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# Comparison of molecular structures of *cis*-bis[8-(dimethylphosphanyl)quinoline]nickel(II) and -platinum(II) complex cations

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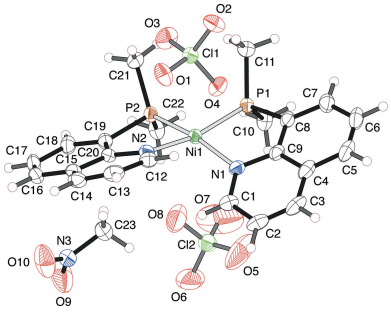
**CCDC references**: 2041421; 2041420

**Supporting information**: this article has supporting information at journals.iucr.org/e

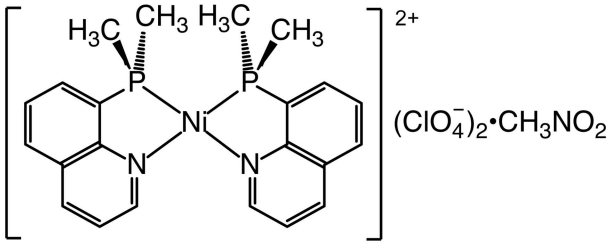
The crystal structures of the complexes (*SP*-4-2)-*cis*-bis[8-(dimethylphosphanyl)quinoline-$\kappa^2N,P$]nickel(II) bis(perchlorate) nitromethane monosolvate, $[Ni(C_{11}H_{12}NP)_2](ClO_4)_2\cdot CH_3NO_2$ (**1**), and (*SP*-4-2)-*cis*-bis[8-(dimethylphosphanyl)quinoline-$\kappa^2N,P$]platinum(II) bis(tetrafluoroborate) acetonitrile monosolvate, $[Pt(C_{11}H_{12}NP)_2](BF_4)_2\cdot C_2H_3N$ (**2**), are reported. In both complex cations, two phosphanylquinolines act as bidentate *P,N*-donating chelate ligands and form the mutually *cis* configuration in the square-planar coordination geometry. The strong *trans* influence of the dimethylphosphanyl donor group is confirmed by the Ni—N bond lengths in **1**, 1.970 (2) and 1.982 (2) Å and, the Pt—N bond lengths of **2**, 2.123 (4) and 2.132 (4) Å, which are relatively long as compared to those in the analogous 8-(diphenylphosphanyl)quinoline complexes. Mutually *cis*-positioned quinoline donor groups would give a severe steric hindrance between their *ortho*-H atoms. In order to reduce such a steric congestion, the $Ni^{II}$ complex in **1** shows a tetrahedral distortion of the coordination geometry, as parameterized by $\tau_4$ = 0.199 (1)°, while the $Pt^{II}$ complex in **2** exhibits a typical square-planar coordination geometry [$\tau_4$ = 0.014 (1)°] with a large bending deformation of the ideally planar $Me_2$Pqn chelate planes. In the crystal structure of **2**, three F atoms of one of the $BF_4^-$ anions are disordered over two sets of positions with refined occupancies of 0.573 (10) and 0.427 (10).

## 1. Chemical context

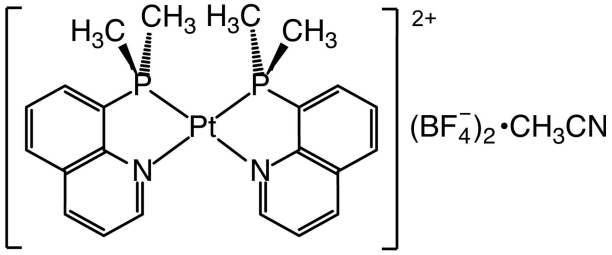
8-Quinolylphosphanes are an intriguing class of ligands because they form a planar asymmetrical five-membered chelate ring *via* coordination through a phosphane-P atom having a strong $\sigma$-donating character and an imine-N atom incorporated in a $\pi$-conjugated quinoline ring (Salem & Wild, 1992; Scattolin *et al.*, 2017; Cai *et al.*, 2018). The electronic properties of these ligands, in particular their $\pi$-bonding nature, may stabilize unusual electronic states of their transition-metal complexes (Suzuki *et al.*, 1995; Hashimoto *et al.*, 2010; Hopkins *et al.*, 2019). In addition, the steric requirement from the planar quinoline moiety often has a significant influence on the properties of their metal complexes. For example, the nickel(II), palladium(II) and platinum(II) complexes containing two 8-(diphenylphosphanyl)quinoline ($Ph_2$Pqn) in the *cis(P,P)* configuration exhibit a severe distortion of the square-planar coordination geometry around $M^{II}$ (*M* = Ni, Pd or Pt; Suzuki, 2004; Hashimoto *et al.*, 2010; Mori *et al.*, 2020). The dimethylphosphanyl analogue, 8-(dimethylphosphanyl)quinoline ($Me_2$Pqn), is an interesting derivative, because it would give a stronger *trans* influence,



which could affect the steric congestion between the intramolecular ligands. However, the transition-metal complexes bearing $Me_2Pqn$ are limited to only those listed in section 4: *Database survey*, all of which were reported by our group. In 1995 we reported the preparation and crystal structure of (*SP*-4-2)-$[Pd(Me_2Pqn)_2](BF_4)_2$ (Suzuki *et al.*, 1995), but the crystal structures of the corresponding $Ni^{II}$ and $Pt^{II}$ complexes were not compared.




**1**




**2**

## 2. Structural commentary

A red block-shaped crystal of the $Ni^{II}$ complex, $[Ni(Me_2Pqn)_2](ClO_4)_2{\cdot}CH_3NO_2$ (**1**), recrystallized from nitromethane/diisopropyl ether and a colorless platelet crystal of the $Pt^{II}$ complex, $[Pt(Me_2Pqn)_2](BF_4)_2{\cdot}CH_3CN$ (**2**), recrystallized from acetonitrile/diisopropyl ether were used for the X-ray diffraction analysis.

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

| | | | |
|---|---|---|---|
| Ni1—N1 | 1.970 (2) | Ni1—P2 | 2.1534 (7) |
| Ni1—N2 | 1.982 (2) | Ni1—P1 | 2.1576 (7) |
| N1—Ni1—N2 | 97.01 (9) | N1—Ni1—P1 | 86.13 (7) |
| N1—Ni1—P2 | 166.27 (7) | N2—Ni1—P1 | 165.68 (6) |
| N2—Ni1—P2 | 85.97 (6) | P2—Ni1—P1 | 94.29 (3) |
| Ni1—P1—C8—C9 | 14.54 (19) | Ni1—P2—C19—C20 | 18.86 (19) |
| Ni1—N1—C9—C8 | −11.8 (3) | Ni1—N2—C20—C19 | −9.7 (3) |

**Table 2**
Selected geometric parameters (Å, °) for **2**.

| | | | |
|---|---|---|---|
| Pt1—N1 | 2.123 (4) | Pt1—P2 | 2.2293 (12) |
| Pt1—N2 | 2.132 (4) | Pt1—P1 | 2.2365 (12) |
| N1—Pt1—N2 | 97.13 (15) | N1—Pt1—P1 | 82.76 (11) |
| N1—Pt1—P2 | 178.51 (11) | N2—Pt1—P1 | 179.55 (11) |
| N2—Pt1—P2 | 81.93 (11) | P2—Pt1—P1 | 98.17 (4) |
| Pt1—P1—C8—C9 | 15.5 (3) | Pt1—P2—C19—C20 | 21.2 (4) |
| Pt1—N1—C9—C8 | −18.9 (5) | Pt1—N2—C20—C19 | −19.0 (5) |

In the crystal structure of **2**, three F atoms of one of the $BF_4^-$ anions show disorder over two sets of positions: (F2*A*, F3*A* and F4*A*) and (F2*B*, F3*B* and F4*B*). The occupancy parameters of these atoms were refined with suitable restrictions and found to be 0.573 (10) and 0.427 (10) for the *A*-set atoms and the *B*-set atoms, respectively.

In both crystals, two $Me_2Pqn$ ligands coordinate to a metal(II) center in the bidentate $\kappa^2P,N$ mode to form a *cis*-isomer of the complex dication, (*SP*-4-2)-$[M(Me_2Pqn)_2]^{2+}$ (*M*

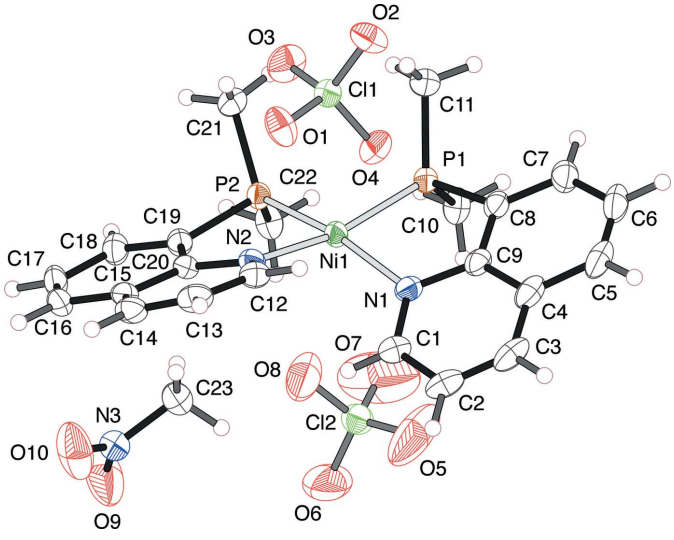



**Figure 1**
An ellipsoid plot of the molecular structures in $[Ni(Me_2Pqn)_2](ClO_4)_2{\cdot}CH_3NO_2$ (**1**), showing the atom-numbering scheme, with ellipsoids drawn at the 50% probability level.

