | 0.7904     | 0.028*      |
| C5   | 0.2814 (4)   | 0.4542 (3)   | 0.8540 (2)  | 0.0298 (13) |
| H5   | 0.2219      | 0.4262      | 0.8268     | 0.036*      |
| C6   | 0.2499 (4)   | 0.4647 (3)   | 0.9147 (2)  | 0.0352 (14) |
| H6   | 0.1705      | 0.4412      | 0.9296     | 0.042*      |
| C7   | 0.3327 (4)   | 0.5092 (3)   | 0.95467 (19)| 0.0346 (12) |
| H7   | 0.3090      | 0.5180      | 0.9964     | 0.042*      |
| C8   | 0.4517 (4)   | 0.5410 (3)   | 0.9326 (2)  | 0.0266 (12) |
| H8   | 0.5093      | 0.5714      | 0.9595     | 0.032*      |
| C9   | 0.7583 (4)   | 0.5316 (3)   | 0.90152 (18)| 0.0171 (11) |
| C10  | 0.7398 (4)   | 0.4525 (3)   | 0.93414 (19)| 0.0250 (12) |
| H10  | 0.6675      | 0.4153      | 0.9252     | 0.030*      |
| C11  | 0.8265 (4)   | 0.4273 (3)   | 0.97990 (18)| 0.0276 (11) |
| H11  | 0.8116      | 0.3741      | 1.0030     | 0.033*      |
| C12  | 0.9337 (4)   | 0.4795 (3)   | 0.9917 (2)  | 0.0285 (12) |
| H12  | 0.9934      | 0.4621      | 1.0226     | 0.034*      |
| C13  | 0.9544 (4)   | 0.5575 (3)   | 0.9584 (2)  | 0.0278 (12) |
| Atom | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|------|-----|-----|-----|-----|-----|-----|
| Pd1  | 0.01207 (12) | 0.01632 (15) | 0.01261 (12) | 0.00130 (15) | 0.00071 (16) | −0.000188 (19) |
| Cl1  | 0.0249 (5) | 0.0193 (6) | 0.0211 (6) | 0.00024 (5) | 0.0007 (5) | −0.00003 (5) |
| P1   | 0.0129 (6) | 0.0181 (7) | 0.0142 (6) | −0.0010 (5) | 0.0009 (5) | −0.0010 (5) |
| O1   | 0.0074 (15) | 0.028 (2) | 0.0212 (17) | 0.0013 (13) | 0.0016 (12) | −0.00099 (15) |

**Atomic displacement parameters (Å²)**

| Atom | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|------|-----|-----|-----|-----|-----|-----|
| Pd1  | 0.01207 (12) | 0.01632 (15) | 0.01261 (12) | 0.00130 (15) | 0.00071 (16) | −0.000188 (19) |
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| O1   | 0.0074 (15) | 0.028 (2) | 0.0212 (17) | 0.0013 (13) | 0.0016 (12) | −0.00099 (15) |
### Geometric parameters (Å, °)

| Bond                  | Length (Å) | Angle (°) |
|-----------------------|------------|-----------|
| Pd1—Cl1               | 2.3564 (11) |           |
| Pd1—P1                | 2.2366 (11) |           |
| Pd1—N1                | 2.100 (3)   |           |

\[\text{data reports}\]

