# Crystal and molecular structures of dichlorido-palladium(II) containing 2-methyl- or 2-phenyl-8-(diphenyphosphanyl)quinoline

**Masatoshi Mori,[a] Atsushi Namioka[a] and Takayoshi Suzuki[b]***

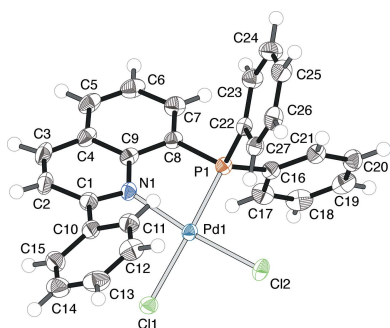[a]Graduate School of Natural Science and Technology, Okayama University, Okayama, 700-8530, Japan, and [b]Research Institute for Interdisciplinary Science, Okayama University, Okayama, 700-8530, Japan. *Correspondence e-mail: suzuki@okayama-u.ac.jp

The crystal structures of dichloridopalladium(II) complexes bearing 2-methyl- and 2-phenyl-8-(diphenylphosphanyl)quinoline, namely, dichlorido[8-(diphenylphosphanyl)-2-methylquinoline-$\kappa^2N,P$]palladium(II), [PdCl$_2$(C$_{22}$H$_{18}$NP)] (**1**) and dichlorido[8-(diphenylphosphanyl)-2-phenylquinoline-$\kappa^2N,P$]palladium(II), [PdCl$_2$(C$_{27}$H$_{20}$NP)] (**2**), were analyzed and compared to that of the 8-(diphenylphosphanyl)quinoline (PQ$^H$) analogue (**3**). In all three complexes, the phosphanylquinoline moiety acts as a bidentate $P,N$-donating chelate ligand. In the PQ$^H$ complex (**3**), the Pd$^{II}$ center has a typical planar coordination environment; however, both the methyl- and phenyl-substituted phosphanylquinoline (PQ$^{Me}$ and PQ$^{Ph}$, respectively) complexes (**1**) and (**2**) exhibit a considerable tetrahedral distortion around the Pd$^{II}$ center, as parameterized by the $\tau_4$ values of 0.1555 (4) and 0.1438 (4) for (**1**) and (**2**), respectively. The steric interaction from the substituted group introduced at the 2-position of the quinoline ring enforces the *cis*-positioned Cl ligand to be displaced from the ideal coordination plane. Also, the ideally planar phosphanylquinoline five-membered chelate ring shows a large bending deformation by the displacement of the Pd$^{II}$ center from the quinoline plane. In addition, in the phenyl-substituted complex (**3**), the coordinating quinolyl and the substituted phenyl rings are not co-planar to each other, having a dihedral angle of 33.08 (7)°. This twist conformation prohibits any intermolecular $\pi$–$\pi$ stacking interaction between the quinoline planes, which is observed in the crystals of complexes (**1**) and (**2**).

## 1. Chemical context

8-Quinolylphosphanes are competent ligands for various functional coordination compounds, because they consist of a strongly $\sigma$-donating phosphane donor group and a $\pi$-conjugated quinoline moiety and form a stable planar five-membered chelate ring on coordination to a metal center (Cai *et al.*, 2018; Hopkins *et al.*, 2019; Scattolin *et al.*, 2017). In one of our previous studies, it was revealed that 8-(diphenylphosphanyl)quinoline (PQ$^H$) in the simplest dichloridopalladium(II) complex, [PdCl$_2$(PQ$^H$)] (**3**), exhibits a strong *trans* influence of the diphenylphosphanyl donor group and an intermolecular $\pi$–$\pi$ stacking interaction between the quinoline ring systems (Suzuki *et al.*, 2015). Also, in the bis(PQ$^H$)-type Ni$^{II}$, Pd$^{II}$ and Pt$^{II}$ ($M^{II}$) complexes, [$M^{II}$(PQ$^H$)$_2$]X$_2$ ($X$ = ClO$_4$, BF$_4$ or CF$_3$SO$_3$), the *cis*(P,P)-isomers are preferably formed due to the above-mentioned *trans* influence, but the mutually *cis*-positioned quinoline groups give a steric congestion between them, causing the coordination environ-

ment around $M^{II}$ to be distorted (Suzuki, 2004; Mori *et al.*, 2020). When a methyl or phenyl group substituted at the *ortho*-position of the quinoline-N atom of $PQ^H$ is used for complexation, for example in 2-methyl-8-(diphenylphosphanyl)quinoline ($PQ^{Me}$) (**1**) or 2-phenyl-8-(diphenylphosphanyl)quinoline ($PQ^{Ph}$) (**2**), a much larger steric hindrance would be expected at the *cis*-position of the coordinating quinoline-N donor site. In the present study we reveal the characteristic structural features of the simplest $PdCl_2$ complexes bearing $PQ^{Me}$ (**1**) and $PQ^{Ph}$ (**2**) chelate ligands.
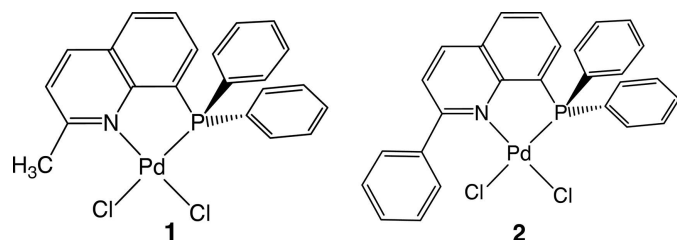
## 2. Structural commentary

In the crystals of (**1**) and (**2**), the quinolylphosphane moiety coordinates to a $Pd^{II}$ center in a bidentate $\kappa^2 P,N$ mode, and the coordination environment around the $Pd^{II}$ center is roughly square-planar with two additional chlorido ligands. The analogous $PQ^H$ complex (**3**) has a typical planar environment (Suzuki *et al.*, 2015); the $\tau_4$ value (Yang *et al.*, 2007) indicating the tetrahedral distortion around the four-coordi-

nate $Pd^{II}$ center is here only 0.0552 (4). The coordination plane (defined by the central Pd and four donor atoms) and the quinoline plane are almost co-planar, with their dihedral angle being 8.58 (3)°. The Pd1—P1 and Pd1—N1 bond lengths in the structure of (**3**) are 2.2026 (6) and 2.065 (2) Å, respectively, and the P1—Pd1—N1 chelate bite angle is 84.75 (6)°. The Pd—Cl1 (*trans* to P1) and Pd1—Cl2 (*trans* to N1) bond lengths are 2.3716 (7) and 2.2885 (8) Å, respectively, indicating a strong *trans* influence of the $Ph_2P–$ donor group.

In the $PQ^{Me}$ complex (**1**) (Fig. 1), the coordination environment around the $Pd^{II}$ center is apparently distorted; the $\tau_4$ value is 0.1555 (4). The steric requirement from the 2-methyl substituent of the coordinating quinoline group causes the Cl ligand in the *cis*-position to be pushed away (Fig. 2). Thus, the Cl1 atom is considerably displaced from the $Pd^{II}$ coordination plane (defined by Pd1, Cl2, P1 and N1) by 0.554 (1) Å, and the P1—Pd1—Cl1 bond angle is 166.74 (2)°, as compared to the N1—Pd1—Cl2 angle of 171.32 (5)°. More importantly, the $PQ^{Me}$ chelate ring is no longer planar. The Pd1 atom is displaced by 0.755 (2) Å from the chelating ligand plane (defined by P1, C8, C9 and N1), and the dihedral angle $\varphi_C$ between the plane [Pd1,P1,N1] and the quinoline plane
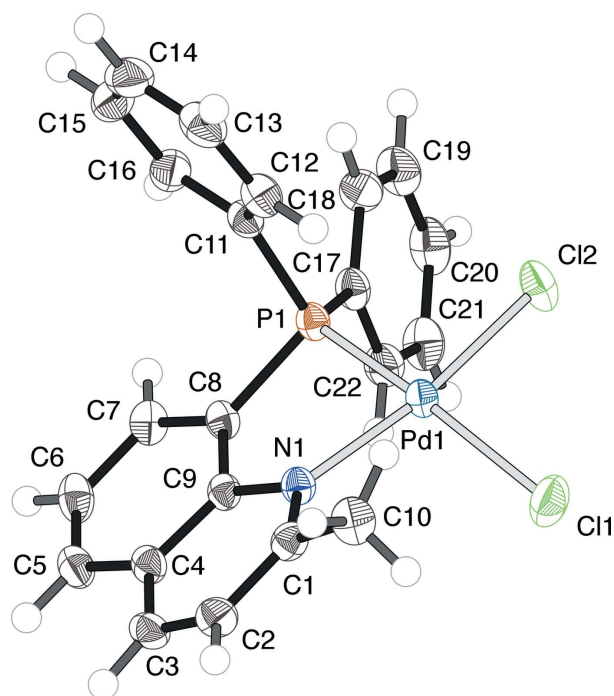