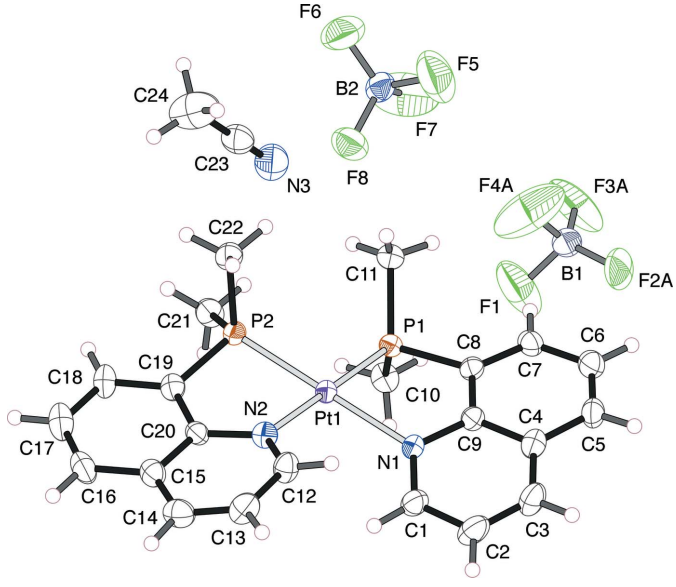



**Figure 2**
An ellipsoid plot of the molecular structures in $[Pt(Me_2Pqn)_2](BF_4)_2{\cdot}CH_3CN$ (**2**), showing the atom-numbering scheme, with ellipsoids drawn at the 50% probability level. The minor component atoms (F2*B*, F3*B* and F4*B*) of the positionally disordered F atoms are omitted for clarity.

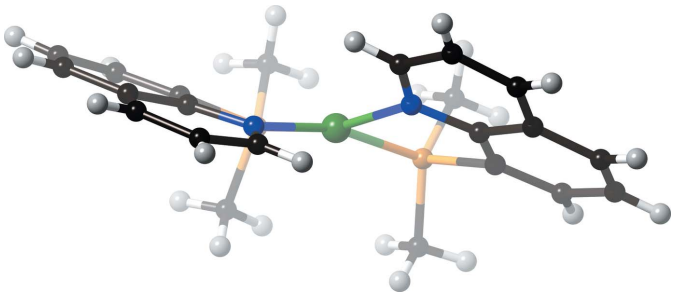


**Figure 3**
A perspective side view (from one of the NiPN coordination planes) of $[Ni(Me_2Pqn)_2](ClO_4)_2{\cdot}CH_3NO_2$ (**1**). Color code: Ni, dark green; P, orange; N, blue; C, black and H, gray.

= Ni or Pt), having a roughly square-planar coordination geometry (Figs. 1 and 2, Tables 1 and 2). For the group 10 metal(II) complexes bearing 8-quinolylphosphanes, it was revealed that most of the bis($\kappa^2P,N$)-type complexes have a similar geometrical structure, except for those of the halide complexes (Suzuki, 2004; Mori *et al.*, 2020), because the strong *trans* influence of the phosphane donor groups makes the mutually *trans(P,P)* configuration thermodynamically unstable. The Ni—N bond lengths in **1** are 1.970 (2) and 1.982 (2) Å, which are slightly longer than those in $[Ni(MePhPqn)_2](BF_4)_2$ [MePhPqn = 8-(methylphenylphosphanyl)quinoline; 1.954 (3) and 1.977 (3) Å] and $[Ni(Ph_2Pqn)_2](BF_4)_2$ [1.954 (6) and 1.949 (5) Å] (Hashimoto *et al.*, 2010), indicating the *trans* influence becomes stronger in the order of $Ph_2Pqn$ < MePhPqn < $Me_2Pqn$. In the case of $Pt^{II}$ complexes, the Pt—N bond lengths in **2** [2.123 (4) and 2.132 (4) Å] are similarly long, as compared to those in $[Pt(Ph_2Pqn)_2](ClO_4)_2$ [2.107 (4) and 2.108 (5) Å; Mori *et al.*, 2020]. By contrast, the Ni—P bond lengths and the P—Ni—N chelate bite angles are comparable among the complexes **1** [2.1576 (7) and 2.1534 (7) Å; 86.13 (7) and 85.97 (6)°], $[Ni(MePhPqn)_2](BF_4)_2$ [2.151 (1) and 2.162 (1) Å; 87.4 (1) and 86.6 (1)°] and $[Ni(Ph_2Pqn)_2](BF_4)_2$ [2.168 (2) and 2.177 (2) Å; 86.6 (1) and 84.6 (1)°]. The Pt—P bond lengths and the P—Pt—N bite angles in **2** [2.2293 (12) and 2.2365 (12) Å; 82.76 (11) and 81.93 (11)°] are also comparable to those in $[Pt(Ph_2Pqn)_2](ClO_4)_2$ [2.2311 (14) and 2.2318 (14) Å; 83.29 (13) and 82.79 (13)°].

Comparison of the $Ni^{II}$ complex cation in **1** and the corresponding $Pt^{II}$ complex cation in **2** shows an obvious

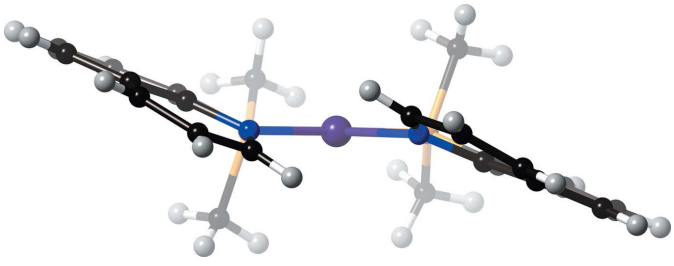


**Figure 4**
A perspective side view (from one of the PtPN coordination planes) of $[Pt(Me_2Pqn)_2](BF_4)_2{\cdot}CH_3CN$ (**2**). Color code: Pt, purple; P, orange; N, blue; C, black and H, gray.

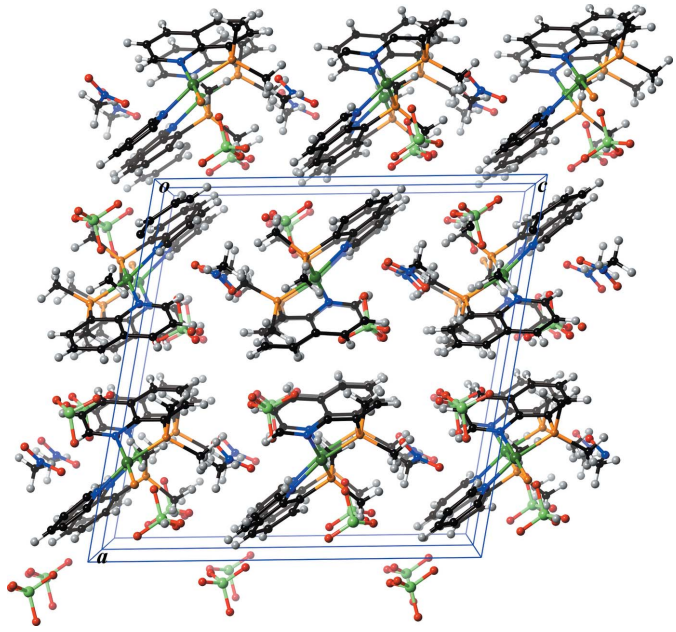



**Figure 5**
A packing drawing of $[Ni(Me_2Pqn)_2](ClO_4)_2CH_3NO_2$ (**1**) along the crystallographic *b* axis (two unit cells are shown). Color code: Ni, dark green; Cl, light green; P, orange; O, red; N, blue; C, black and H, gray.

difference in their coordination geometry (Figs. 3 and 4). The four-coordinate $Ni^{II}$ center in **1** exhibits a large tetrahedral distortion, as indicated by the $\tau_4$ value (Yang *et al.*, 2007) of 0.199 (1)°. This is due to the steric requirement from the planar quinoline moiety located in the mutually *cis* positions around the $Ni^{II}$ center. In the analogous MePhPqn and $Ph_2Pqn$ complexes, the $\tau_4$ values are 0.273 (1)° and 0.189 (2)°, respectively. By contrast, the $\tau_4$ value of the $Pt^{II}$ complex in **2** is only 0.014 (1)°, indicating a nearly perfect planar coordination geometry around the $Pt^{II}$ center. The corresponding value in $[Pt(Ph_2Pqn)_2](BF_4)_2$ is 0.149 (2)° (Mori *et al.*, 2020). It is obvious that the present planar structure of the $Pt^{II}$ center in **2** is a rare example. In this complex, the interligand steric interaction expected for the mutually *cis*-positioned quinoline groups could be reduced by envelope-type bending of the planar $Me_2Pqn$ chelate coordination, that is, the displacement of the $Pt^{II}$ metal center from the ideal plane defined by the chelate ring of 8-quinolylphosphanes. The dihedral angle, $\varphi_C$, between the [Pt,P,N] coordination plane and the [PCCN] phosphanylquinoline planes in **2** are 21.53 (16) and 24.76 (16)°, and the displacement of the Pt1 atom from the ideal quinoline [$C_9H_6N$] planes is 0.579 (5) and 0.550 (5) Å. The two quinoline planes are nearly parallel, with the dihedral angle between them being only 7.99 (10)°. Such a synchronized bending deformation of two chelate coordination (Fig. 4) acts to reduce the steric congestion effectively. The corresponding $\varphi_C$ values for **1** are 17.44 (9) and 19.76 (9)°, and the dihedral angle between the two quinoline planes is obviously large, at 33.35 (6)°. Interestingly, the analogous palladium(II) complex, $[Pd(Me_2Pqn)_2](BF_4)_2$, has a $\tau_4$ value of 0.096 (2)° (Suzuki *et al.*, 1995), which is in between those of the present $Ni^{II}$ and $Pt^{II}$ complexes.

## 3. Supramolecular features

In the crystal structure of **1**, there are two $ClO_4^-$ anions and a $CH_3NO_2$ solvent molecule, in addition to the $[Ni(Me_2Pqn)_2]^{2+}$ complex cation in the asymmetric unit. The asymmetric unit of the $Pt^{II}$ complex, **2**, contains a $[Pt(Me_2Pqn)_2]^{2+}$ complex cation, two $BF_4^-$ anions (in one of which the positions of three F atoms are disordered) and a $CH_3CN$ solvent molecule. In the crystal structures of both **1** and **2** (Figs. 5 and 6, respectively), no remarkable intermolecular stacking or hydrogen-bonding interactions are observed.