\[\text{IUCrData (2021). 6, x211171}\]
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|
| Pd1—P2       | 2.2577 (12)  | C13—H13      | 0.9500       |
| P1—C1        | 1.828 (4)    | C13—C14      | 1.385 (6)    |
| P1—C3        | 1.821 (4)    | C14—H14      | 0.9500       |
| P1—C9        | 1.814 (4)    | C15—C16      | 1.392 (6)    |
| O1—C32       | 1.233 (4)    | C15—C20      | 1.391 (5)    |
| N1—C27       | 1.352 (5)    | C16—H16      | 0.9500       |
| N1—C31       | 1.343 (5)    | C16—C17      | 1.394 (5)    |
| C1—H1A       | 0.9900       | C17—H17      | 0.9500       |
| C1—H1B       | 0.9900       | C17—C18      | 1.379 (6)    |
| C1—C2        | 1.530 (5)    | C18—H18      | 0.9500       |
| P2—C2        | 1.829 (4)    | C18—C19      | 1.391 (6)    |
| P2—C15       | 1.823 (4)    | C19—H19      | 0.9500       |
| P2—C21       | 1.820 (4)    | C19—C20      | 1.402 (5)    |
| O2—N3        | 1.259 (4)    | C20—H20      | 0.9500       |
| N2—H2C       | 0.8800       | C21—C22      | 1.390 (6)    |
| N2—H2D       | 0.8800       | C21—C26      | 1.401 (5)    |
| N2—C32       | 1.333 (5)    | C22—H22      | 0.9500       |
| C2—H2A       | 0.9900       | C22—C23      | 1.394 (6)    |
| C2—H2B       | 0.9900       | C23—H23      | 0.9500       |
| O3—N3        | 1.260 (4)    | C23—C24      | 1.396 (6)    |
| N3—O4        | 1.247 (4)    | C24—H24      | 0.9500       |
| C3—C4        | 1.401 (5)    | C24—C25      | 1.376 (6)    |
| C3—C8        | 1.378 (5)    | C25—H25      | 0.9500       |
| N4—C33       | 1.140 (6)    | C25—C26      | 1.383 (5)    |
| C4—H4        | 0.9500       | C26—H26      | 0.9500       |
| C4—C5        | 1.390 (5)    | C27—H27      | 0.9500       |
| C5—H5        | 0.9500       | C27—C28      | 1.373 (5)    |
| C5—C6        | 1.371 (6)    | C28—H28      | 0.9500       |
| C6—H6        | 0.9500       | C28—C29      | 1.379 (5)    |
| C6—C7        | 1.388 (6)    | C29—C30      | 1.395 (5)    |
| C7—H7        | 0.9500       | C29—C32      | 1.505 (5)    |
| C7—C8        | 1.403 (6)    | C30—H30      | 0.9500       |
| C8—H8        | 0.9500       | C30—C31      | 1.376 (5)    |
| C9—C10       | 1.387 (6)    | C31—H31      | 0.9500       |
| C9—C14       | 1.393 (5)    | C33—C34      | 1.463 (7)    |
| C10—H10      | 0.9500       | C34—H34A     | 0.9800       |
| C10—C11      | 1.391 (6)    | C34—H34B     | 0.9800       |
| C11—H11      | 0.9500       | C34—H34C     | 0.9800       |
| P1—Pd1—C11   | 90.06 (4)    | C13—C12—H12  | 120.1        |
| P1—Pd1—P2    | 86.24 (4)    | C12—C13—H13  | 119.8        |
| N1—Pd1—C11   | 86.98 (9)    | C12—C13—C14  | 120.4 (4)    |
| N1—Pd1—P1    | 176.86 (9)   | C14—C13—H13  | 119.8        |
| N1—Pd1—P2    | 96.81 (9)    | C9—C14—H14   | 120.0        |
| P2—Pd1—C11   | 173.44 (4)   | C13—C14—C9   | 120.1 (4)    |
| C1—P1—Pd1    | 109.20 (13)  | C13—C14—H14  | 120.0        |
| C3—P1—Pd1    | 110.82 (14)  | C16—C15—P2   | 121.9 (3)    |
| C3—P1—C1     | 107.71 (18)  | C20—C15—P2   | 117.1 (3)    |
| Bond              | Value   | Bond              | Value   | Bond              | Value   |
|------------------|---------|------------------|---------|------------------|---------|
| C9—P1—Pd1        | 116.11  | C20—C15—C16     | 121.0   | C15—C16—H16     | 120.6   |
| C9—P1—C1         | 107.14  | C15—C16—C17     | 118.8   | C15—C16—H16     | 120.6   |
| C9—P1—C3         | 105.48  | C16—C17—H17     | 119.6   | C15—C16—H17     | 120.6   |
| C27—N1—Pd1       | 120.0   | C17—C16—H16     | 120.6   | C17—C17—H17     | 119.6   |
| C31—N1—Pd1       | 120.1   | C18—C17—C16     | 120.8   | C17—C17—H17     | 119.6   |
| C31—N1—C27       | 118.3   | C18—C17—H18     | 119.9   | C17—C17—H18     | 119.9   |
| P1—C1—H1A        | 109.8   | C18—C17—H18     | 119.9   | C17—C18—C19     | 120.2   |
| P1—C1—H1B        | 109.8   | C18—C19—H19     | 120.1   | C18—C19—C20     | 119.7   |
