

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

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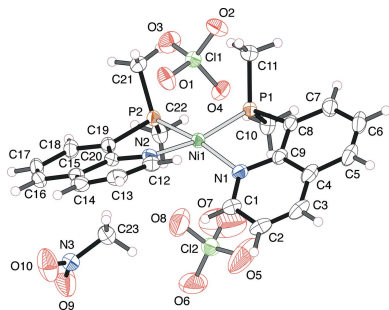
Supporting information: this article has supporting information at journals.iucr.org/e

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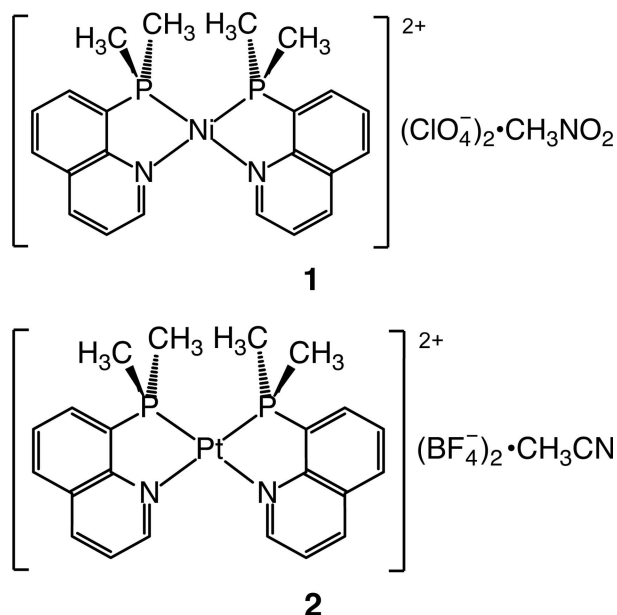
The crystal structures of the complexes (*SP*-4-2)-*cis*-bis[8-(dimethylphosphanyl)quinoline- κ^2N,P]nickel(II) bis(perchlorate) nitromethane monosolvate, $[\text{Ni}(\text{C}_{11}\text{H}_{12}\text{NP})_2](\text{ClO}_4)_2 \cdot \text{CH}_3\text{NO}_2$ (**1**), and (*SP*-4-2)-*cis*-bis[8-(dimethylphosphanyl)quinoline- κ^2N,P]platinum(II) bis(tetrafluoroborate) acetonitrile monosolvate, $[\text{Pt}(\text{C}_{11}\text{H}_{12}\text{NP})_2](\text{BF}_4)_2 \cdot \text{C}_2\text{H}_3\text{N}$ (**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 Me₂Pqn chelate planes. In the crystal structure of **2**, three F atoms of one of the BF₄[−] anions are disordered over two sets of positions with refined occupancies of 0.573 (10) and 0.427 (10).

1. Chemical context

8-Quinolyolphosphanes 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 σ -donating character and an imine-N atom incorporated in a π -conjugated quinoline ring (Salem & Wild, 1992; Scattolin *et al.*, 2017; Cai *et al.*, 2018). The electronic properties of these ligands, in particular their π -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 (Ph₂Pqn) 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 (Me₂Pqn), 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 Me₂Pqn 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(Me₂Pqn)₂](BF₄)₂ (Suzuki *et al.*, 1995), but the crystal structures of the corresponding Ni^{II} and Pt^{II} complexes were not compared.



2. Structural commentary

A red block-shaped crystal of the Ni^{II} complex, [Ni(Me₂Pqn)₂](ClO₄)₂·CH₃NO₂ (**1**), recrystallized from nitromethane/diisopropyl ether and a colorless platelet crystal of the Pt^{II} complex, [Pt(Me₂Pqn)₂](BF₄)₂·CH₃CN (**2**), recryst-