## 4. Database survey

Metal complexes containing $Me_2Pqn$ have been reported by us, *e.g.*, *cis*-$[Pd(Me_2Pqn)_2](BF_4)_2$ (refcode ZIFPUZ in the CSD database, version 5.41, last update May 2020; Groom *et al.*, 2016) and $[Pd_2Cl_2(Me_2Pqn)_2]$ (ZIFQAG; Suzuki *et al.*, 1995), $[Cu(Me_2Pqn)_2]PF_6$ (OZILAL; Suzuki *et al.*, 2011), $[Ru(bpy)_{3-n}(Me_2Pqn)_n](PF_6)_2$ (bpy = 2,2′-bipyridine; HUTRIV, HUTPCB, HUTPUH and HUTQAO; Suzuki *et al.*, 2003), and $[Pt(ppy)(Me_2Pqn)]BF_4$ (ppy = 2-(2′-pyridyl)phenyl; Mori & Suzuki, 2020). Some of the related bis(8-quinolyl-phosphanes) complexes are: $[Ni(Ph_2Pqn)_2](BF_4)_n$ ($n$ = 1 or 2; BUGDAJ, BUGDEN and BUGDOX) and $[Ni(MePhPqn)_2](BF_4)_2$ (BUGDIR; Hashimoto *et al.*, 2010), $[Pd(Ph_2Pqn)_2]X_2$ ($X_2$ = $Cl_2$, $Br_2$ or $ClBF_4$; FERZOS, FERZUY and FESBAH; Suzuki, 2004), $[Cu(Ph_2Pqn)_2]BF_4$ (OZILEP and OZILEP01; Suzuki *et al.*, 2011) and $[Cu(Ph_2Pqn)_2]PF_6$ (NOPNIQ; Tsukuda *et al.*, 2009).

## 5. Synthesis and crystallization

The ligand, $Me_2Pqn$, and the nickel(II) complexes, $[Ni(Me_2Pqn)_2](ClO_4)_2$, were prepared according to the method reported previously (Suzuki *et al.*, 1995). Single crystals of **1** suitable for an X-ray diffraction study were obtained by recrystallization from nitromethane by diffusion of diisopropyl ether. The platinum(II) complex, $[Pt(Me_2Pqn)_2](BF_4)_2$, was prepared by the following method. A methanol (5 ml) solution of $Me_2Pqn$ (0.76 mmol) was added dropwise with stirring to a dichloromethane solution (10 ml) of $[PtCl_2(EtCN)_2]$ (0.105 g, 0.278 mmol), and the mixture was stirred for 24 h at room temperature. After removal of the resulting precipitate, the filtrate was concentrated to *ca* 5 ml using a rotary evaporator. A large excess amount of a methanol solution of $NaBF_4$ was added, and the mixture was stirred for 1 h at room temperature. The resulting pale-yellow precipitate was collected by filtration, washed with water (5 ml) and diethyl ether (10 ml), and dried *in vacuo*. Colorless platelet-shaped crystals of $[Pt(Me_2Pqn)_2](BF_4)_2{\cdot}CH_3CN$ (**2**) were obtained by recrystallization from an acetonitrile solution by diffusion of diisopropyl ether. Yield: 0.126 g (61%). Analysis calculated for $C_{24}H_{27}B_2F_8N_3P_2Pt$: C, 35.37; H, 3.24; N, 3.75%. Found (after completely drying): C, 35.39; H, 2.89; N, 3.74%.

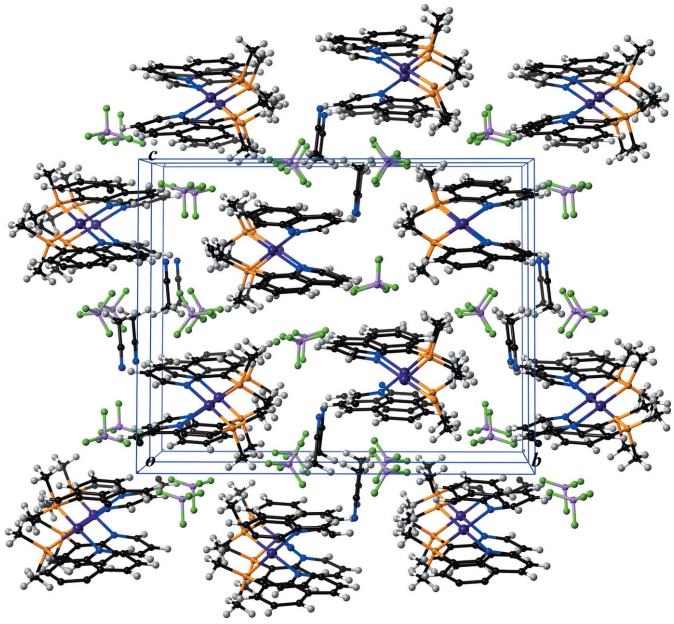



**Figure 6**
A packing drawing of $[Pt(Me_2Pqn)_2](BF_4)_2{\cdot}CH_3CN$ (**2**) along the crystallographic *a* axis (two unit cells are shown). Color code: Pt, purple; P, orange; F, green; N, blue; C, black; B, pale purple and H, gray.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were refined using a riding model, with C—H = 0.95 (aromatic) or 0.98 (methyl) Å and $U_{iso}(H) = 1.2U_{eq}(C)$. In the analysis of **2**, two sets of F atoms for one of the two $BF_4^-$ anions were introduced as positionally disordered atoms, and their occupation parameters were refined with suitable restrictions [the final major:minor occupancy ratio was 0.573 (10):0.427 (10)].

## Funding information

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**Table 3**
Experimental details.

| | **1** | **2** |
|---|---|---|
| Crystal data | | |
| Chemical formula | $[Ni(C_{11}H_{12}NP)_2](ClO_4)_2{\cdot}CH_3NO_2$ | $[Pt(C_{11}H_{12}NP)_2](BF_4)_2{\cdot}C_2H_3N$ |
| $M_r$ | 697.02 | 788.13 |
| Crystal system, space group | Monoclinic, $P2_1/c$ | Monoclinic, $P2_1/n$ |
| Temperature (K) | 188 | 188 |
| $a, b, c$ (Å) | 17.8114 (13), 8.9398 (6), 18.0245 (14) | 7.9102 (3), 21.0833 (5), 16.7519 (4) |
| $\beta$ (°) | 100.524 (3) | 95.3931 (11) |
| $V$ (Å$^3$) | 2821.8 (4) | 2781.42 (15) |
| $Z$ | 4 | 4 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.05 | 5.23 |
| Crystal size (mm) | 0.70 × 0.50 × 0.20 | 0.30 × 0.30 × 0.10 |
| Data collection | | |
| Diffractometer | Rigaku R-AXIS RAPID | Rigaku R-AXIS RAPID |
| Absorption correction | Multi-scan (*ABSCOR*; Rigaku, 1995) | Numerical (*NUMABS*; Rigaku, 1999) |
| $T_{min}$, $T_{max}$ | 0.379, 0.811 | 0.338, 0.594 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26671, 6459, 5440 | 43967, 6350, 5435 |
| $R_{int}$ | 0.041 | 0.042 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.649 | 0.649 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.043, 0.117, 1.05 | 0.033, 0.084, 1.07 |
| No. of reflections | 6459 | 6350 |
| No. of parameters | 370 | 366 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.03, −0.49 | 1.42, −1.45 |

Computer programs: RAPID AUTO (Rigaku, 1998), *CrystalStructure* (Rigaku, 2010), *SIR2011* (Burla *et al.*, 2012), *SHELXL2013* (Sheldrick, 2015) and *CrystalMaker* (CrystalMaker Software, 2017).


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# supporting information

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## Comparison of molecular structures of *cis*-bis[8-(dimethylphosphanyl)quinoline]nickel(II) and -platinum(II) complex cations

**Masatoshi Mori and Takayoshi Suzuki**

### Computing details

For both structures, data collection: RAPID AUTO (Rigaku, 1998); cell refinement: RAPID AUTO (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku, 2010); program(s) used to solve structure: *SIR2011* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (CrystalMaker Software, 2017); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015).

### (*SP*-4-2)-*cis*-Bis[8-(dimethylphosphanyl)quinoline-$\kappa^2N,P$]nickel(II) bis(perchlorate) nitromethane monosolvate (1)

*Crystal data*

$[Ni(C_{11}H_{12}NP)_2](ClO_4)_2{\cdot}CH_3NO_2$
$M_r$ = 697.02
Monoclinic, $P2_1/c$
$a$ = 17.8114 (13) Å
$b$ = 8.9398 (6) Å
$c$ = 18.0245 (14) Å
$\beta$ = 100.524 (3)°
$V$ = 2821.8 (4) Å$^3$
$Z$ = 4
$F(000)$ = 1432
$D_x$ = 1.641 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71075 Å
Cell parameters from 20058 reflections
$\theta$ = 3.2–27.6°
$\mu$ = 1.05 mm$^{-1}$
$T$ = 188 K
Block, red
0.70 × 0.50 × 0.20 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
$T_{min}$ = 0.379, $T_{max}$ = 0.811
26671 measured reflections
6459 independent reflections
5440 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 3.2°
$h$ = −23→23
$k$ = −11→10
$l$ = −23→23