| H1A—C1—H1B       | 108.2   | C18—C19—H19     | 120.1   | C18—C19—C20     | 119.7   |
| C2—C1—P1         | 109.4   | C19—C18—H18     | 119.9   | C19—C18—H19     | 120.1   |
| C2—C1—H1A        | 109.8   | C19—C18—H19     | 120.1   | C19—C18—H19     | 120.1   |
| C2—C1—H1B        | 109.8   | C19—C18—H19     | 120.1   | C19—C18—H19     | 120.1   |
| C2—P2—Pd1        | 107.89  | C20—C19—H20     | 120.3   | C20—C19—H20     | 120.3   |
| C15—P2—Pd1       | 112.25  | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C15—P2—C2        | 109.45  | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C21—P2—Pd1       | 117.25  | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C21—P2—C2        | 104.05  | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| H2C—N2—H2D       | 120.0   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C2—C1—H2A        | 109.6   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C1—C2—P2         | 110.4   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C1—C2—H2A        | 109.6   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C1—C2—H2B        | 109.6   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| P2—C2—H2A        | 109.6   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| C2—C2—H2B        | 109.6   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| H2A—C2—H2B       | 108.1   | C21—C20—C19     | 119.3   | C21—C20—C19     | 119.3   |
| O2—N3—O3         | 118.8   | C25—C24—H24     | 119.8   | C25—C24—H24     | 119.8   |
| O4—N3—O2         | 120.7   | C24—C25—H25     | 119.7   | C24—C25—H25     | 119.7   |
| O4—N3—O3         | 120.5   | C24—C25—H25     | 119.7   | C24—C25—H25     | 119.7   |
| C4—C3—P1         | 118.4   | C26—C25—H25     | 119.7   | C26—C25—H25     | 119.7   |
| C8—C3—P1         | 121.6   | C26—C25—H25     | 119.7   | C26—C25—H25     | 119.7   |
| C8—C3—C4         | 119.9   | C26—C25—H25     | 119.7   | C26—C25—H25     | 119.7   |
| C3—C4—H4         | 120.2   | C25—C24—H24     | 119.8   | C25—C24—H24     | 119.8   |
| C5—C4—C3         | 119.5   | N1—C27—H27      | 119.3   | N1—C27—H27      | 119.3   |
| C5—C4—H4         | 120.2   | N1—C27—C28      | 121.5   | N1—C27—C28      | 121.5   |
| C4—C5—H5         | 119.9   | C28—C27—H27     | 119.3   | C28—C27—H27     | 119.3   |
| C6—C5—C4         | 120.3   | C27—C28—H28     | 119.8   | C27—C28—H28     | 119.8   |
| C6—C5—H5         | 119.9   | C27—C28—H28     | 119.8   | C27—C28—H28     | 119.8   |
| C5—C6—H6         | 119.6   | C29—C28—H28     | 119.8   | C29—C28—H28     | 119.8   |
| C6—C7—C8         | 119.1   | C29—C30—C32     | 123.9   | C29—C30—C32     | 123.9   |
| C8—C7—H7         | 120.5   | C30—C29—C32     | 123.9   | C30—C29—C32     | 123.9   |
| C3—C8—C7         | 120.3   | C31—C30—C32     | 118.7   | C31—C30—C32     | 118.7   |
| C3—C8—H8         | 119.9   | C31—C30—C32     | 118.7   | C31—C30—C32     | 118.7   |
| C7—C8—H8         | 119.9   | N1—C31—H31      | 118.5   | N1—C31—H31      | 118.5   |
| Bond                  | Bond Angle (deg) | Bond Angle (deg) |
|----------------------|------------------|------------------|
| C10—C9—P1           | 119.3 (3)        | C30—C31—H31     | 118.5 |
| C10—C9—C14          | 119.1 (4)        | O1—C32—N2       | 122.4 (3) |
| C14—C9—P1           | 121.5 (3)        | O1—C32—C29      | 119.9 (4) |
| C9—C10—H10          | 119.8            | N2—C32—C29      | 117.6 (3) |
| C9—C10—C11          | 120.5 (4)        | N4—C33—C34      | 178.7 (6) |
| C11—C10—H10         | 119.8            | C33—C34—H34A    | 109.5 |
| C10—C11—H11         | 120.0            | C33—C34—H34B    | 109.5 |
| C12—C11—C10         | 120.0 (4)        | C33—C34—H34C    | 109.5 |
| C12—C11—H11         | 120.0            | H34A—C34—H34B   | 109.5 |
| C11—C12—H12         | 120.1            | H34A—C34—H34C   | 109.5 |
| C11—C12—C13         | 119.9 (4)        | H34B—C34—H34C   | 109.5 |