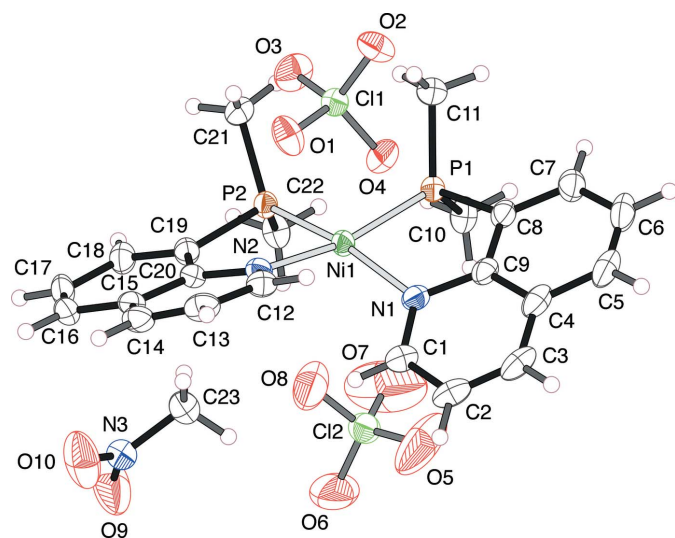


Figure 1
An ellipsoid plot of the molecular structures in [Ni(Me₂Pqn)₂](ClO₄)₂·CH₃NO₂ (**1**), showing the atom-numbering scheme, with ellipsoids drawn at the 50% probability level.

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)

tallized from acetonitrile/diisopropyl ether were used for the X-ray diffraction analysis.

In the crystal structure of **2**, three F atoms of one of the BF₄[−] anions show disorder over two sets of positions: (F2A, F3A and F4A) and (F2B, F3B and F4B). 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 Me₂Pqn ligands coordinate to a metal(II) center in the bidentate κ²P,N mode to form a *cis*-isomer of the complex dication, (SP-4-2)-[M(Me₂Pqn)₂]²⁺ (*M*

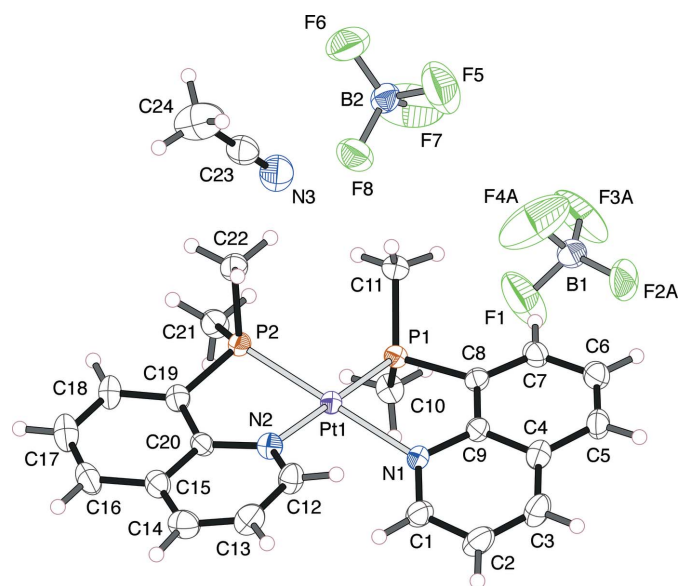


Figure 2
An ellipsoid plot of the molecular structures in [Pt(Me₂Pqn)₂](BF₄)₂·CH₃CN (**2**), showing the atom-numbering scheme, with ellipsoids drawn at the 50% probability level. The minor component atoms (F2B, F3B and F4B) of the positionally disordered F atoms are omitted for clarity.