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
$S$ = 1.05
6459 reflections
370 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 2.7492P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.03$ e Å$^{-3}$
$\Delta\rho_{min} = -0.49$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.74556 (2) | 0.21692 (3) | 0.05020 (2) | 0.02369 (10) |
| Cl1 | 0.60962 (3) | 0.03126 (7) | −0.11398 (3) | 0.02893 (15) |
| Cl2 | 0.90376 (4) | 0.47701 (8) | 0.15809 (4) | 0.03678 (16) |
| P1 | 0.79934 (4) | 0.00551 (7) | 0.08449 (4) | 0.02582 (15) |
| P2 | 0.68019 (4) | 0.22150 (7) | 0.13957 (3) | 0.02357 (14) |
| O1 | 0.57753 (13) | 0.1576 (2) | −0.15803 (13) | 0.0477 (5) |
| O2 | 0.59943 (13) | −0.1010 (2) | −0.15961 (11) | 0.0409 (5) |
| O3 | 0.57362 (13) | 0.0136 (3) | −0.04995 (12) | 0.0495 (6) |
| O4 | 0.68979 (11) | 0.0582 (3) | −0.08854 (13) | 0.0475 (5) |
| O5 | 0.94703 (18) | 0.4498 (6) | 0.1033 (2) | 0.1249 (18) |
| O6 | 0.9264 (2) | 0.6110 (4) | 0.1969 (2) | 0.1026 (13) |
| O7 | 0.9117 (3) | 0.3654 (5) | 0.2115 (3) | 0.156 (2) |
| O8 | 0.82342 (15) | 0.4791 (4) | 0.12503 (17) | 0.0726 (8) |
| O9 | 0.77720 (18) | 0.6729 (4) | −0.1337 (2) | 0.1098 (15) |
| O10 | 0.70736 (19) | 0.6516 (3) | −0.24168 (17) | 0.0800 (10) |
| N1 | 0.82335 (12) | 0.2389 (2) | −0.01392 (12) | 0.0267 (4) |
| N2 | 0.67687 (12) | 0.3788 (2) | 0.00323 (11) | 0.0251 (4) |
| N3 | 0.75088 (15) | 0.7214 (3) | −0.19493 (17) | 0.0435 (6) |
| C1 | 0.83949 (15) | 0.3680 (3) | −0.04390 (15) | 0.0334 (6) |
| H1 | 0.8160 | 0.4564 | −0.0300 | 0.040* |
| C2 | 0.88960 (16) | 0.3797 (4) | −0.09511 (16) | 0.0408 (7) |
| H2 | 0.9004 | 0.4747 | −0.1144 | 0.049* |
| C3 | 0.92279 (16) | 0.2540 (4) | −0.11705 (16) | 0.0408 (7) |
| H3 | 0.9538 | 0.2594 | −0.1546 | 0.049* |
| C4 | 0.91060 (14) | 0.1157 (4) | −0.08344 (15) | 0.0349 (6) |
| C5 | 0.94656 (15) | −0.0205 (4) | −0.09839 (17) | 0.0413 (7) |
| H5 | 0.9771 | −0.0228 | −0.1364 | 0.050* |
| C6 | 0.93793 (16) | −0.1476 (4) | −0.05907 (18) | 0.0429 (7) |
| H6 | 0.9621 | −0.2375 | −0.0702 | 0.051* |
| C7 | 0.89332 (15) | −0.1466 (3) | −0.00189 (17) | 0.0364 (6) |
| H7 | 0.8894 | −0.2343 | 0.0270 | 0.044* |
| C8 | 0.85549 (14) | −0.0183 (3) | 0.01185 (15) | 0.0286 (5) |
| C9 | 0.86259 (13) | 0.1132 (3) | −0.02987 (14) | 0.0277 (5) |
| C10 | 0.86537 (16) | −0.0119 (3) | 0.17317 (16) | 0.0370 (6) |
| H10A | 0.9035 | 0.0681 | 0.1772 | 0.044* |
| H10B | 0.8910 | −0.1092 | 0.1753 | 0.044* |

| | | | | |
|---|---|---|---|---|
| H10C | 0.8373 | −0.0040 | 0.2150 | 0.044* |
| C11 | 0.73838 (16) | −0.1577 (3) | 0.07758 (19) | 0.0391 (6) |
| H11A | 0.7694 | −0.2480 | 0.0768 | 0.047* |
| H11B | 0.7002 | −0.1523 | 0.0311 | 0.047* |
| H11C | 0.7126 | −0.1611 | 0.1212 | 0.047* |
| C12 | 0.66794 (15) | 0.4179 (3) | −0.06857 (14) | 0.0298 (5) |
| H12 | 0.6936 | 0.3612 | −0.1009 | 0.036* |
| C13 | 0.62244 (16) | 0.5391 (3) | −0.09962 (16) | 0.0354 (6) |
| H13 | 0.6166 | 0.5605 | −0.1520 | 0.042* |
| C14 | 0.58701 (15) | 0.6251 (3) | −0.05472 (16) | 0.0349 (6) |
| H14 | 0.5590 | 0.7111 | −0.0745 | 0.042* |
| C15 | 0.59216 (14) | 0.5853 (3) | 0.02189 (15) | 0.0287 (5) |
| C16 | 0.55524 (15) | 0.6643 (3) | 0.07288 (17) | 0.0343 (6) |
| H16 | 0.5277 | 0.7531 | 0.0569 | 0.041* |
| C17 | 0.55876 (15) | 0.6142 (3) | 0.14475 (17) | 0.0357 (6) |
| H17 | 0.5353 | 0.6702 | 0.1791 | 0.043* |
| C18 | 0.59706 (15) | 0.4793 (3) | 0.16850 (16) | 0.0320 (6) |
| H18 | 0.5962 | 0.4416 | 0.2176 | 0.038* |
| C19 | 0.63542 (14) | 0.4026 (3) | 0.12141 (14) | 0.0262 (5) |
| C20 | 0.63564 (14) | 0.4568 (3) | 0.04816 (14) | 0.0250 (5) |
| C21 | 0.60140 (15) | 0.0941 (3) | 0.13956 (17) | 0.0348 (6) |
| H21A | 0.5720 | 0.0851 | 0.0882 | 0.042* |
| H21B | 0.5683 | 0.1325 | 0.1731 | 0.042* |
| H21C | 0.6212 | −0.0044 | 0.1573 | 0.042* |
| C22 | 0.73083 (16) | 0.2268 (3) | 0.23602 (14) | 0.0332 (6) |
| H22A | 0.6946 | 0.2457 | 0.2698 | 0.040* |
| H22B | 0.7690 | 0.3069 | 0.2416 | 0.040* |
| H22C | 0.7563 | 0.1306 | 0.2489 | 0.040* |
| C23 | 0.77162 (18) | 0.8734 (3) | −0.21331 (18) | 0.0415 (7) |
| H23A | 0.7415 | 0.9028 | −0.2622 | 0.050* |
| H23B | 0.8261 | 0.8769 | −0.2158 | 0.050* |
| H23C | 0.7611 | 0.9425 | −0.1742 | 0.050* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.02478 (17) | 0.02146 (17) | 0.02684 (18) | 0.00232 (12) | 0.00998 (12) | 0.00229 (11) |
| Cl1 | 0.0286 (3) | 0.0280 (3) | 0.0311 (3) | 0.0003 (2) | 0.0078 (2) | −0.0003 (2) |
| Cl2 | 0.0402 (4) | 0.0324 (3) | 0.0390 (4) | −0.0014 (3) | 0.0107 (3) | −0.0005 (3) |
| P1 | 0.0232 (3) | 0.0227 (3) | 0.0327 (3) | 0.0020 (2) | 0.0082 (2) | 0.0015 (2) |
| P2 | 0.0240 (3) | 0.0233 (3) | 0.0246 (3) | 0.0029 (2) | 0.0078 (2) | 0.0016 (2) |
| O1 | 0.0566 (13) | 0.0350 (11) | 0.0505 (13) | 0.0162 (10) | 0.0072 (11) | 0.0061 (9) |
| O2 | 0.0594 (13) | 0.0287 (10) | 0.0360 (11) | −0.0060 (9) | 0.0123 (10) | −0.0034 (8) |
| O3 | 0.0531 (13) | 0.0633 (15) | 0.0376 (12) | −0.0076 (11) | 0.0227 (10) | −0.0053 (10) |
| O4 | 0.0267 (10) | 0.0517 (13) | 0.0637 (14) | −0.0025 (9) | 0.0070 (9) | −0.0069 (11) |
| O5 | 0.0573 (18) | 0.220 (5) | 0.107 (3) | −0.033 (2) | 0.0413 (19) | −0.094 (3) |
| O6 | 0.091 (2) | 0.082 (2) | 0.149 (3) | −0.041 (2) | 0.059 (2) | −0.062 (2) |
| O7 | 0.164 (4) | 0.120 (4) | 0.159 (4) | −0.038 (3) | −0.041 (3) | 0.091 (3) |

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|---|---|---|---|---|---|---|
| O8 | 0.0430 (14) | 0.095 (2) | 0.080 (2) | 0.0072 (14) | 0.0111 (13) | −0.0257 (16) |
| O9 | 0.070 (2) | 0.103 (3) | 0.139 (3) | −0.0263 (18) | −0.029 (2) | 0.086 (2) |
| O10 | 0.110 (2) | 0.0643 (17) | 0.0767 (19) | −0.0462 (18) | 0.0471 (18) | −0.0385 (15) |
| N1 | 0.0243 (10) | 0.0289 (10) | 0.0280 (11) | −0.0045 (9) | 0.0071 (8) | −0.0013 (8) |
| N2 | 0.0278 (10) | 0.0213 (10) | 0.0271 (10) | −0.0013 (8) | 0.0074 (8) | 0.0013 (8) |
| N3 | 0.0373 (13) | 0.0317 (13) | 0.0643 (18) | 0.0005 (11) | 0.0165 (13) | 0.0012 (12) |
| C1 | 0.0315 (13) | 0.0354 (14) | 0.0337 (14) | −0.0072 (11) | 0.0073 (11) | 0.0006 (11) |
| C2 | 0.0332 (14) | 0.0522 (18) | 0.0378 (15) | −0.0148 (13) | 0.0088 (12) | 0.0072 (13) |
| C3 | 0.0261 (13) | 0.066 (2) | 0.0326 (14) | −0.0110 (14) | 0.0113 (11) | −0.0016 (14) |
| C4 | 0.0211 (11) | 0.0549 (18) | 0.0286 (13) | −0.0042 (12) | 0.0043 (10) | −0.0086 (12) |
| C5 | 0.0213 (12) | 0.066 (2) | 0.0377 (15) | 0.0004 (13) | 0.0072 (11) | −0.0178 (14) |
| C6 | 0.0263 (13) | 0.0550 (19) | 0.0467 (17) | 0.0075 (13) | 0.0051 (12) | −0.0227 (15) |
| C7 | 0.0275 (13) | 0.0372 (15) | 0.0432 (16) | 0.0036 (12) | 0.0026 (11) | −0.0096 (12) |
| C8 | 0.0204 (11) | 0.0324 (13) | 0.0328 (13) | −0.0007 (10) | 0.0044 (10) | −0.0071 (10) |
| C9 | 0.0205 (11) | 0.0343 (13) | 0.0282 (12) | −0.0036 (10) | 0.0038 (9) | −0.0080 (10) |
| C10 | 0.0324 (14) | 0.0433 (16) | 0.0354 (15) | 0.0106 (12) | 0.0069 (11) | 0.0035 (12) |
| C11 | 0.0338 (14) | 0.0282 (13) | 0.0570 (18) | −0.0022 (12) | 0.0128 (13) | 0.0031 (13) |
| C12 | 0.0320 (13) | 0.0285 (12) | 0.0295 (13) | −0.0043 (11) | 0.0068 (10) | 0.0019 (10) |
| C13 | 0.0365 (14) | 0.0350 (14) | 0.0332 (14) | −0.0058 (12) | 0.0023 (11) | 0.0129 (11) |
| C14 | 0.0321 (13) | 0.0256 (13) | 0.0450 (16) | −0.0024 (11) | 0.0014 (12) | 0.0106 (11) |
| C15 | 0.0244 (11) | 0.0212 (11) | 0.0394 (14) | −0.0027 (10) | 0.0029 (10) | 0.0006 (10) |
| C16 | 0.0273 (12) | 0.0226 (12) | 0.0517 (17) | 0.0033 (10) | 0.0035 (12) | −0.0029 (11) |
| C17 | 0.0292 (13) | 0.0324 (14) | 0.0457 (16) | 0.0073 (11) | 0.0075 (11) | −0.0120 (12) |
| C18 | 0.0288 (12) | 0.0345 (14) | 0.0330 (14) | 0.0043 (11) | 0.0065 (10) | −0.0053 (11) |
| C19 | 0.0247 (11) | 0.0256 (12) | 0.0279 (12) | 0.0022 (10) | 0.0039 (9) | −0.0016 (9) |
| C20 | 0.0239 (11) | 0.0199 (11) | 0.0309 (12) | −0.0014 (9) | 0.0043 (9) | −0.0015 (9) |
| C21 | 0.0294 (13) | 0.0337 (14) | 0.0436 (15) | −0.0020 (11) | 0.0128 (11) | 0.0019 (12) |
| C22 | 0.0383 (14) | 0.0352 (14) | 0.0256 (13) | 0.0099 (12) | 0.0047 (11) | 0.0011 (10) |
| C23 | 0.0407 (15) | 0.0336 (15) | 0.0501 (17) | −0.0029 (13) | 0.0081 (13) | 0.0051 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ni1—N1 | 1.970 (2) | C6—C7 | 1.412 (4) |
| Ni1—N2 | 1.982 (2) | C6—H6 | 0.9500 |
| Ni1—P2 | 2.1534 (7) | C7—C8 | 1.376 (4) |
| Ni1—P1 | 2.1576 (7) | C7—H7 | 0.9500 |
| Cl1—O3 | 1.428 (2) | C8—C9 | 1.413 (4) |
| Cl1—O2 | 1.433 (2) | C10—H10A | 0.9800 |
| Cl1—O1 | 1.438 (2) | C10—H10B | 0.9800 |
| Cl1—O4 | 1.438 (2) | C10—H10C | 0.9800 |
| Cl2—O7 | 1.376 (4) | C11—H11A | 0.9800 |
| Cl2—O5 | 1.381 (3) | C11—H11B | 0.9800 |
| Cl2—O6 | 1.408 (3) | C11—H11C | 0.9800 |
| Cl2—O8 | 1.446 (3) | C12—C13 | 1.406 (4) |
| P1—C8 | 1.800 (3) | C12—H12 | 0.9500 |
| P1—C11 | 1.809 (3) | C13—C14 | 1.353 (4) |
| P1—C10 | 1.810 (3) | C13—H13 | 0.9500 |
| P2—C22 | 1.807 (3) | C14—C15 | 1.413 (4) |