Figure 1
The molecular structure of $[PdCl_2(PQ^{Me})]$ (**1**), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.
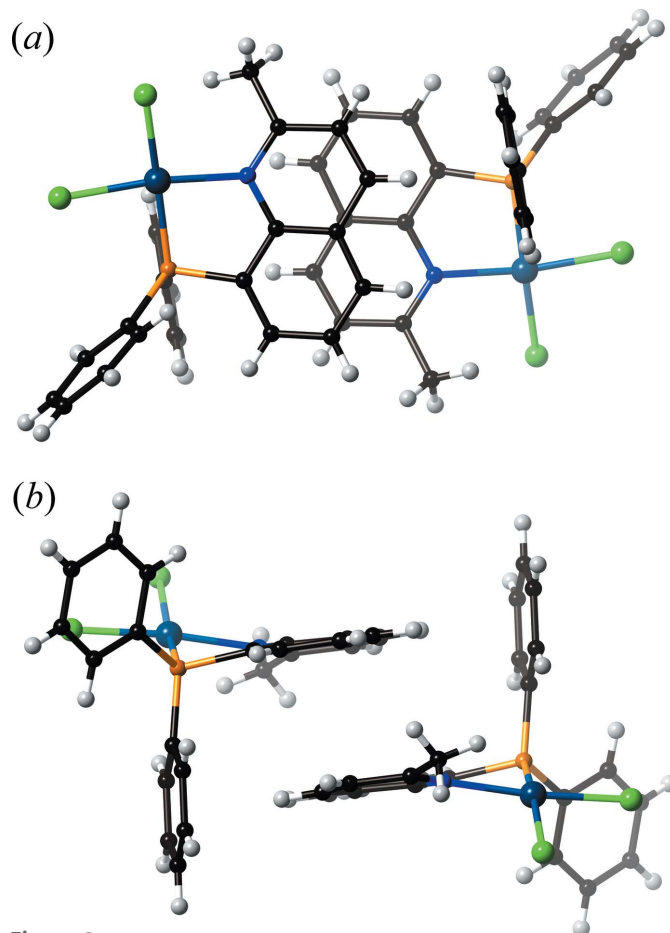


Figure 2
Perspective (*a*) top and (*b*) side views of a dimeric unit of (**1**), showing the distortion of the coordination environment around $Pd^{II}$ and the intermolecular $\pi$–$\pi$ stacking interaction between the quinoline ring systems. Color code: Pd, blueish purple; P, orange; N, blue; C, black and H, gray.

| Pd1—N1 | 2.0971 (17) | Pd1—Cl2 | 2.2823 (6) |
| Pd1—P1 | 2.1910 (5) | Pd1—Cl1 | 2.3742 (6) |
| | | | |
| N1—Pd1—P1 | 83.52 (5) | N1—Pd1—Cl1 | 98.30 (5) |
| N1—Pd1—Cl2 | 171.32 (5) | P1—Pd1—Cl1 | 166.74 (2) |
| P1—Pd1—Cl2 | 88.25 (2) | Cl2—Pd1—Cl1 | 90.34 (2) |

| Pd1—N1 | 2.0806 (15) | Pd1—Cl2 | 2.2769 (5) |
| Pd1—P1 | 2.2036 (6) | Pd1—Cl1 | 2.3738 (6) |
| | | | |
| N1—Pd1—P1 | 83.24 (5) | N1—Pd1—Cl1 | 94.56 (5) |
| N1—Pd1—Cl2 | 173.78 (5) | P1—Pd1—Cl1 | 165.930 (19) |
| P1—Pd1—Cl2 | 90.56 (2) | Cl2—Pd1—Cl1 | 91.57 (2) |

(defined by N1 and C1–C9) is 25.35 (3)°. Thus, an envelope-type deformation of the chelate ring is observed. This distortion would weaken the Pd—N bond, because the direction of the lone-pair electrons on the N atom does not match with the $Pd^{II}$ acceptor $d$-orbital. In fact, the Pd1—N1 bond length of 2.0971 (17) Å in (**1**) is slightly longer than that in (**3**). Other coordination bonds and angles are collated in Table 1 and are comparable to those in (**3**).

The $PQ^{Ph}$ complex (**2**) shows a more explicit distortion of the coordination environment on the quinolylphosphane ligand due to the 2-phenyl substitution group (Figs. 3 and 4). The $\tau_4$ value is 0.1438 (4), and the Cl1 atom is displaced from the $Pd^{II}$ coordination plane (defined by Pd1, Cl2, P1 and N1) by 0.571 (1) Å. The P1—Pd1—Cl1 and N1—Pd1—Cl2 bond angles are 165.930 (19) and 173.78 (5)°, respectively. The Pd1 atom is displaced by 0.864 (2) Å from the chelating ligand plane (defined by P1, C8, C9 and N1), and the dihedral angle $\varphi_C$ between the plane [Pd1,P1,N1] and the quinoline plane

(defined by N1 and C1–C9) is 32.56 (3)°. In addition, the substituted phenyl plane is twisted from the attached quinoline plane with a dihedral angle of 33.08 (7)°. Table 2 lists selected bond lengths and angles.

## 3. Supramolecular features

In the crystal structure, the molecular $PQ^H$ complex (**3**) forms a dimer by an intermolecular $\pi$–$\pi$ stacking interaction between the quinoline ring systems. A similar stacking interaction is observed in the crystal structure of the $PQ^{Me}$ complex (**1**) (Fig. 2). The shortest intermolecular contact distance is 3.322 (3) Å for C2$\cdots$C6$^i$ [symmetry code: (i) $-x + 1$, $-y + 1$, $-z$]. By contrast, the $PQ^{Ph}$ complex (**2**) does not show a similar stacking interaction to the above examples, because the twist motion of the attached phenyl group prohibits a full $\pi$–$\pi$ stacking interaction between the molecules (Fig. 4). The shortest intermolecular contact distance in (**2**) is 3.549 (3) Å for C2$\cdots$C3$^{ii}$ [symmetry code (ii) $-x + 1$, $-y + 2$, $-z + 1$]. There are no other obvious supramolecular features in the crystal structures of (**1**) and (**2**) (Figs. 5 and 6).

## 4. Database survey

Crystal structures of the following transition-metal complexes containing $PQ^{Me}$ or $PQ^{Ph}$ were retrieved from the Cambridge Structural Database (CSD, version 5.41, last update May 2020; Groom *et al.*, 2016): $[Cu(PQ^{Me})_2]PF_6$ (refcode NOPNOW;



**Figure 3**
The molecular structure of $[PdCl_2(PQ^{Ph})]$ (**2**), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.
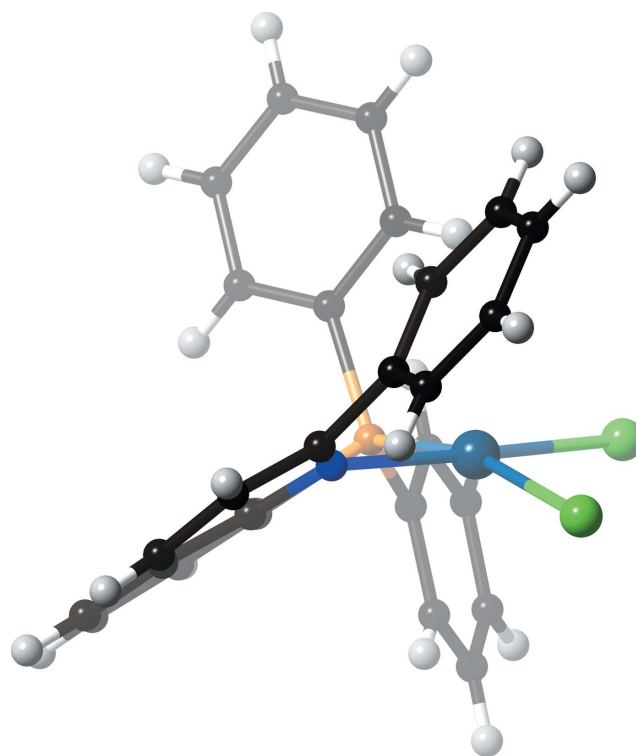