| Bond                  | Bond Angle (deg) |
|----------------------|------------------|
| C9—P1—C1—C2         | 34.8 (3)         |
| Pd1—P1—C1—C2        | −9.3 (4)         |
| C9—P1—C3—C4         | 167.7 (3)        |
| C9—P1—C9—C10        | −86.2 (3)        |
| C9—P1—C9—C14        | 91.1 (3)         |
| Pd1—N1—C27—C28      | 167.1 (3)        |
| Pd1—N1—C31—C30      | −166.1 (3)       |
| Pd1—P2—C2—C1        | 36.2 (3)         |
| Pd1—P2—C2—C1        | −109.9 (3)       |
| Pd1—P2—C15—C16      | 68.4 (3)         |
| Pd1—P2—C2—C1        | −147.5 (3)       |
| Pd1—P2—C2—C1        | 37.5 (4)         |
| P1—C1—C2—P2         | −45.1 (3)        |
| P1—C3—C4—C5         | 177.5 (3)        |
| P1—C3—C8—C7         | −176.4 (3)       |
| P1—C9—C10—C11       | −179.5 (3)       |
| P1—C9—C14—C13       | 180.0 (3)        |
| N1—C27—C28—C29      | −1.7 (6)         |
| C1—P1—C3—C4         | 110.1 (3)        |
| P1—C3—C4—C5         | −72.9 (4)        |
| C1—P1—C3—C8         | 151.5 (3)        |
| C1—P1—C9—C10        | −31.2 (4)        |
| C1—P1—C9—C14        | 178.1 (3)        |
| P2—C15—C16—C17      | −178.7 (3)       |
| P2—C21—C22—C23      | −175.8 (3)       |
| P2—C21—C26—C25      | 174.8 (3)        |
| C2—P2—C15—C16       | 9.9 (4)          |
| C2—P2—C15—C20       | −171.8 (3)       |
| C2—P2—C21—C22       | 93.5 (4)         |
| C2—P2—C21—C26       | −81.5 (3)        |
| C3—P1—C1—C2         | −85.6 (3)        |
| C3—P1—C9—C10        | 145.8 (3)        |
| C3—P1—C9—C14        | −2.3 (7)         |
| C3—C4—C5—C6         | 0.6 (7)          |
| C4—C3—C8—C7         | 3.2 (7)          |

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| Bond                        | Angle (°) |
|-----------------------------|-----------|
| C5—C6—C7—C8                | -2.1 (7)  |
| C6—C7—C8—C3                | 0.2 (7)   |
| C8—C3—C4—C5                | 0.5 (6)   |
| C31—N1—C27—C28             | 1.1 (6)   |
| C32—C29—C30—C31            | 178.9 (4) |

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|-------|-------|---------|
| N2—H2C···O2 | 0.88 | 2.04  | 2.891 (4) | 163     |
| N2—H2D···O1i | 0.88 | 2.19  | 3.047 (4) | 163     |
| C28—H28···O3ii | 0.95 | 2.39  | 3.082 (5) | 129     |

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