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|---|---|---|---|
| P2—C21 | 1.807 (3) | C14—H14 | 0.9500 |
| P2—C19 | 1.808 (3) | C15—C16 | 1.413 (4) |
| O9—N3 | 1.199 (4) | C15—C20 | 1.417 (3) |
| O10—N3 | 1.209 (4) | C16—C17 | 1.361 (4) |
| N1—C1 | 1.327 (3) | C16—H16 | 0.9500 |
| N1—C9 | 1.381 (3) | C17—C18 | 1.413 (4) |
| N2—C12 | 1.322 (3) | C17—H17 | 0.9500 |
| N2—C20 | 1.378 (3) | C18—C19 | 1.367 (3) |
| N3—C23 | 1.462 (4) | C18—H18 | 0.9500 |
| C1—C2 | 1.400 (4) | C19—C20 | 1.407 (3) |
| C1—H1 | 0.9500 | C21—H21A | 0.9800 |
| C2—C3 | 1.362 (5) | C21—H21B | 0.9800 |
| C2—H2 | 0.9500 | C21—H21C | 0.9800 |
| C3—C4 | 1.411 (4) | C22—H22A | 0.9800 |
| C3—H3 | 0.9500 | C22—H22B | 0.9800 |
| C4—C9 | 1.402 (3) | C22—H22C | 0.9800 |
| C4—C5 | 1.424 (4) | C23—H23A | 0.9800 |
| C5—C6 | 1.363 (5) | C23—H23B | 0.9800 |
| C5—H5 | 0.9500 | C23—H23C | 0.9800 |

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|---|---|---|---|
| N1—Ni1—N2 | 97.01 (9) | C9—C8—P1 | 113.84 (18) |
| N1—Ni1—P2 | 166.27 (7) | N1—C9—C4 | 121.7 (2) |
| N2—Ni1—P2 | 85.97 (6) | N1—C9—C8 | 117.9 (2) |
| N1—Ni1—P1 | 86.13 (7) | C4—C9—C8 | 120.3 (2) |
| N2—Ni1—P1 | 165.68 (6) | P1—C10—H10A | 109.5 |
| P2—Ni1—P1 | 94.29 (3) | P1—C10—H10B | 109.5 |
| O3—Cl1—O2 | 110.15 (13) | H10A—C10—H10B | 109.5 |
| O3—Cl1—O1 | 109.95 (14) | P1—C10—H10C | 109.5 |
| O2—Cl1—O1 | 109.60 (13) | H10A—C10—H10C | 109.5 |
| O3—Cl1—O4 | 109.09 (14) | H10B—C10—H10C | 109.5 |
| O2—Cl1—O4 | 109.61 (13) | P1—C11—H11A | 109.5 |
| O1—Cl1—O4 | 108.41 (14) | P1—C11—H11B | 109.5 |
| O7—Cl2—O5 | 111.9 (4) | H11A—C11—H11B | 109.5 |
| O7—Cl2—O6 | 106.6 (3) | P1—C11—H11C | 109.5 |
| O5—Cl2—O6 | 111.0 (2) | H11A—C11—H11C | 109.5 |
| O7—Cl2—O8 | 105.4 (3) | H11B—C11—H11C | 109.5 |
| O5—Cl2—O8 | 110.3 (2) | N2—C12—C13 | 123.4 (2) |
| O6—Cl2—O8 | 111.5 (2) | N2—C12—H12 | 118.3 |
| C8—P1—C11 | 105.12 (13) | C13—C12—H12 | 118.3 |
| C8—P1—C10 | 105.93 (12) | C14—C13—C12 | 119.8 (3) |
| C11—P1—C10 | 106.05 (15) | C14—C13—H13 | 120.1 |
| C8—P1—Ni1 | 99.90 (9) | C12—C13—H13 | 120.1 |
| C11—P1—Ni1 | 117.20 (10) | C13—C14—C15 | 119.2 (2) |
| C10—P1—Ni1 | 120.75 (10) | C13—C14—H14 | 120.4 |
| C22—P2—C21 | 105.52 (14) | C15—C14—H14 | 120.4 |
| C22—P2—C19 | 106.08 (12) | C14—C15—C16 | 123.7 (2) |
| C21—P2—C19 | 104.32 (12) | C14—C15—C20 | 117.7 (2) |
| C22—P2—Ni1 | 118.50 (10) | C16—C15—C20 | 118.6 (2) |

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|---|---|---|---|
| C21—P2—Ni1 | 120.92 (10) | C17—C16—C15 | 120.6 (2) |
| C19—P2—Ni1 | 99.35 (8) | C17—C16—H16 | 119.7 |
| C1—N1—C9 | 117.8 (2) | C15—C16—H16 | 119.7 |
| C1—N1—Ni1 | 123.61 (18) | C16—C17—C18 | 120.3 (2) |
| C9—N1—Ni1 | 118.53 (17) | C16—C17—H17 | 119.8 |
| C12—N2—C20 | 117.4 (2) | C18—C17—H17 | 119.8 |
| C12—N2—Ni1 | 124.45 (18) | C19—C18—C17 | 120.6 (3) |
| C20—N2—Ni1 | 118.18 (16) | C19—C18—H18 | 119.7 |
| O9—N3—O10 | 123.2 (3) | C17—C18—H18 | 119.7 |
| O9—N3—C23 | 118.2 (3) | C18—C19—C20 | 119.8 (2) |
| O10—N3—C23 | 118.6 (3) | C18—C19—P2 | 126.2 (2) |
| N1—C1—C2 | 123.0 (3) | C20—C19—P2 | 113.68 (18) |
| N1—C1—H1 | 118.5 | N2—C20—C19 | 118.0 (2) |
| C2—C1—H1 | 118.5 | N2—C20—C15 | 122.1 (2) |
| C3—C2—C1 | 119.5 (3) | C19—C20—C15 | 119.8 (2) |
| C3—C2—H2 | 120.3 | P2—C21—H21A | 109.5 |
| C1—C2—H2 | 120.3 | P2—C21—H21B | 109.5 |
| C2—C3—C4 | 119.3 (2) | H21A—C21—H21B | 109.5 |
| C2—C3—H3 | 120.3 | P2—C21—H21C | 109.5 |
| C4—C3—H3 | 120.3 | H21A—C21—H21C | 109.5 |
| C9—C4—C3 | 118.1 (3) | H21B—C21—H21C | 109.5 |
| C9—C4—C5 | 117.9 (3) | P2—C22—H22A | 109.5 |
| C3—C4—C5 | 123.9 (3) | P2—C22—H22B | 109.5 |
| C6—C5—C4 | 121.1 (3) | H22A—C22—H22B | 109.5 |
| C6—C5—H5 | 119.4 | P2—C22—H22C | 109.5 |
| C4—C5—H5 | 119.4 | H22A—C22—H22C | 109.5 |
| C5—C6—C7 | 120.4 (3) | H22B—C22—H22C | 109.5 |
| C5—C6—H6 | 119.8 | N3—C23—H23A | 109.5 |
| C7—C6—H6 | 119.8 | N3—C23—H23B | 109.5 |
| C8—C7—C6 | 119.7 (3) | H23A—C23—H23B | 109.5 |
| C8—C7—H7 | 120.1 | N3—C23—H23C | 109.5 |
| C6—C7—H7 | 120.1 | H23A—C23—H23C | 109.5 |
| C7—C8—C9 | 120.2 (2) | H23B—C23—H23C | 109.5 |
| C7—C8—P1 | 125.8 (2) | | |