**Figure 4**
A perspective side view of (**2**), showing the distortion of the coordination environment around $Pd^{II}$. Color code: Pd, blueish purple; P, orange; N, blue; C, black and H, gray.
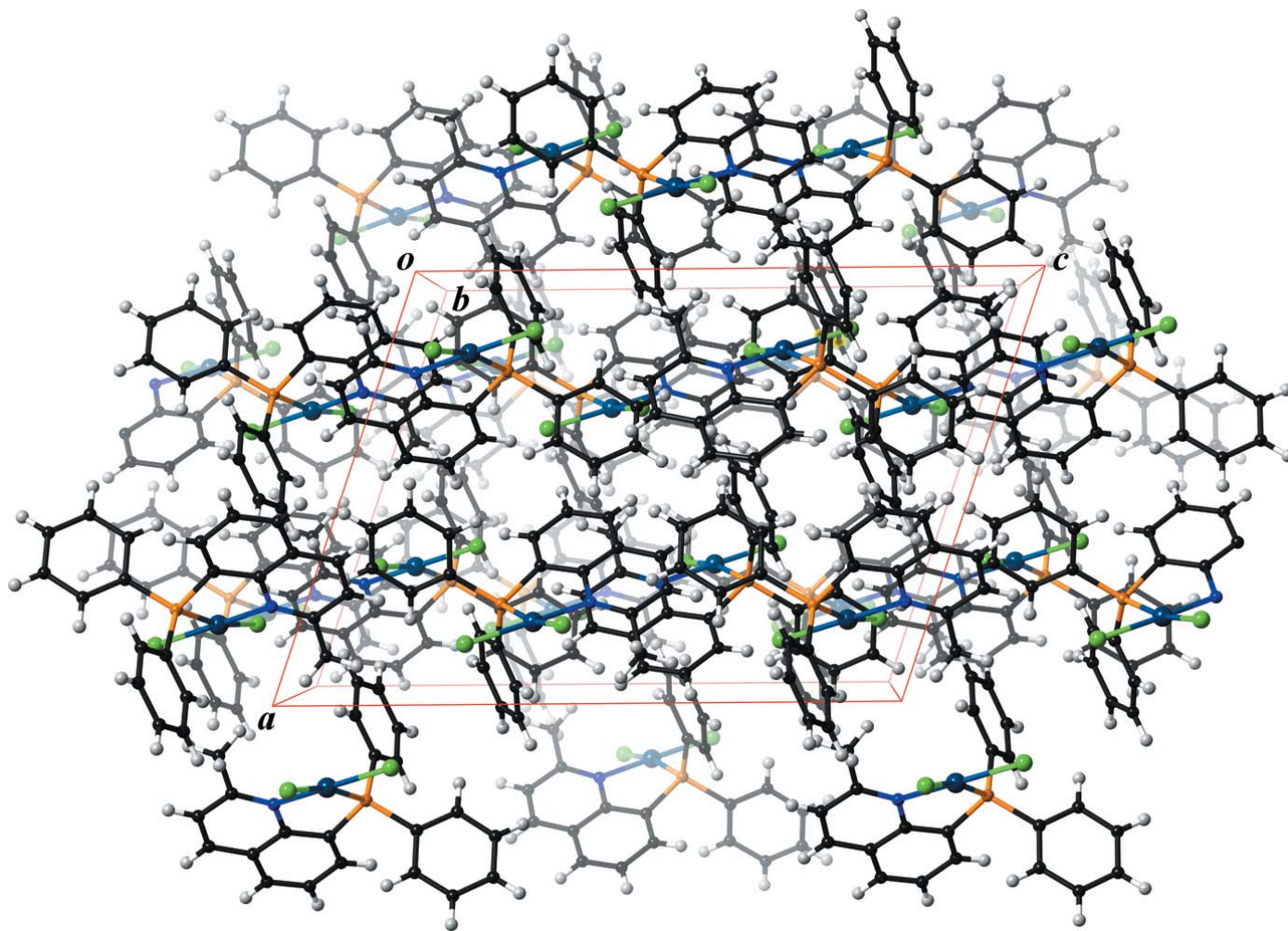
**Figure 5**
The packing of [PdCl$_2$(PQ$^{Me}$)] (**1**), viewed along the *b* axis. Color code: Pd, blueish purple; P, orange; N, blue; C, black and H, gray.
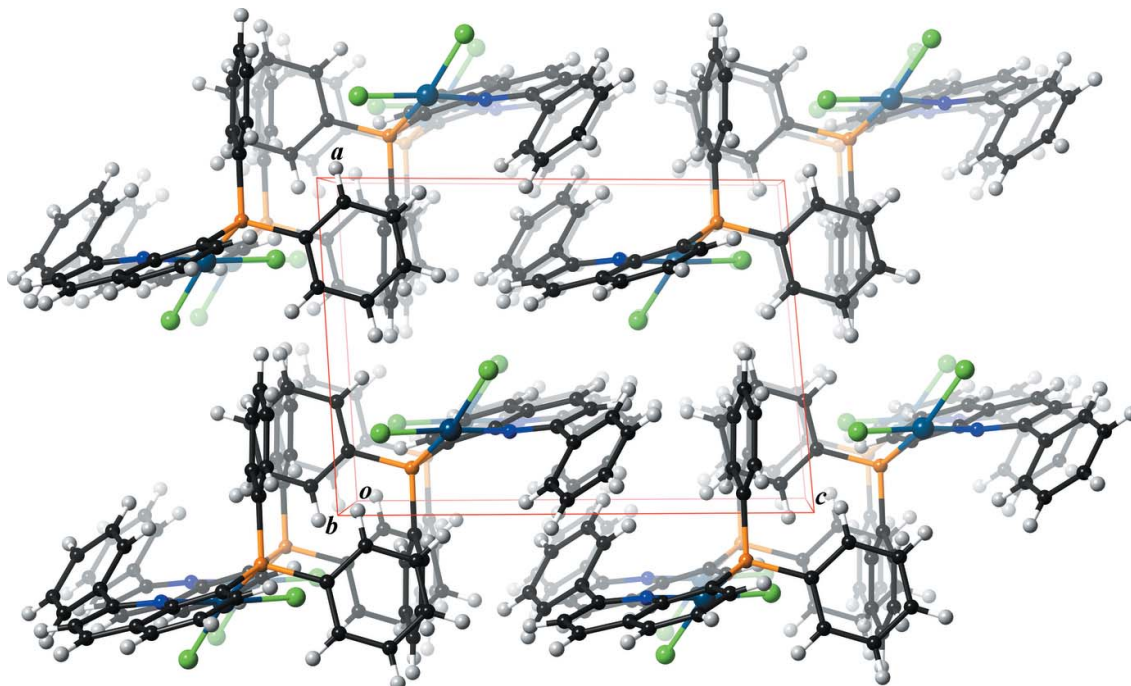


**Figure 6**
The packing of [PdCl$_2$(PQ$^{Ph}$)] (**2**), viewed along the *b* axis. Color code: Pd, blueish purple; P, orange; N, blue; C, black and H, gray.

**Table 3**
Experimental details.

| | Complex (**1**) | Complex (**2**) |
|---|---|---|
| **Crystal data** | | |
| Chemical formula | $[PdCl_2(C_{22}H_{18}NP)]$ | $[PdCl_2(C_{27}H_{20}NP)]$ |
| $M_r$ | 504.64 | 566.71 |
| Crystal system, space group | Monoclinic, $C2/c$ | Triclinic, $P\bar{1}$ |
| Temperature (K) | 188 | 188 |
| $a, b, c$ (Å) | 13.8153 (5), 15.5676 (8), 18.9683 (5) | 9.6582 (13), 9.8765 (14), 13.0748 (14) |
| $\alpha, \beta, \gamma$ (°) | 90, 108.733 (2), 90 | 102.011 (4), 90.426 (4), 109.827 (4) |
| $V$ (Å$^3$) | 3863.4 (3) | 1143.4 (3) |
| $Z$ | 8 | 2 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.33 | 1.13 |
| Crystal size (mm) | $0.50 \times 0.20 \times 0.15$ | $0.30 \times 0.20 \times 0.20$ |
| | | |
| **Data collection** | | |
| Diffractometer | Rigaku R-AXIS RAPID | Rigaku R-AXIS RAPID |
| Absorption correction | Numerical (*NUMABS*; Rigaku, 1999) | Numerical (*NUMABS*; Rigaku, 1999) |
| $T_{min}, T_{max}$ | 0.662, 0.819 | 0.640, 0.797 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 18561, 4438, 3976 | 11339, 5194, 4682 |
| $R_{int}$ | 0.039 | 0.027 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.649 | 0.649 |
| | | |
| **Refinement** | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.025, 0.063, 1.05 | 0.025, 0.064, 1.06 |
| No. of reflections | 4438 | 5192 |
| No. of parameters | 245 | 289 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{max}, \Delta\rho_{min}$ (e Å$^{-3}$) | 0.46, −0.34 | 0.74, −0.59 |

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *CrystalStructure* (Rigaku, 2010), *DIRDIF99* (Beurskens *et al.*, 1999), *Il Milione* (Burla *et al.*, 2012), *SHELXL2014/7* (Sheldrick, 2015), *CrystalMaker* (CrystalMaker, 2017), and *publCIF* (Westrip, 2010).

Tsukuda *et al.*, 2009), [Cu(PQ$^{Me}$){(Ph$_2$PC$_6$H$_4$)$_2$O}]BF$_4$·CH$_2$Cl$_2$ (OGUYEV; Qin *et al.*, 2009), [{Ni(PQ$^{Me}$)Cl}$_2$($\mu$-Cl)$_2$]·CH$_2$Cl$_2$ (MUMDAZ; Sun *et al.*, 2002), two organometallic Pd$^{II}$ complexes (BUPMIK and BUPMOQ; Canovese *et al.*, 2015). We have recently reported some Ni$^{II}$, Pd$^{II}$ and Pt$^{II}$ ($M^{II}$) complexes bearing PQ$^R$: [$M$(PQ$^R$)$_2$]$X_2$ ($X$ = Br, BF$_4$ or CF$_3$SO$_3$) (Mori *et al.*, 2020) and [Pt(ppy)(PQ$^R$)]BF$_4$ [ppy = 2-(2′-pyridyl)phenyl; Mori & Suzuki, 2020]. A related palladium(II) complex containing 2-methyl-8-(methylphenylphosphanyl)quinoline has also been reported (PUMDAD; Bock *et al.*, 2010).

## 5. Synthesis and crystallization

The ligands, PQ$^{Me}$ and PQ$^{Ph}$, were prepared according to the methods reported previously (Mori & Suzuki, 2020). Complex (**1**) was prepared as follows: under a nitrogen atmosphere, a dichloromethane solution (10 ml) of PQ$^{Me}$ (0.109 g, 0.334 mmol) was added under stirring to a dichloromethane solution (8 ml) of [PdCl$_2$(PhCN)$_2$] (PhCN = benzonitrile) (0.121 g, 0.315 mmol), and the mixture was stirred overnight at room temperature. The resulting solution was concentrated using a rotary evaporator, and diethyl ether was added under stirring to the concentrate, giving a yellow precipitate, which was collected by filtration, washed with diethyl ether (10 ml), and dried *in vacuo*. Yield: 0.142 g (92%). Analysis found: C, 51.03; H, 3.67; N, 2.99%. Calculated for C$_{22}$H$_{18}$Cl$_2$NPPd·0.7H$_2$O: C, 51.08; H, 3.78; N, 2.71%. Yellow needle-like crys-

tals of (**1**) were obtained by recrystallization from an acetonitrile solution by diffusion of diisopropyl ether.

Complex (**2**) was prepared as follows: under a nitrogen atmosphere, a dichloromethane solution (10 ml) of PQ$^{Ph}$ (0.071 g, 0.18 mmol) was added under stirring to a dichloromethane solution (10 ml) of [PdCl$_2$(PhCN)$_2$] (0.070 g, 0.18 mmol), and the mixture was stirred overnight at room temperature. The resulting brown precipitate was filtered off, and the filtrate was concentrated under reduced pressure. Diethyl ether was added under stirring to the concentrate, giving a yellow precipitate, which was collected by filtration, washed with diethyl ether (10 ml), and dried *in vacuo*. Yield: 0.041 g (40%). Analysis found: C, 56.23; H, 3.50; N, 2.56%. Calculated for C$_{27}$H$_{20}$Cl$_2$NPPd: C, 57.22; H, 3.56; N, 2.47%. Yellow block-like crystals of (**2**) were obtained by recrystallization from an acetonitrile solution by diffusion of diisopropyl ether.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 (aromatic) or 0.98 (methyl) Å and $U_{iso} = 1.2U_{eq}$(C). For the refinement of (**2**), two reflections (4$\bar{1}$1, $\bar{7}$98) were omitted because they showed a significantly lower intensity than calculated, most probably caused by obstruction from the beam stop.

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# Crystal and molecular structures of dichloridopalladium(II) containing 2-methyl- or 2-phenyl-8-(diphenyphosphanyl)quinoline

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**Computing details**

For both structures, data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku, 2010). Program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999) for complex1; *Il Milione* (Burla *et al.*, 2012) for complex2. For both structures, program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (*CrystalMaker*, 2017); software used to prepare material for publication: *publCIF* (Westrip, 2010).

**Dichlorido[8-(diphenylphosphanyl)-2-methylquinoline-$\kappa^2 N,P$]palladium(II) (complex1)**

*Crystal data*

| | |
|---|---|
| [PdCl$_2$(C$_{22}$H$_{18}$NP)] | $F(000) = 2016$ |
| $M_r = 504.64$ | $D_x = 1.735$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *Kα* radiation, $\lambda = 0.71075$ Å |
| $a = 13.8153$ (5) Å | Cell parameters from 15062 reflections |
| $b = 15.5676$ (8) Å | $\theta = 3.1$–27.6° |
| $c = 18.9683$ (5) Å | $\mu = 1.33$ mm$^{-1}$ |
| $\beta = 108.733$ (2)° | $T = 188$ K |
| $V = 3863.4$ (3) Å$^3$ | Needle, yellow |
| $Z = 8$ | $0.50 \times 0.20 \times 0.15$ mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 18561 measured reflections |
| Radiation source: fine-focus sealed tube | 4438 independent reflections |
| Detector resolution: 10.000 pixels mm$^{-1}$ | 3976 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.039$ |
| Absorption correction: numerical (NUMABS; Rigaku, 1999) | $\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$ |
| | $h = -17 \rightarrow 17$ |
| $T_{min} = 0.662$, $T_{max} = 0.819$ | $k = -20 \rightarrow 20$ |
| | $l = -23 \rightarrow 25$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.025$ | Secondary atom site location: difference Fourier map |
| $wR(F^2) = 0.063$ | |
| $S = 1.05$ | Hydrogen site location: inferred from neighbouring sites |
| 4438 reflections | |
| 245 parameters | H-atom parameters constrained |
| 0 restraints | |

$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 5.1054P]$

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

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

$\Delta\rho_{max} = 0.46$ e Å$^{-3}$

$\Delta\rho_{min} = -0.34$ 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 (Å$^2$)*

|  | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 0.18958 (2) | 0.00853 (2) | 0.12906 (2) | 0.02335 (6) |
| Cl1 | 0.18633 (5) | −0.13050 (4) | 0.07691 (4) | 0.04342 (15) |
| Cl2 | 0.14113 (5) | −0.04783 (4) | 0.22366 (3) | 0.03709 (14) |
| P1 | 0.22803 (4) | 0.12790 (3) | 0.19320 (3) | 0.02356 (11) |
| N1 | 0.23191 (12) | 0.07847 (11) | 0.04910 (9) | 0.0238 (3) |
| C1 | 0.20531 (16) | 0.06113 (14) | −0.02343 (12) | 0.0274 (4) |
| C2 | 0.26023 (17) | 0.09721 (15) | −0.06751 (12) | 0.0314 (5) |
| H2 | 0.2439 | 0.0806 | −0.1182 | 0.038* |
| C3 | 0.33556 (16) | 0.15490 (15) | −0.03855 (12) | 0.0308 (5) |
| H3 | 0.3744 | 0.1764 | −0.0679 | 0.037* |
| C4 | 0.35637 (15) | 0.18305 (14) | 0.03552 (12) | 0.0269 (4) |
| C5 | 0.42756 (16) | 0.24877 (15) | 0.06901 (13) | 0.0314 (5) |
| H5 | 0.4667 | 0.2742 | 0.0415 | 0.038* |
| C6 | 0.44088 (16) | 0.27612 (15) | 0.13956 (13) | 0.0334 (5) |
| H6 | 0.4893 | 0.3199 | 0.1610 | 0.040* |
| C7 | 0.38300 (16) | 0.23959 (14) | 0.18060 (12) | 0.0303 (5) |
| H7 | 0.3902 | 0.2604 | 0.2291 | 0.036* |
| C8 | 0.31559 (15) | 0.17359 (13) | 0.15078 (11) | 0.0249 (4) |
| C9 | 0.30212 (14) | 0.14371 (13) | 0.07806 (11) | 0.0232 (4) |
| C10 | 0.11417 (19) | 0.00666 (15) | −0.06008 (13) | 0.0354 (5) |
| H10A | 0.0587 | 0.0218 | −0.0406 | 0.042* |
| H10B | 0.1321 | −0.0540 | −0.0497 | 0.042* |
| H10C | 0.0919 | 0.0164 | −0.1140 | 0.042* |
| C11 | 0.12787 (16) | 0.20610 (14) | 0.17993 (12) | 0.0268 (4) |
| C12 | 0.03231 (17) | 0.18947 (16) | 0.12721 (13) | 0.0340 (5) |
| H12 | 0.0190 | 0.1349 | 0.1037 | 0.041* |
| C13 | −0.04303 (18) | 0.25209 (18) | 0.10918 (15) | 0.0405 (6) |
| H13 | −0.1078 | 0.2408 | 0.0733 | 0.049* |
| C14 | −0.0230 (2) | 0.33035 (18) | 0.14365 (15) | 0.0447 (6) |
| H14 | −0.0744 | 0.3735 | 0.1318 | 0.054* |
| C15 | 0.0717 (2) | 0.34742 (17) | 0.19588 (15) | 0.0425 (6) |
| H15 | 0.0843 | 0.4023 | 0.2190 | 0.051* |
| C16 | 0.14790 (18) | 0.28583 (15) | 0.21475 (13) | 0.0338 (5) |
| H16 | 0.2124 | 0.2977 | 0.2506 | 0.041* |
| C17 | 0.29830 (16) | 0.11805 (14) | 0.29131 (11) | 0.0270 (4) |
| C18 | 0.25801 (18) | 0.14295 (16) | 0.34621 (13) | 0.0349 (5) |