| | | | |
|---|---|---|---|
| C9—N1—C1—C2 | 5.1 (4) | C20—N2—C12—C13 | 3.7 (4) |
| Ni1—N1—C1—C2 | −173.7 (2) | Ni1—N2—C12—C13 | −175.97 (19) |
| N1—C1—C2—C3 | 1.3 (4) | N2—C12—C13—C14 | 2.1 (4) |
| C1—C2—C3—C4 | −4.8 (4) | C12—C13—C14—C15 | −4.3 (4) |
| C2—C3—C4—C9 | 1.8 (4) | C13—C14—C15—C16 | −177.8 (3) |
| C2—C3—C4—C5 | −175.6 (3) | C13—C14—C15—C20 | 0.9 (4) |
| C9—C4—C5—C6 | −3.4 (4) | C14—C15—C16—C17 | 175.8 (3) |
| C3—C4—C5—C6 | 173.9 (3) | C20—C15—C16—C17 | −2.8 (4) |
| C4—C5—C6—C7 | −0.5 (4) | C15—C16—C17—C18 | −2.4 (4) |
| C5—C6—C7—C8 | 3.0 (4) | C16—C17—C18—C19 | 4.4 (4) |
| C6—C7—C8—C9 | −1.5 (4) | C17—C18—C19—C20 | −1.2 (4) |
| C6—C7—C8—P1 | −177.4 (2) | C17—C18—C19—P2 | −174.3 (2) |
| C11—P1—C8—C7 | −47.4 (3) | C22—P2—C19—C18 | −44.2 (3) |

| | | | |
|---|---|---|---|
| C10—P1—C8—C7 | 64.6 (3) | C21—P2—C19—C18 | 67.0 (3) |
| Ni1—P1—C8—C7 | −169.2 (2) | Ni1—P2—C19—C18 | −167.6 (2) |
| C11—P1—C8—C9 | 136.4 (2) | C22—P2—C19—C20 | 142.27 (19) |
| C10—P1—C8—C9 | −111.6 (2) | C21—P2—C19—C20 | −106.6 (2) |
| Ni1—P1—C8—C9 | 14.54 (19) | Ni1—P2—C19—C20 | 18.86 (19) |
| C1—N1—C9—C4 | −8.2 (4) | C12—N2—C20—C19 | 170.6 (2) |
| Ni1—N1—C9—C4 | 170.70 (18) | Ni1—N2—C20—C19 | −9.7 (3) |
| C1—N1—C9—C8 | 169.3 (2) | C12—N2—C20—C15 | −7.3 (3) |
| Ni1—N1—C9—C8 | −11.8 (3) | Ni1—N2—C20—C15 | 172.42 (18) |
| C3—C4—C9—N1 | 4.8 (4) | C18—C19—C20—N2 | 178.1 (2) |
| C5—C4—C9—N1 | −177.7 (2) | P2—C19—C20—N2 | −8.0 (3) |
| C3—C4—C9—C8 | −172.6 (2) | C18—C19—C20—C15 | −4.0 (4) |
| C5—C4—C9—C8 | 4.9 (4) | P2—C19—C20—C15 | 169.96 (18) |
| C7—C8—C9—N1 | 179.9 (2) | C14—C15—C20—N2 | 5.1 (4) |
| P1—C8—C9—N1 | −3.6 (3) | C16—C15—C20—N2 | −176.2 (2) |
| C7—C8—C9—C4 | −2.6 (4) | C14—C15—C20—C19 | −172.7 (2) |
| P1—C8—C9—C4 | 173.89 (19) | C16—C15—C20—C19 | 6.0 (4) |

**(*SP*-4-2)-*cis*-Bis[8-(dimethylphosphanyl)quinoline-$\kappa^2N,P$]platinum(II) bis(tetrafluoroborate) acetonitrile monosolvate (2)**

*Crystal data*

$[Pt(C_{11}H_{12}NP)_2](BF_4)_2 \cdot C_2H_3N$
$M_r = 788.13$
Monoclinic, $P2_1/n$
$a = 7.9102$ (3) Å
$b = 21.0833$ (5) Å
$c = 16.7519$ (4) Å
$\beta = 95.3931$ (11)°
$V = 2781.42$ (15) Å$^3$
$Z = 4$
$F(000) = 1528$
$D_x = 1.882$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 31045 reflections
$\theta = 3.1$–27.5°
$\mu = 5.23$ mm$^{-1}$
$T = 188$ K
Platelet, colorless
0.30 × 0.30 × 0.10 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: numerical (NUMABS; Rigaku, 1999)
$T_{min} = 0.338$, $T_{max} = 0.594$
43967 measured reflections
6350 independent reflections
5435 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -10 \rightarrow 10$
$k = -27 \rightarrow 27$
$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.084$
$S = 1.07$
6350 reflections
366 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 9.8949P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.42$ e Å$^{-3}$
$\Delta\rho_{min} = -1.44$ 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)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pt1 | 0.64274 (2) | 0.17364 (2) | 0.20553 (2) | 0.02183 (7) | |
| P1 | 0.50347 (15) | 0.24824 (5) | 0.26806 (7) | 0.0237 (2) | |
| P2 | 0.80277 (15) | 0.23745 (6) | 0.13781 (7) | 0.0247 (2) | |
| F1 | 1.2369 (6) | −0.1256 (2) | 0.0823 (5) | 0.136 (3) | |
| F2A | 1.5089 (15) | −0.1511 (5) | 0.0808 (7) | 0.089 (2) | 0.573 (10) |
| F3A | 1.4191 (13) | −0.0455 (4) | 0.0691 (7) | 0.089 (2) | 0.573 (10) |
| F4A | 1.3835 (12) | −0.1067 (4) | 0.1779 (6) | 0.089 (2) | 0.573 (10) |
| F2B | 1.4392 (16) | −0.1049 (8) | 0.0213 (10) | 0.121 (4) | 0.427 (10) |
| F3B | 1.4100 (18) | −0.0423 (9) | 0.1216 (12) | 0.121 (4) | 0.427 (10) |
| F4B | 1.520 (2) | −0.1430 (9) | 0.1262 (12) | 0.121 (4) | 0.427 (10) |
| F5 | 0.0397 (6) | 0.3460 (3) | −0.0167 (5) | 0.115 (2) | |
| F6 | 0.2266 (7) | 0.4071 (2) | −0.0644 (3) | 0.0883 (15) | |
| F7 | 0.1968 (10) | 0.4023 (3) | 0.0675 (3) | 0.126 (3) | |
| F8 | 0.3139 (5) | 0.31996 (17) | 0.0067 (2) | 0.0566 (10) | |
| N1 | 0.4883 (5) | 0.11161 (18) | 0.2672 (2) | 0.0256 (8) | |
| N2 | 0.7738 (5) | 0.10240 (18) | 0.1453 (2) | 0.0270 (8) | |
| N3 | 0.8437 (7) | −0.0443 (3) | 0.3316 (4) | 0.0521 (13) | |
| C1 | 0.5191 (7) | 0.0503 (2) | 0.2795 (3) | 0.0342 (11) | |
| H1 | 0.6285 | 0.0343 | 0.2714 | 0.041* | |
| C2 | 0.3965 (8) | 0.0078 (3) | 0.3041 (3) | 0.0411 (13) | |
| H2 | 0.4219 | −0.0361 | 0.3103 | 0.049* | |
| C3 | 0.2415 (7) | 0.0304 (3) | 0.3190 (3) | 0.0395 (12) | |
| H3 | 0.1547 | 0.0020 | 0.3317 | 0.047* | |
| C4 | 0.2103 (6) | 0.0963 (2) | 0.3155 (3) | 0.0310 (10) | |
| C5 | 0.0599 (6) | 0.1251 (3) | 0.3391 (3) | 0.0350 (11) | |
| H5 | −0.0327 | 0.0992 | 0.3512 | 0.042* | |
| C6 | 0.0477 (7) | 0.1893 (3) | 0.3444 (3) | 0.0346 (11) | |
| H6 | −0.0519 | 0.2077 | 0.3620 | 0.042* | |
| C7 | 0.1812 (6) | 0.2289 (2) | 0.3239 (3) | 0.0307 (10) | |
| H7 | 0.1727 | 0.2736 | 0.3298 | 0.037* | |
| C8 | 0.3228 (6) | 0.2031 (2) | 0.2955 (3) | 0.0253 (9) | |
| C9 | 0.3391 (6) | 0.1368 (2) | 0.2909 (3) | 0.0254 (9) | |
| C10 | 0.6062 (6) | 0.2807 (2) | 0.3599 (3) | 0.0328 (11) | |
| H10A | 0.6548 | 0.2461 | 0.3938 | 0.039* | |
| H10B | 0.6968 | 0.3097 | 0.3474 | 0.039* | |
| H10C | 0.5227 | 0.3038 | 0.3884 | 0.039* | |
| C11 | 0.4207 (7) | 0.3163 (2) | 0.2120 (3) | 0.0353 (11) | |
| H11A | 0.3625 | 0.3023 | 0.1609 | 0.042* | |
| H11B | 0.3403 | 0.3389 | 0.2429 | 0.042* | |