| | | | |
|---|---|---|---|
| H18 | 0.1928 | 0.1697 | 0.3333 | 0.042* |
| C19 | 0.3144 (2) | 0.12828 (17) | 0.42099 (13) | 0.0404 (6) |
| H19 | 0.2880 | 0.1471 | 0.4589 | 0.048* |
| C20 | 0.4061 (2) | 0.08758 (16) | 0.44024 (13) | 0.0402 (6) |
| H20 | 0.4427 | 0.0771 | 0.4912 | 0.048* |
| C21 | 0.44627 (18) | 0.06140 (16) | 0.38595 (13) | 0.0384 (5) |
| H21 | 0.5102 | 0.0325 | 0.3994 | 0.046* |
| C22 | 0.39295 (17) | 0.07739 (15) | 0.31183 (13) | 0.0325 (5) |
| H22 | 0.4213 | 0.0604 | 0.2745 | 0.039* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.02644 (9) | 0.02137 (9) | 0.02156 (9) | −0.00327 (6) | 0.00677 (6) | 0.00066 (6) |
| Cl1 | 0.0661 (4) | 0.0244 (3) | 0.0403 (3) | −0.0008 (3) | 0.0178 (3) | −0.0036 (2) |
| Cl2 | 0.0465 (3) | 0.0371 (3) | 0.0281 (3) | −0.0135 (2) | 0.0126 (2) | 0.0043 (2) |
| P1 | 0.0270 (3) | 0.0234 (3) | 0.0196 (2) | −0.0033 (2) | 0.00651 (19) | 0.00029 (19) |
| N1 | 0.0253 (8) | 0.0235 (8) | 0.0218 (8) | −0.0011 (7) | 0.0062 (6) | 0.0011 (7) |
| C1 | 0.0313 (10) | 0.0252 (10) | 0.0247 (10) | 0.0031 (8) | 0.0075 (8) | 0.0007 (8) |
| C2 | 0.0386 (12) | 0.0347 (12) | 0.0215 (10) | 0.0043 (10) | 0.0103 (9) | 0.0026 (9) |
| C3 | 0.0327 (11) | 0.0361 (12) | 0.0273 (11) | 0.0065 (9) | 0.0148 (9) | 0.0089 (9) |
| C4 | 0.0256 (10) | 0.0276 (10) | 0.0279 (11) | 0.0037 (8) | 0.0089 (8) | 0.0078 (8) |
| C5 | 0.0249 (10) | 0.0320 (11) | 0.0377 (12) | −0.0006 (9) | 0.0106 (9) | 0.0096 (9) |
| C6 | 0.0271 (10) | 0.0286 (11) | 0.0394 (13) | −0.0060 (9) | 0.0034 (9) | 0.0062 (9) |
| C7 | 0.0299 (10) | 0.0285 (11) | 0.0285 (11) | −0.0026 (9) | 0.0037 (8) | 0.0009 (9) |
| C8 | 0.0242 (10) | 0.0249 (10) | 0.0244 (10) | −0.0014 (8) | 0.0061 (8) | 0.0037 (8) |
| C9 | 0.0228 (9) | 0.0223 (9) | 0.0236 (10) | 0.0011 (8) | 0.0060 (7) | 0.0038 (8) |
| C10 | 0.0394 (13) | 0.0378 (13) | 0.0252 (12) | −0.0055 (10) | 0.0049 (9) | −0.0021 (9) |
| C11 | 0.0292 (10) | 0.0283 (10) | 0.0247 (10) | −0.0004 (8) | 0.0110 (8) | 0.0039 (8) |
| C12 | 0.0313 (11) | 0.0362 (12) | 0.0348 (12) | −0.0044 (10) | 0.0112 (9) | 0.0020 (10) |
| C13 | 0.0300 (11) | 0.0514 (16) | 0.0405 (14) | 0.0025 (11) | 0.0119 (10) | 0.0120 (12) |
| C14 | 0.0473 (14) | 0.0491 (16) | 0.0450 (15) | 0.0180 (12) | 0.0249 (12) | 0.0143 (12) |
| C15 | 0.0608 (16) | 0.0334 (13) | 0.0396 (14) | 0.0096 (12) | 0.0250 (12) | 0.0037 (11) |
| C16 | 0.0408 (12) | 0.0312 (12) | 0.0302 (12) | 0.0009 (10) | 0.0128 (9) | −0.0003 (9) |
| C17 | 0.0327 (11) | 0.0252 (10) | 0.0217 (10) | −0.0050 (8) | 0.0068 (8) | 0.0008 (8) |
| C18 | 0.0418 (13) | 0.0364 (12) | 0.0272 (11) | 0.0009 (10) | 0.0122 (9) | 0.0004 (10) |
| C19 | 0.0567 (15) | 0.0411 (14) | 0.0244 (12) | −0.0079 (12) | 0.0145 (10) | −0.0019 (10) |
| C20 | 0.0528 (15) | 0.0378 (13) | 0.0218 (11) | −0.0103 (11) | 0.0006 (10) | 0.0043 (10) |
| C21 | 0.0358 (12) | 0.0373 (13) | 0.0347 (13) | −0.0025 (10) | 0.0012 (10) | 0.0072 (10) |
| C22 | 0.0351 (11) | 0.0324 (12) | 0.0294 (12) | −0.0014 (9) | 0.0095 (9) | 0.0020 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—N1 | 2.0971 (17) | C10—H10B | 0.9800 |
| Pd1—P1 | 2.1910 (5) | C10—H10C | 0.9800 |
| Pd1—Cl2 | 2.2823 (6) | C11—C16 | 1.391 (3) |
| Pd1—Cl1 | 2.3742 (6) | C11—C12 | 1.401 (3) |
| P1—C11 | 1.799 (2) | C12—C13 | 1.386 (3) |

| | | | |
|---|---|---|---|
| P1—C8 | 1.800 (2) | C12—H12 | 0.9500 |
| P1—C17 | 1.808 (2) | C13—C14 | 1.368 (4) |
| N1—C1 | 1.333 (3) | C13—H13 | 0.9500 |
| N1—C9 | 1.390 (3) | C14—C15 | 1.390 (4) |
| C1—C2 | 1.413 (3) | C14—H14 | 0.9500 |
| C1—C10 | 1.492 (3) | C15—C16 | 1.384 (3) |
| C2—C3 | 1.351 (3) | C15—H15 | 0.9500 |
| C2—H2 | 0.9500 | C16—H16 | 0.9500 |
| C3—C4 | 1.410 (3) | C17—C18 | 1.384 (3) |
| C3—H3 | 0.9500 | C17—C22 | 1.391 (3) |
| C4—C9 | 1.406 (3) | C18—C19 | 1.401 (3) |
| C4—C5 | 1.420 (3) | C18—H18 | 0.9500 |
| C5—C6 | 1.359 (3) | C19—C20 | 1.358 (4) |
| C5—H5 | 0.9500 | C19—H19 | 0.9500 |
| C6—C7 | 1.403 (3) | C20—C21 | 1.379 (4) |
| C6—H6 | 0.9500 | C20—H20 | 0.9500 |
| C7—C8 | 1.380 (3) | C21—C22 | 1.384 (3) |
| C7—H7 | 0.9500 | C21—H21 | 0.9500 |
| C8—C9 | 1.410 (3) | C22—H22 | 0.9500 |
| C10—H10A | 0.9800 | | |
| | | | |
| N1—Pd1—P1 | 83.52 (5) | C1—C10—H10A | 109.5 |
| N1—Pd1—Cl2 | 171.32 (5) | C1—C10—H10B | 109.5 |
| P1—Pd1—Cl2 | 88.25 (2) | H10A—C10—H10B | 109.5 |
| N1—Pd1—Cl1 | 98.30 (5) | C1—C10—H10C | 109.5 |
| P1—Pd1—Cl1 | 166.74 (2) | H10A—C10—H10C | 109.5 |
| Cl2—Pd1—Cl1 | 90.34 (2) | H10B—C10—H10C | 109.5 |
| C11—P1—C8 | 105.50 (10) | C16—C11—C12 | 120.1 (2) |
| C11—P1—C17 | 109.64 (10) | C16—C11—P1 | 120.69 (17) |
| C8—P1—C17 | 106.13 (10) | C12—C11—P1 | 118.75 (17) |
| C11—P1—Pd1 | 117.25 (7) | C13—C12—C11 | 120.5 (2) |
| C8—P1—Pd1 | 99.48 (7) | C13—C12—H12 | 119.8 |
| C17—P1—Pd1 | 116.99 (7) | C11—C12—H12 | 119.8 |
| C1—N1—C9 | 118.82 (18) | C14—C13—C12 | 119.2 (2) |
| C1—N1—Pd1 | 126.37 (14) | C14—C13—H13 | 120.4 |
| C9—N1—Pd1 | 114.50 (13) | C12—C13—H13 | 120.4 |
| N1—C1—C2 | 120.5 (2) | C13—C14—C15 | 120.7 (2) |
| N1—C1—C10 | 120.52 (19) | C13—C14—H14 | 119.7 |
| C2—C1—C10 | 118.9 (2) | C15—C14—H14 | 119.7 |
| C3—C2—C1 | 120.9 (2) | C16—C15—C14 | 121.1 (2) |
| C3—C2—H2 | 119.6 | C16—C15—H15 | 119.5 |
| C1—C2—H2 | 119.6 | C14—C15—H15 | 119.5 |
| C2—C3—C4 | 119.7 (2) | C15—C16—C11 | 118.5 (2) |
| C2—C3—H3 | 120.1 | C15—C16—H16 | 120.8 |
| C4—C3—H3 | 120.1 | C11—C16—H16 | 120.8 |
| C9—C4—C3 | 117.4 (2) | C18—C17—C22 | 119.1 (2) |
| C9—C4—C5 | 118.5 (2) | C18—C17—P1 | 122.53 (17) |
| C3—C4—C5 | 124.0 (2) | C22—C17—P1 | 118.19 (16) |

| C6—C5—C4 | 121.4 (2) | C17—C18—C19 | 119.3 (2) |
| C6—C5—H5 | 119.3 | C17—C18—H18 | 120.4 |
| C4—C5—H5 | 119.3 | C19—C18—H18 | 120.4 |
| C5—C6—C7 | 119.9 (2) | C20—C19—C18 | 121.1 (2) |
| C5—C6—H6 | 120.1 | C20—C19—H19 | 119.5 |
| C7—C6—H6 | 120.1 | C18—C19—H19 | 119.5 |
| C8—C7—C6 | 120.3 (2) | C19—C20—C21 | 120.1 (2) |
| C8—C7—H7 | 119.9 | C19—C20—H20 | 119.9 |
| C6—C7—H7 | 119.9 | C21—C20—H20 | 119.9 |
| C7—C8—C9 | 120.40 (19) | C20—C21—C22 | 119.7 (2) |
| C7—C8—P1 | 124.94 (17) | C20—C21—H21 | 120.2 |
| C9—C8—P1 | 114.22 (15) | C22—C21—H21 | 120.2 |
| N1—C9—C4 | 121.63 (19) | C21—C22—C17 | 120.8 (2) |
| N1—C9—C8 | 118.93 (18) | C21—C22—H22 | 119.6 |
| C4—C9—C8 | 119.37 (19) | C17—C22—H22 | 119.6 |
| | | | |
| C9—N1—C1—C2 | 11.2 (3) | C7—C8—C9—C4 | −1.4 (3) |
| Pd1—N1—C1—C2 | −162.19 (16) | P1—C8—C9—C4 | 171.46 (15) |
| C9—N1—C1—C10 | −165.95 (19) | C8—P1—C11—C16 | −66.1 (2) |
| Pd1—N1—C1—C10 | 20.7 (3) | C17—P1—C11—C16 | 47.8 (2) |
| N1—C1—C2—C3 | −5.1 (3) | Pd1—P1—C11—C16 | −175.63 (15) |
| C10—C1—C2—C3 | 172.1 (2) | C8—P1—C11—C12 | 106.50 (18) |
| C1—C2—C3—C4 | −3.3 (3) | C17—P1—C11—C12 | −139.61 (17) |
| C2—C3—C4—C9 | 5.1 (3) | Pd1—P1—C11—C12 | −3.1 (2) |
| C2—C3—C4—C5 | −174.3 (2) | C16—C11—C12—C13 | 0.1 (3) |
| C9—C4—C5—C6 | −2.6 (3) | P1—C11—C12—C13 | −172.52 (18) |
| C3—C4—C5—C6 | 176.8 (2) | C11—C12—C13—C14 | −0.2 (4) |
| C4—C5—C6—C7 | −0.5 (3) | C12—C13—C14—C15 | 0.3 (4) |
| C5—C6—C7—C8 | 2.6 (3) | C13—C14—C15—C16 | −0.4 (4) |
| C6—C7—C8—C9 | −1.7 (3) | C14—C15—C16—C11 | 0.3 (4) |
| C6—C7—C8—P1 | −173.74 (17) | C12—C11—C16—C15 | −0.1 (3) |
| C11—P1—C8—C7 | 74.4 (2) | P1—C11—C16—C15 | 172.32 (18) |
| C17—P1—C8—C7 | −41.9 (2) | C11—P1—C17—C18 | 20.9 (2) |
| Pd1—P1—C8—C7 | −163.70 (17) | C8—P1—C17—C18 | 134.36 (19) |
| C11—P1—C8—C9 | −98.03 (17) | Pd1—P1—C17—C18 | −115.78 (18) |
| C17—P1—C8—C9 | 145.66 (15) | C11—P1—C17—C22 | −164.51 (17) |
| Pd1—P1—C8—C9 | 23.84 (16) | C8—P1—C17—C22 | −51.0 (2) |
| C1—N1—C9—C4 | −9.3 (3) | Pd1—P1—C17—C22 | 58.83 (19) |
| Pd1—N1—C9—C4 | 164.82 (15) | C22—C17—C18—C19 | 1.3 (3) |
| C1—N1—C9—C8 | 167.77 (19) | P1—C17—C18—C19 | 175.92 (18) |
| Pd1—N1—C9—C8 | −18.1 (2) | C17—C18—C19—C20 | −2.2 (4) |
| C3—C4—C9—N1 | 1.1 (3) | C18—C19—C20—C21 | 1.3 (4) |
| C5—C4—C9—N1 | −179.45 (18) | C19—C20—C21—C22 | 0.5 (4) |
| C3—C4—C9—C8 | −175.94 (19) | C20—C21—C22—C17 | −1.3 (4) |
| C5—C4—C9—C8 | 3.5 (3) | C18—C17—C22—C21 | 0.4 (3) |
| C7—C8—C9—N1 | −178.54 (19) | P1—C17—C22—C21 | −174.44 (18) |
| P1—C8—C9—N1 | −5.7 (2) | | |

**Dichlorido[8-(diphenylphosphanyl)-2-phenylquinoline-$\kappa^2N$</i.,P]palladium(II) (complex2)**

*Crystal data*

| | |
|---|---|
| [PdCl$_2$(C$_{27}$H$_{20}$NP)] | $Z = 2$ |
| $M_r = 566.71$ | $F(000) = 568$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.646$ Mg m$^{-3}$ |
| $a = 9.6582$ (13) Å | Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å |
| $b = 9.8765$ (14) Å | Cell parameters from 9246 reflections |
| $c = 13.0748$ (14) Å | $\theta = 3.0$–27.5° |
| $\alpha = 102.011$ (4)° | $\mu = 1.13$ mm$^{-1}$ |
| $\beta = 90.426$ (4)° | $T = 188$ K |
| $\gamma = 109.827$ (4)° | Block, yellow |
| $V = 1143.4$ (3) Å$^3$ | 0.30 × 0.20 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 11339 measured reflections |
| Radiation source: fine-focus sealed tube | 5194 independent reflections |
| Detector resolution: 10.000 pixels mm$^{-1}$ | 4682 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.027$ |
| Absorption correction: numerical (NUMABS; Rigaku, 1999) | $\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$ |
| | $h = -10 \rightarrow 12$ |
| | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.640$, $T_{max} = 0.797$ | $l = -16 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.025$ | H-atom parameters constrained |
| $wR(F^2) = 0.064$ | $w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.2021P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | |
| 5192 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 289 parameters | $\Delta\rho_{max} = 0.74$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.59$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 0.25082 (2) | 1.07058 (2) | 0.24836 (2) | 0.02194 (6) |
| Cl1 | 0.43029 (5) | 1.29486 (5) | 0.34148 (4) | 0.02876 (11) |
| Cl2 | 0.24428 (6) | 1.16677 (6) | 0.10529 (4) | 0.03346 (12) |
| P1 | 0.13193 (5) | 0.84625 (6) | 0.15446 (4) | 0.02330 (11) |
| N1 | 0.24296 (17) | 0.96063 (18) | 0.36894 (12) | 0.0247 (3) |
| C1 | 0.2588 (2) | 1.0232 (2) | 0.47079 (15) | 0.0286 (4) |
| C2 | 0.3092 (2) | 0.9587 (3) | 0.54451 (16) | 0.0352 (5) |
| H2 | 0.3254 | 1.0066 | 0.6168 | 0.042* |