| | | | | |
|---|---|---|---|---|
| H11C | 0.5144 | 0.3447 | 0.2019 | 0.042* |
| C12 | 0.7232 (7) | 0.0429 (2) | 0.1333 (3) | 0.0333 (11) |
| H12 | 0.6088 | 0.0325 | 0.1405 | 0.040* |
| C13 | 0.8316 (7) | −0.0059 (2) | 0.1104 (3) | 0.0380 (12) |
| H13 | 0.7911 | −0.0482 | 0.1044 | 0.046* |
| C14 | 0.9946 (7) | 0.0083 (3) | 0.0970 (3) | 0.0392 (12) |
| H14 | 1.0717 | −0.0244 | 0.0861 | 0.047* |
| C15 | 1.0478 (6) | 0.0725 (2) | 0.0996 (3) | 0.0311 (10) |
| C16 | 1.2074 (6) | 0.0932 (3) | 0.0757 (3) | 0.0392 (12) |
| H16 | 1.2897 | 0.0628 | 0.0632 | 0.047* |
| C17 | 1.2421 (7) | 0.1564 (3) | 0.0707 (3) | 0.0409 (13) |
| H17 | 1.3472 | 0.1696 | 0.0530 | 0.049* |
| C18 | 1.1258 (6) | 0.2021 (3) | 0.0913 (3) | 0.0350 (11) |
| H18 | 1.1518 | 0.2459 | 0.0865 | 0.042* |
| C19 | 0.9729 (6) | 0.1843 (2) | 0.1186 (3) | 0.0268 (10) |
| C20 | 0.9326 (6) | 0.1191 (2) | 0.1230 (3) | 0.0256 (9) |
| C21 | 0.8949 (7) | 0.3084 (2) | 0.1834 (3) | 0.0349 (11) |
| H21A | 0.8043 | 0.3379 | 0.1944 | 0.042* |
| H21B | 0.9617 | 0.2974 | 0.2338 | 0.042* |
| H21C | 0.9688 | 0.3284 | 0.1469 | 0.042* |
| C22 | 0.7056 (7) | 0.2620 (3) | 0.0406 (3) | 0.0354 (11) |
| H22A | 0.6527 | 0.2252 | 0.0124 | 0.042* |
| H22B | 0.6189 | 0.2942 | 0.0476 | 0.042* |
| H22C | 0.7926 | 0.2798 | 0.0091 | 0.042* |
| C23 | 0.8162 (8) | −0.0480 (3) | 0.3952 (4) | 0.0437 (13) |
| C24 | 0.7834 (13) | −0.0553 (4) | 0.4779 (4) | 0.078 (2) |
| H24A | 0.7717 | −0.0134 | 0.5021 | 0.094* |
| H24B | 0.8781 | −0.0780 | 0.5071 | 0.094* |
| H24C | 0.6783 | −0.0794 | 0.4808 | 0.094* |
| B1 | 1.3953 (8) | −0.1035 (3) | 0.0979 (4) | 0.0361 (13) |
| B2 | 0.2039 (8) | 0.3716 (3) | 0.0001 (4) | 0.0370 (13) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pt1 | 0.02079 (9) | 0.02222 (10) | 0.02284 (10) | 0.00020 (6) | 0.00396 (6) | 0.00096 (7) |
| P1 | 0.0234 (6) | 0.0233 (5) | 0.0243 (6) | 0.0018 (4) | 0.0025 (4) | 0.0014 (5) |
| P2 | 0.0221 (6) | 0.0261 (6) | 0.0258 (6) | −0.0021 (4) | 0.0023 (4) | 0.0032 (5) |
| F1 | 0.040 (2) | 0.051 (3) | 0.317 (10) | −0.003 (2) | 0.017 (4) | 0.009 (4) |
| F2A | 0.104 (4) | 0.057 (3) | 0.106 (5) | 0.009 (3) | 0.014 (4) | 0.015 (3) |
| F3A | 0.104 (4) | 0.057 (3) | 0.106 (5) | 0.009 (3) | 0.014 (4) | 0.015 (3) |
| F4A | 0.104 (4) | 0.057 (3) | 0.106 (5) | 0.009 (3) | 0.014 (4) | 0.015 (3) |
| F2B | 0.071 (5) | 0.136 (8) | 0.158 (10) | −0.024 (5) | 0.031 (6) | −0.015 (7) |
| F3B | 0.071 (5) | 0.136 (8) | 0.158 (10) | −0.024 (5) | 0.031 (6) | −0.015 (7) |
| F4B | 0.071 (5) | 0.136 (8) | 0.158 (10) | −0.024 (5) | 0.031 (6) | −0.015 (7) |
| F5 | 0.052 (3) | 0.081 (3) | 0.215 (7) | 0.001 (2) | 0.032 (4) | 0.012 (4) |
| F6 | 0.108 (4) | 0.087 (3) | 0.075 (3) | 0.032 (3) | 0.037 (3) | 0.040 (3) |
| F7 | 0.207 (7) | 0.110 (4) | 0.057 (3) | 0.077 (5) | −0.008 (4) | −0.027 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F8 | 0.053 (2) | 0.054 (2) | 0.062 (2) | 0.0172 (17) | 0.0060 (18) | 0.0040 (18) |
| N1 | 0.0241 (19) | 0.0264 (19) | 0.0269 (19) | 0.0009 (15) | 0.0066 (15) | 0.0044 (16) |
| N2 | 0.028 (2) | 0.027 (2) | 0.0252 (19) | −0.0004 (16) | 0.0028 (16) | −0.0020 (16) |
| N3 | 0.052 (3) | 0.049 (3) | 0.057 (3) | 0.003 (2) | 0.013 (3) | 0.004 (3) |
| C1 | 0.040 (3) | 0.028 (2) | 0.037 (3) | 0.004 (2) | 0.012 (2) | 0.004 (2) |
| C2 | 0.058 (4) | 0.026 (3) | 0.042 (3) | 0.000 (2) | 0.018 (3) | 0.006 (2) |
| C3 | 0.045 (3) | 0.034 (3) | 0.042 (3) | −0.010 (2) | 0.014 (2) | 0.003 (2) |
| C4 | 0.030 (2) | 0.037 (3) | 0.026 (2) | −0.005 (2) | 0.0045 (19) | 0.000 (2) |
| C5 | 0.025 (2) | 0.049 (3) | 0.032 (3) | −0.003 (2) | 0.007 (2) | 0.004 (2) |
| C6 | 0.030 (3) | 0.047 (3) | 0.028 (2) | 0.009 (2) | 0.006 (2) | 0.005 (2) |
| C7 | 0.030 (2) | 0.038 (3) | 0.025 (2) | 0.006 (2) | 0.0046 (19) | 0.001 (2) |
| C8 | 0.026 (2) | 0.031 (2) | 0.019 (2) | 0.0008 (18) | 0.0018 (17) | 0.0029 (18) |
| C9 | 0.026 (2) | 0.029 (2) | 0.022 (2) | 0.0007 (18) | 0.0033 (18) | 0.0014 (18) |
| C10 | 0.032 (3) | 0.036 (3) | 0.030 (2) | 0.000 (2) | 0.001 (2) | −0.007 (2) |
| C11 | 0.033 (3) | 0.031 (3) | 0.043 (3) | 0.004 (2) | 0.006 (2) | 0.009 (2) |
| C12 | 0.035 (3) | 0.030 (2) | 0.036 (3) | −0.004 (2) | 0.010 (2) | −0.004 (2) |
| C13 | 0.052 (3) | 0.025 (2) | 0.038 (3) | 0.000 (2) | 0.013 (2) | −0.004 (2) |
| C14 | 0.047 (3) | 0.038 (3) | 0.033 (3) | 0.013 (2) | 0.007 (2) | −0.002 (2) |
| C15 | 0.029 (2) | 0.039 (3) | 0.025 (2) | 0.006 (2) | 0.0046 (19) | −0.003 (2) |
| C16 | 0.026 (3) | 0.057 (3) | 0.034 (3) | 0.009 (2) | 0.004 (2) | −0.004 (3) |
| C17 | 0.026 (3) | 0.062 (4) | 0.035 (3) | −0.007 (2) | 0.007 (2) | −0.010 (3) |
| C18 | 0.028 (2) | 0.045 (3) | 0.033 (3) | −0.007 (2) | 0.008 (2) | −0.003 (2) |
| C19 | 0.024 (2) | 0.033 (2) | 0.024 (2) | −0.0016 (18) | 0.0028 (18) | −0.0035 (19) |
| C20 | 0.022 (2) | 0.031 (2) | 0.023 (2) | 0.0034 (18) | 0.0017 (17) | 0.0004 (19) |
| C21 | 0.030 (3) | 0.029 (2) | 0.046 (3) | −0.004 (2) | 0.001 (2) | −0.002 (2) |
| C22 | 0.034 (3) | 0.043 (3) | 0.029 (2) | −0.001 (2) | 0.000 (2) | 0.007 (2) |
| C23 | 0.044 (3) | 0.030 (3) | 0.057 (4) | −0.006 (2) | 0.005 (3) | −0.001 (3) |
| C24 | 0.125 (7) | 0.057 (4) | 0.054 (4) | −0.025 (5) | 0.020 (5) | 0.005 (4) |
| B1 | 0.038 (3) | 0.028 (3) | 0.044 (4) | 0.003 (2) | 0.010 (3) | −0.002 (3) |
| B2 | 0.043 (3) | 0.034 (3) | 0.036 (3) | 0.005 (3) | 0.014 (3) | 0.001 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pt1—N1 | 2.123 (4) | C6—C7 | 1.414 (7) |
| Pt1—N2 | 2.132 (4) | C6—H6 | 0.9500 |
| Pt1—P2 | 2.2293 (12) | C7—C8 | 1.371 (6) |
| Pt1—P1 | 2.2365 (12) | C7—H7 | 0.9500 |
| P1—C11 | 1.804 (5) | C8—C9 | 1.405 (7) |
| P1—C10 | 1.805 (5) | C10—H10A | 0.9800 |
| P1—C8 | 1.812 (5) | C10—H10B | 0.9800 |
| P2—C21 | 1.802 (5) | C10—H10C | 0.9800 |
| P2—C19 | 1.804 (5) | C11—H11A | 0.9800 |
| P2—C22 | 1.810 (5) | C11—H11B | 0.9800 |
| F1—B1 | 1.340 (8) | C11—H11C | 0.9800 |
| F2A—B1 | 1.395 (13) | C12—C13 | 1.416 (7) |
| F3A—B1 | 1.334 (11) | C12—H12 | 0.9500 |
| F4A—B1 | 1.353 (11) | C13—C14 | 1.363 (8) |
| F2B—B1 | 1.361 (17) | C13—H13 | 0.9500 |

| | | | |
|---|---|---|---|
| F3B—B1 | 1.351 (18) | C14—C15 | 1.416 (8) |
| F4B—B1 | 1.35 (2) | C14—H14 | 0.9500 |
| F5—B2 | 1.410 (8) | C15—C20 | 1.421 (6) |
| F6—B2 | 1.341 (7) | C15—C16 | 1.428 (7) |
| F7—B2 | 1.309 (8) | C16—C17 | 1.366 (8) |
| F8—B2 | 1.391 (7) | C16—H16 | 0.9500 |
| N1—C1 | 1.329 (6) | C17—C18 | 1.398 (8) |
| N1—C9 | 1.386 (6) | C17—H17 | 0.9500 |
| N2—C12 | 1.326 (6) | C18—C19 | 1.384 (7) |
| N2—C20 | 1.389 (6) | C18—H18 | 0.9500 |
| N3—C23 | 1.110 (8) | C19—C20 | 1.414 (6) |
| C1—C2 | 1.409 (7) | C21—H21A | 0.9800 |
| C1—H1 | 0.9500 | C21—H21B | 0.9800 |
| C2—C3 | 1.360 (8) | C21—H21C | 0.9800 |
| C2—H2 | 0.9500 | C22—H22A | 0.9800 |
| C3—C4 | 1.410 (7) | C22—H22B | 0.9800 |
| C3—H3 | 0.9500 | C22—H22C | 0.9800 |
| C4—C9 | 1.421 (7) | C23—C24 | 1.441 (9) |
| C4—C5 | 1.424 (7) | C24—H24A | 0.9800 |
| C5—C6 | 1.361 (8) | C24—H24B | 0.9800 |
| C5—H5 | 0.9500 | C24—H24C | 0.9800 |