| C3 | 0.3343 (2) | 0.8301 (3) | 0.51319 (16) | 0.0358 (5) |
|---|---|---|---|---|
| H3 | 0.3758 | 0.7927 | 0.5622 | 0.043* |
| C4 | 0.2985 (2) | 0.7512 (2) | 0.40669 (16) | 0.0307 (4) |
| C5 | 0.3080 (2) | 0.6111 (3) | 0.36724 (18) | 0.0363 (5) |
| H5 | 0.3435 | 0.5647 | 0.4130 | 0.044* |
| C6 | 0.2671 (2) | 0.5404 (3) | 0.26407 (19) | 0.0380 (5) |
| H6 | 0.2758 | 0.4465 | 0.2386 | 0.046* |
| C7 | 0.2116 (2) | 0.6075 (2) | 0.19524 (17) | 0.0332 (5) |
| H7 | 0.1802 | 0.5566 | 0.1243 | 0.040* |
| C8 | 0.2030 (2) | 0.7453 (2) | 0.23036 (15) | 0.0263 (4) |
| C9 | 0.2492 (2) | 0.8205 (2) | 0.33623 (15) | 0.0258 (4) |
| C10 | 0.2157 (2) | 1.1546 (2) | 0.50524 (15) | 0.0295 (4) |
| C11 | 0.0945 (2) | 1.1650 (2) | 0.45270 (16) | 0.0323 (4) |
| H11 | 0.0402 | 1.0879 | 0.3954 | 0.039* |
| C12 | 0.0535 (3) | 1.2877 (3) | 0.48423 (18) | 0.0404 (5) |
| H12 | −0.0279 | 1.2952 | 0.4476 | 0.049* |
| C13 | 0.1302 (3) | 1.3993 (3) | 0.56847 (19) | 0.0467 (6) |
| H13 | 0.1011 | 1.4829 | 0.5901 | 0.056* |
| C14 | 0.2493 (3) | 1.3890 (3) | 0.62121 (18) | 0.0452 (6) |
| H14 | 0.3026 | 1.4663 | 0.6788 | 0.054* |
| C15 | 0.2915 (2) | 1.2678 (3) | 0.59103 (16) | 0.0371 (5) |
| H15 | 0.3725 | 1.2609 | 0.6287 | 0.045* |
| C16 | 0.1809 (2) | 0.8010 (2) | 0.02145 (15) | 0.0259 (4) |
| C17 | 0.3276 (2) | 0.8225 (2) | 0.00430 (17) | 0.0353 (5) |
| H17 | 0.3998 | 0.8545 | 0.0622 | 0.042* |
| C18 | 0.3692 (3) | 0.7974 (3) | −0.09724 (19) | 0.0414 (5) |
| H18 | 0.4695 | 0.8110 | −0.1090 | 0.050* |
| C19 | 0.2635 (3) | 0.7524 (3) | −0.18145 (17) | 0.0399 (5) |
| H19 | 0.2919 | 0.7352 | −0.2510 | 0.048* |
| C20 | 0.1189 (3) | 0.7325 (3) | −0.16542 (16) | 0.0373 (5) |
| H20 | 0.0476 | 0.7019 | −0.2238 | 0.045* |
| C21 | 0.0756 (2) | 0.7571 (2) | −0.06359 (15) | 0.0294 (4) |
| H21 | −0.0248 | 0.7440 | −0.0524 | 0.035* |
| C22 | −0.0677 (2) | 0.7813 (2) | 0.14853 (14) | 0.0242 (4) |
| C23 | −0.1542 (2) | 0.6327 (2) | 0.12208 (16) | 0.0332 (5) |
| H23 | −0.1087 | 0.5599 | 0.1105 | 0.040* |
| C24 | −0.3069 (3) | 0.5900 (3) | 0.11247 (18) | 0.0415 (5) |
| H24 | −0.3660 | 0.4882 | 0.0948 | 0.050* |
| C25 | −0.3732 (2) | 0.6962 (3) | 0.12869 (17) | 0.0387 (5) |
| H25 | −0.4778 | 0.6668 | 0.1215 | 0.046* |
| C26 | −0.2891 (2) | 0.8431 (3) | 0.15501 (16) | 0.0343 (5) |
| H26 | −0.3355 | 0.9151 | 0.1665 | 0.041* |
| C27 | −0.1357 (2) | 0.8872 (2) | 0.16492 (15) | 0.0283 (4) |
| H27 | −0.0774 | 0.9893 | 0.1828 | 0.034* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.02264 (9) | 0.02275 (9) | 0.02375 (9) | 0.01079 (6) | 0.00033 (5) | 0.00750 (6) |
| Cl1 | 0.0271 (2) | 0.0258 (3) | 0.0334 (2) | 0.00800 (19) | −0.00090 (17) | 0.00894 (18) |
| Cl2 | 0.0398 (3) | 0.0379 (3) | 0.0305 (3) | 0.0188 (2) | −0.00031 (19) | 0.0154 (2) |
| P1 | 0.0233 (3) | 0.0241 (3) | 0.0258 (2) | 0.0119 (2) | 0.00061 (17) | 0.00659 (18) |
| N1 | 0.0238 (8) | 0.0290 (9) | 0.0236 (8) | 0.0101 (7) | 0.0007 (6) | 0.0094 (6) |
| C1 | 0.0221 (10) | 0.0328 (11) | 0.0306 (10) | 0.0069 (8) | 0.0027 (7) | 0.0108 (8) |
| C2 | 0.0312 (12) | 0.0494 (14) | 0.0277 (10) | 0.0127 (10) | 0.0002 (8) | 0.0168 (9) |
| C3 | 0.0289 (11) | 0.0514 (14) | 0.0353 (11) | 0.0155 (10) | 0.0012 (8) | 0.0247 (10) |
| C4 | 0.0226 (10) | 0.0373 (12) | 0.0399 (11) | 0.0133 (9) | 0.0051 (8) | 0.0205 (9) |
| C5 | 0.0278 (11) | 0.0397 (13) | 0.0532 (14) | 0.0174 (10) | 0.0063 (9) | 0.0265 (10) |
| C6 | 0.0337 (12) | 0.0306 (12) | 0.0593 (14) | 0.0185 (10) | 0.0079 (10) | 0.0185 (10) |
| C7 | 0.0319 (12) | 0.0304 (12) | 0.0416 (12) | 0.0156 (9) | 0.0028 (8) | 0.0098 (9) |
| C8 | 0.0243 (10) | 0.0252 (10) | 0.0333 (10) | 0.0113 (8) | 0.0026 (7) | 0.0103 (8) |
| C9 | 0.0202 (10) | 0.0280 (10) | 0.0343 (10) | 0.0110 (8) | 0.0044 (7) | 0.0137 (8) |
| C10 | 0.0280 (11) | 0.0336 (11) | 0.0256 (10) | 0.0073 (9) | 0.0067 (7) | 0.0097 (8) |
| C11 | 0.0298 (11) | 0.0328 (12) | 0.0333 (11) | 0.0096 (9) | 0.0053 (8) | 0.0074 (8) |
| C12 | 0.0358 (13) | 0.0418 (14) | 0.0495 (13) | 0.0179 (11) | 0.0133 (10) | 0.0148 (10) |
| C13 | 0.0548 (16) | 0.0330 (13) | 0.0522 (14) | 0.0156 (12) | 0.0187 (11) | 0.0083 (10) |
| C14 | 0.0531 (16) | 0.0355 (13) | 0.0358 (12) | 0.0040 (11) | 0.0104 (10) | 0.0034 (9) |
| C15 | 0.0349 (12) | 0.0411 (13) | 0.0290 (11) | 0.0055 (10) | 0.0037 (8) | 0.0073 (9) |
| C16 | 0.0278 (10) | 0.0238 (10) | 0.0289 (10) | 0.0129 (8) | 0.0035 (7) | 0.0054 (7) |
| C17 | 0.0281 (11) | 0.0368 (13) | 0.0430 (12) | 0.0150 (10) | 0.0037 (8) | 0.0067 (9) |
| C18 | 0.0336 (13) | 0.0388 (13) | 0.0566 (15) | 0.0172 (10) | 0.0203 (10) | 0.0126 (10) |
| C19 | 0.0546 (15) | 0.0323 (12) | 0.0373 (12) | 0.0196 (11) | 0.0190 (10) | 0.0091 (9) |
| C20 | 0.0477 (14) | 0.0367 (13) | 0.0286 (11) | 0.0163 (11) | 0.0048 (9) | 0.0069 (9) |
| C21 | 0.0299 (11) | 0.0307 (11) | 0.0315 (10) | 0.0141 (9) | 0.0045 (8) | 0.0090 (8) |
| C22 | 0.0236 (10) | 0.0295 (10) | 0.0225 (9) | 0.0111 (8) | 0.0028 (7) | 0.0087 (7) |
| C23 | 0.0337 (12) | 0.0301 (12) | 0.0393 (11) | 0.0147 (9) | 0.0030 (8) | 0.0091 (9) |
| C24 | 0.0353 (13) | 0.0332 (13) | 0.0512 (14) | 0.0048 (10) | 0.0013 (10) | 0.0115 (10) |
| C25 | 0.0241 (11) | 0.0519 (15) | 0.0429 (12) | 0.0123 (10) | 0.0031 (8) | 0.0184 (10) |
| C26 | 0.0321 (12) | 0.0459 (14) | 0.0342 (11) | 0.0230 (10) | 0.0043 (8) | 0.0127 (9) |
| C27 | 0.0292 (11) | 0.0300 (11) | 0.0288 (10) | 0.0132 (9) | 0.0010 (7) | 0.0085 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—N1 | 2.0806 (15) | C12—H12 | 0.9500 |
| Pd1—P1 | 2.2036 (6) | C13—C14 | 1.380 (4) |
| Pd1—Cl2 | 2.2769 (5) | C13—H13 | 0.9500 |
| Pd1—Cl1 | 2.3738 (6) | C14—C15 | 1.376 (4) |
| P1—C22 | 1.8094 (19) | C14—H14 | 0.9500 |
| P1—C16 | 1.8112 (19) | C15—H15 | 0.9500 |
| P1—C8 | 1.821 (2) | C16—C17 | 1.387 (3) |
| N1—C1 | 1.330 (2) | C16—C21 | 1.394 (3) |
| N1—C9 | 1.383 (3) | C17—C18 | 1.387 (3) |
| C1—C2 | 1.425 (3) | C17—H17 | 0.9500 |

| | | | |
|---|---|---|---|
| C1—C10 | 1.479 (3) | C18—C19 | 1.387 (3) |
| C2—C3 | 1.354 (3) | C18—H18 | 0.9500 |
| C2—H2 | 0.9500 | C19—C20 | 1.367 (3) |
| C3—C4 | 1.423 (3) | C19—H19 | 0.9500 |
| C3—H3 | 0.9500 | C20—C21 | 1.396 (3) |
| C4—C5 | 1.406 (3) | C20—H20 | 0.9500 |
| C4—C9 | 1.422 (3) | C21—H21 | 0.9500 |
| C5—C6 | 1.370 (3) | C22—C23 | 1.388 (3) |
| C5—H5 | 0.9500 | C22—C27 | 1.395 (3) |
| C6—C7 | 1.420 (3) | C23—C24 | 1.387 (3) |
| C6—H6 | 0.9500 | C23—H23 | 0.9500 |
| C7—C8 | 1.374 (3) | C24—C25 | 1.385 (3) |
| C7—H7 | 0.9500 | C24—H24 | 0.9500 |
| C8—C9 | 1.416 (3) | C25—C26 | 1.368 (3) |
| C10—C15 | 1.398 (3) | C25—H25 | 0.9500 |
| C10—C11 | 1.398 (3) | C26—C27 | 1.392 (3) |
| C11—C12 | 1.383 (3) | C26—H26 | 0.9500 |
| C11—H11 | 0.9500 | C27—H27 | 0.9500 |
| C12—C13 | 1.380 (3) | | |
| | | | |
| N1—Pd1—P1 | 83.24 (5) | C13—C12—C11 | 120.5 (2) |
| N1—Pd1—Cl2 | 173.78 (5) | C13—C12—H12 | 119.8 |
| P1—Pd1—Cl2 | 90.56 (2) | C11—C12—H12 | 119.8 |
| N1—Pd1—Cl1 | 94.56 (5) | C12—C13—C14 | 119.8 (2) |
| P1—Pd1—Cl1 | 165.930 (19) | C12—C13—H13 | 120.1 |
| Cl2—Pd1—Cl1 | 91.57 (2) | C14—C13—H13 | 120.1 |
| C22—P1—C16 | 106.75 (9) | C15—C14—C13 | 120.5 (2) |
| C22—P1—C8 | 110.11 (9) | C15—C14—H14 | 119.7 |
| C16—P1—C8 | 106.83 (9) | C13—C14—H14 | 119.7 |
| C22—P1—Pd1 | 117.05 (7) | C14—C15—C10 | 120.3 (2) |
| C16—P1—Pd1 | 117.40 (7) | C14—C15—H15 | 119.9 |
| C8—P1—Pd1 | 97.85 (7) | C10—C15—H15 | 119.9 |
| C1—N1—C9 | 119.93 (16) | C17—C16—C21 | 119.90 (18) |
| C1—N1—Pd1 | 124.98 (14) | C17—C16—P1 | 119.09 (15) |
| C9—N1—Pd1 | 113.93 (11) | C21—C16—P1 | 120.78 (15) |
| N1—C1—C2 | 119.8 (2) | C18—C17—C16 | 120.1 (2) |
| N1—C1—C10 | 118.68 (17) | C18—C17—H17 | 119.9 |
| C2—C1—C10 | 121.43 (18) | C16—C17—H17 | 119.9 |
| C3—C2—C1 | 121.03 (19) | C17—C18—C19 | 119.6 (2) |
| C3—C2—H2 | 119.5 | C17—C18—H18 | 120.2 |
| C1—C2—H2 | 119.5 | C19—C18—H18 | 120.2 |
| C2—C3—C4 | 119.82 (18) | C20—C19—C18 | 120.7 (2) |
| C2—C3—H3 | 120.1 | C20—C19—H19 | 119.7 |
| C4—C3—H3 | 120.1 | C18—C19—H19 | 119.7 |
| C5—C4—C3 | 124.78 (19) | C19—C20—C21 | 120.2 (2) |
| C5—C4—C9 | 118.47 (19) | C19—C20—H20 | 119.9 |
| C3—C4—C9 | 116.74 (19) | C21—C20—H20 | 119.9 |
| C6—C5—C4 | 121.20 (19) | C16—C21—C20 | 119.4 (2) |

| | | | |
|---|---|---|---|
| C6—C5—H5 | 119.4 | C16—C21—H21 | 120.3 |
| C4—C5—H5 | 119.4 | C20—C21—H21 | 120.3 |
| C5—C6—C7 | 120.0 (2) | C23—C22—C27 | 119.44 (19) |
| C5—C6—H6 | 120.0 | C23—C22—P1 | 122.85 (16) |
| C7—C6—H6 | 120.0 | C27—C22—P1 | 117.58 (15) |
| C8—C7—C6 | 120.6 (2) | C24—C23—C22 | 120.2 (2) |
| C8—C7—H7 | 119.7 | C24—C23—H23 | 119.9 |
| C6—C7—H7 | 119.7 | C22—C23—H23 | 119.9 |
| C7—C8—C9 | 119.58 (17) | C25—C24—C23 | 119.9 (2) |
| C7—C8—P1 | 126.59 (15) | C25—C24—H24 | 120.1 |
| C9—C8—P1 | 113.81 (14) | C23—C24—H24 | 120.1 |
| N1—C9—C8 | 118.45 (16) | C26—C25—C24 | 120.5 (2) |
| N1—C9—C4 | 121.43 (17) | C26—C25—H25 | 119.8 |
| C8—C9—C4 | 120.11 (18) | C24—C25—H25 | 119.8 |
| C15—C10—C11 | 118.9 (2) | C25—C26—C27 | 120.2 (2) |
| C15—C10—C1 | 121.50 (19) | C25—C26—H26 | 119.9 |
| C11—C10—C1 | 119.55 (18) | C27—C26—H26 | 119.9 |
| C12—C11—C10 | 120.0 (2) | C26—C27—C22 | 119.9 (2) |
| C12—C11—H11 | 120.0 | C26—C27—H27 | 120.1 |
| C10—C11—H11 | 120.0 | C22—C27—H27 | 120.1 |
| | | | |
| C9—N1—C1—C2 | 11.7 (3) | C15—C10—C11—C12 | 1.6 (3) |
| Pd1—N1—C1—C2 | −155.23 (15) | C1—C10—C11—C12 | −179.87 (19) |
| C9—N1—C1—C10 | −165.13 (17) | C10—C11—C12—C13 | −1.0 (3) |
| Pd1—N1—C1—C10 | 28.0 (2) | C11—C12—C13—C14 | 0.5 (4) |
| N1—C1—C2—C3 | −3.4 (3) | C12—C13—C14—C15 | −0.6 (4) |
| C10—C1—C2—C3 | 173.3 (2) | C13—C14—C15—C10 | 1.2 (3) |
| C1—C2—C3—C4 | −5.3 (3) | C11—C10—C15—C14 | −1.7 (3) |
| C2—C3—C4—C5 | −174.4 (2) | C1—C10—C15—C14 | 179.83 (19) |
| C2—C3—C4—C9 | 5.5 (3) | C22—P1—C16—C17 | −172.40 (17) |
| C3—C4—C5—C6 | 178.0 (2) | C8—P1—C16—C17 | −54.62 (19) |
| C9—C4—C5—C6 | −1.8 (3) | Pd1—P1—C16—C17 | 53.89 (19) |
| C4—C5—C6—C7 | −1.0 (3) | C22—P1—C16—C21 | 13.03 (19) |
| C5—C6—C7—C8 | 2.1 (3) | C8—P1—C16—C21 | 130.82 (17) |
| C6—C7—C8—C9 | −0.3 (3) | Pd1—P1—C16—C21 | −120.67 (16) |
| C6—C7—C8—P1 | −178.71 (17) | C21—C16—C17—C18 | −1.4 (3) |
| C22—P1—C8—C7 | 80.9 (2) | P1—C16—C17—C18 | −175.99 (17) |
| C16—P1—C8—C7 | −34.6 (2) | C16—C17—C18—C19 | 0.8 (3) |
| Pd1—P1—C8—C7 | −156.42 (18) | C17—C18—C19—C20 | 0.0 (4) |
| C22—P1—C8—C9 | −97.56 (16) | C18—C19—C20—C21 | −0.1 (4) |
| C16—P1—C8—C9 | 146.89 (14) | C17—C16—C21—C20 | 1.2 (3) |
| Pd1—P1—C8—C9 | 25.08 (15) | P1—C16—C21—C20 | 175.74 (16) |
| C1—N1—C9—C8 | 167.48 (18) | C19—C20—C21—C16 | −0.5 (3) |
| Pd1—N1—C9—C8 | −24.2 (2) | C16—P1—C22—C23 | 66.97 (18) |
| C1—N1—C9—C4 | −11.5 (3) | C8—P1—C22—C23 | −48.63 (19) |
| Pd1—N1—C9—C4 | 156.78 (15) | Pd1—P1—C22—C23 | −159.13 (14) |
| C7—C8—C9—N1 | 178.38 (19) | C16—P1—C22—C27 | −108.83 (15) |
| P1—C8—C9—N1 | −3.0 (2) | C8—P1—C22—C27 | 135.57 (15) |

| | | | |
|---|---|---|---|
| C7—C8—C9—C4 | −2.6 (3) | Pd1—P1—C22—C27 | 25.07 (16) |
| P1—C8—C9—C4 | 176.01 (15) | C27—C22—C23—C24 | −0.2 (3) |
| C5—C4—C9—N1 | −177.37 (18) | P1—C22—C23—C24 | −175.97 (16) |
| C3—C4—C9—N1 | 2.8 (3) | C22—C23—C24—C25 | 0.4 (3) |
| C5—C4—C9—C8 | 3.7 (3) | C23—C24—C25—C26 | −0.5 (3) |
| C3—C4—C9—C8 | −176.20 (18) | C24—C25—C26—C27 | 0.5 (3) |
| N1—C1—C10—C15 | −146.2 (2) | C25—C26—C27—C22 | −0.3 (3) |
| C2—C1—C10—C15 | 37.0 (3) | C23—C22—C27—C26 | 0.2 (3) |
| N1—C1—C10—C11 | 35.3 (3) | P1—C22—C27—C26 | 176.17 (15) |
| C2—C1—C10—C11 | −141.5 (2) | | |