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| N1—Pt1—N2 | 97.13 (15) | N2—C12—H12 | 118.4 |
| N1—Pt1—P2 | 178.51 (11) | C13—C12—H12 | 118.4 |
| N2—Pt1—P2 | 81.93 (11) | C14—C13—C12 | 119.4 (5) |
| N1—Pt1—P1 | 82.76 (11) | C14—C13—H13 | 120.3 |
| N2—Pt1—P1 | 179.55 (11) | C12—C13—H13 | 120.3 |
| P2—Pt1—P1 | 98.17 (4) | C13—C14—C15 | 119.2 (5) |
| C11—P1—C10 | 104.7 (3) | C13—C14—H14 | 120.4 |
| C11—P1—C8 | 107.1 (2) | C15—C14—H14 | 120.4 |
| C10—P1—C8 | 106.6 (2) | C14—C15—C20 | 118.3 (5) |
| C11—P1—Pt1 | 119.12 (19) | C14—C15—C16 | 123.4 (5) |
| C10—P1—Pt1 | 117.60 (17) | C20—C15—C16 | 118.2 (5) |
| C8—P1—Pt1 | 100.60 (16) | C17—C16—C15 | 120.2 (5) |
| C21—P2—C19 | 108.2 (2) | C17—C16—H16 | 119.9 |
| C21—P2—C22 | 105.4 (3) | C15—C16—H16 | 119.9 |
| C19—P2—C22 | 106.1 (2) | C16—C17—C18 | 121.2 (5) |
| C21—P2—Pt1 | 120.76 (19) | C16—C17—H17 | 119.4 |
| C19—P2—Pt1 | 100.65 (16) | C18—C17—H17 | 119.4 |
| C22—P2—Pt1 | 114.64 (18) | C19—C18—C17 | 120.6 (5) |
| C1—N1—C9 | 118.5 (4) | C19—C18—H18 | 119.7 |
| C1—N1—Pt1 | 124.7 (3) | C17—C18—H18 | 119.7 |
| C9—N1—Pt1 | 116.6 (3) | C18—C19—C20 | 119.3 (4) |
| C12—N2—C20 | 117.8 (4) | C18—C19—P2 | 125.4 (4) |
| C12—N2—Pt1 | 125.8 (3) | C20—C19—P2 | 114.7 (3) |
| C20—N2—Pt1 | 116.2 (3) | N2—C20—C19 | 118.3 (4) |
| N1—C1—C2 | 122.9 (5) | N2—C20—C15 | 121.2 (4) |
| N1—C1—H1 | 118.6 | C19—C20—C15 | 120.3 (4) |

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| C2—C1—H1 | 118.6 | P2—C21—H21A | 109.5 |
| C3—C2—C1 | 119.2 (5) | P2—C21—H21B | 109.5 |
| C3—C2—H2 | 120.4 | H21A—C21—H21B | 109.5 |
| C1—C2—H2 | 120.4 | P2—C21—H21C | 109.5 |
| C2—C3—C4 | 119.7 (5) | H21A—C21—H21C | 109.5 |
| C2—C3—H3 | 120.2 | H21B—C21—H21C | 109.5 |
| C4—C3—H3 | 120.2 | P2—C22—H22A | 109.5 |
| C3—C4—C9 | 118.5 (5) | P2—C22—H22B | 109.5 |
| C3—C4—C5 | 123.8 (5) | H22A—C22—H22B | 109.5 |
| C9—C4—C5 | 117.6 (5) | P2—C22—H22C | 109.5 |
| C6—C5—C4 | 120.6 (5) | H22A—C22—H22C | 109.5 |
| C6—C5—H5 | 119.7 | H22B—C22—H22C | 109.5 |
| C4—C5—H5 | 119.7 | N3—C23—C24 | 177.7 (7) |
| C5—C6—C7 | 120.8 (5) | C23—C24—H24A | 109.5 |
| C5—C6—H6 | 119.6 | C23—C24—H24B | 109.5 |
| C7—C6—H6 | 119.6 | H24A—C24—H24B | 109.5 |
| C8—C7—C6 | 120.2 (5) | C23—C24—H24C | 109.5 |
| C8—C7—H7 | 119.9 | H24A—C24—H24C | 109.5 |
| C6—C7—H7 | 119.9 | H24B—C24—H24C | 109.5 |
| C7—C8—C9 | 119.8 (4) | F3A—B1—F1 | 114.2 (7) |
| C7—C8—P1 | 124.7 (4) | F1—B1—F4B | 119.8 (9) |
| C9—C8—P1 | 115.5 (3) | F1—B1—F3B | 116.3 (8) |
| N1—C9—C8 | 118.8 (4) | F4B—B1—F3B | 116.6 (12) |
| N1—C9—C4 | 120.3 (4) | F3A—B1—F4A | 115.4 (8) |
| C8—C9—C4 | 120.7 (4) | F1—B1—F4A | 91.4 (7) |
| P1—C10—H10A | 109.5 | F1—B1—F2B | 97.2 (8) |
| P1—C10—H10B | 109.5 | F4B—B1—F2B | 94.3 (11) |
| H10A—C10—H10B | 109.5 | F3B—B1—F2B | 106.0 (11) |
| P1—C10—H10C | 109.5 | F3A—B1—F2A | 118.0 (8) |
| H10A—C10—H10C | 109.5 | F1—B1—F2A | 108.5 (7) |
| H10B—C10—H10C | 109.5 | F4A—B1—F2A | 105.8 (7) |
| P1—C11—H11A | 109.5 | F7—B2—F6 | 116.0 (6) |
| P1—C11—H11B | 109.5 | F7—B2—F8 | 113.3 (6) |
| H11A—C11—H11B | 109.5 | F6—B2—F8 | 111.8 (5) |
| P1—C11—H11C | 109.5 | F7—B2—F5 | 104.4 (6) |
| H11A—C11—H11C | 109.5 | F6—B2—F5 | 104.1 (6) |
| H11B—C11—H11C | 109.5 | F8—B2—F5 | 105.9 (5) |
| N2—C12—C13 | 123.2 (5) | | |

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| C9—N1—C1—C2 | 10.0 (7) | C20—N2—C12—C13 | 9.6 (7) |
| Pt1—N1—C1—C2 | −165.3 (4) | Pt1—N2—C12—C13 | −164.6 (4) |
| N1—C1—C2—C3 | −2.5 (8) | N2—C12—C13—C14 | −2.3 (8) |
| C1—C2—C3—C4 | −4.8 (8) | C12—C13—C14—C15 | −5.4 (8) |
| C2—C3—C4—C9 | 4.3 (8) | C13—C14—C15—C20 | 5.4 (7) |
| C2—C3—C4—C5 | −172.4 (5) | C13—C14—C15—C16 | −171.1 (5) |
| C3—C4—C5—C6 | 171.1 (5) | C14—C15—C16—C17 | 172.3 (5) |
| C9—C4—C5—C6 | −5.6 (7) | C20—C15—C16—C17 | −4.2 (7) |
| C4—C5—C6—C7 | 2.3 (8) | C15—C16—C17—C18 | 2.2 (8) |

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| C5—C6—C7—C8 | 2.4 (7) | C16—C17—C18—C19 | 1.1 (8) |
| C6—C7—C8—C9 | −3.5 (7) | C17—C18—C19—C20 | −2.1 (7) |
| C6—C7—C8—P1 | −179.3 (4) | C17—C18—C19—P2 | −173.6 (4) |
| C11—P1—C8—C7 | −43.4 (5) | C21—P2—C19—C18 | −39.4 (5) |
| C10—P1—C8—C7 | 68.3 (4) | C22—P2—C19—C18 | 73.3 (5) |
| Pt1—P1—C8—C7 | −168.5 (4) | Pt1—P2—C19—C18 | −167.0 (4) |
| C11—P1—C8—C9 | 140.6 (4) | C21—P2—C19—C20 | 148.8 (4) |
| C10—P1—C8—C9 | −107.7 (4) | C22—P2—C19—C20 | −98.5 (4) |
| Pt1—P1—C8—C9 | 15.5 (3) | Pt1—P2—C19—C20 | 21.2 (4) |
| C1—N1—C9—C8 | 165.5 (4) | C12—N2—C20—C19 | 166.2 (4) |
| Pt1—N1—C9—C8 | −18.9 (5) | Pt1—N2—C20—C19 | −19.0 (5) |
| C1—N1—C9—C4 | −10.1 (7) | C12—N2—C20—C15 | −9.3 (7) |
| Pt1—N1—C9—C4 | 165.5 (3) | Pt1—N2—C20—C15 | 165.4 (3) |
| C7—C8—C9—N1 | −175.6 (4) | C18—C19—C20—N2 | −175.7 (4) |
| P1—C8—C9—N1 | 0.6 (5) | P2—C19—C20—N2 | −3.3 (6) |
| C7—C8—C9—C4 | −0.1 (7) | C18—C19—C20—C15 | −0.1 (7) |
| P1—C8—C9—C4 | 176.2 (3) | P2—C19—C20—C15 | 172.3 (4) |
| C3—C4—C9—N1 | 3.1 (7) | C14—C15—C20—N2 | 2.0 (7) |
| C5—C4—C9—N1 | −179.9 (4) | C16—C15—C20—N2 | 178.6 (4) |
| C3—C4—C9—C8 | −172.4 (5) | C14—C15—C20—C19 | −173.5 (4) |
| C5—C4—C9—C8 | 4.6 (7) | C16—C15—C20—C19 | 3.2 (7) |