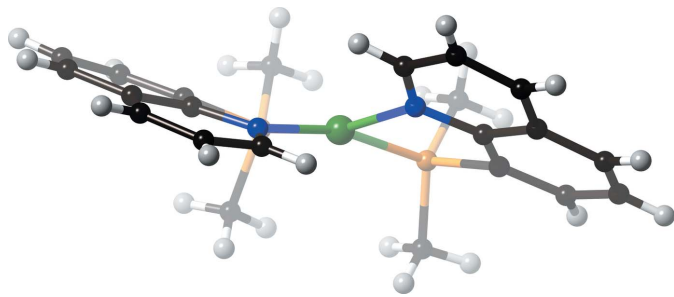


Figure 3

A perspective side view (from one of the NiPN coordination planes) of $[\text{Ni}(\text{Me}_2\text{Pqn})_2](\text{ClO}_4)_2 \cdot \text{CH}_3\text{NO}_2$ (**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(κ^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 $[\text{Ni}(\text{MePhPqn})_2](\text{BF}_4)_2$ [MePhPqn = 8-(methylphenylphosphanyl)quinoline; 1.954 (3) and 1.977 (3) Å] and $[\text{Ni}(\text{Ph}_2\text{Pqn})_2](\text{BF}_4)_2$ [1.954 (6) and 1.949 (5) Å] (Hashimoto *et al.*, 2010), indicating the *trans* influence becomes stronger in the order of $\text{Ph}_2\text{Pqn} < \text{MePhPqn} < \text{Me}_2\text{Pqn}$. 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 $[\text{Pt}(\text{Ph}_2\text{Pqn})_2](\text{ClO}_4)_2$ [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)°], $[\text{Ni}(\text{MePhPqn})_2](\text{BF}_4)_2$ [2.151 (1) and 2.162 (1) Å; 87.4 (1) and 86.6 (1)°] and $[\text{Ni}(\text{Ph}_2\text{Pqn})_2](\text{BF}_4)_2$ [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 $[\text{Pt}(\text{Ph}_2\text{Pqn})_2](\text{ClO}_4)_2$ [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

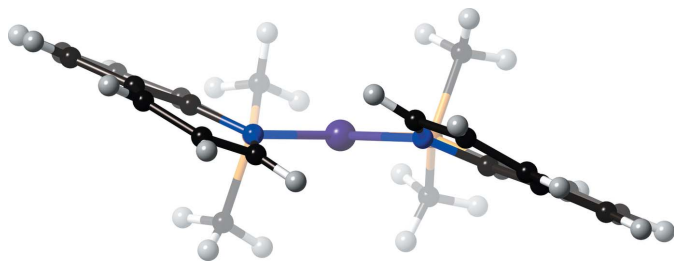


Figure 4

A perspective side view (from one of the PtPN coordination planes) of $[\text{Pt}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2 \cdot \text{CH}_3\text{CN}$ (**2**). Color code: Pt, purple; P, orange; N, blue; C, black and H, gray.

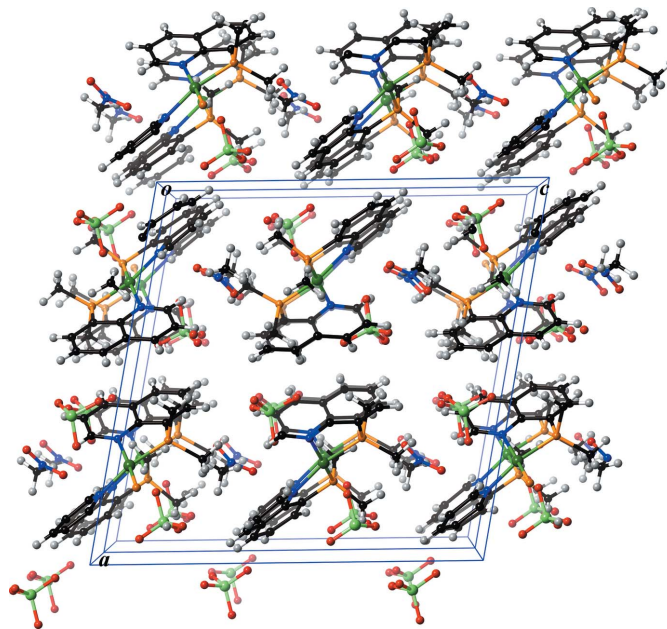


Figure 5

A packing drawing of $[\text{Ni}(\text{Me}_2\text{Pqn})_2](\text{ClO}_4)_2 \cdot \text{CH}_3\text{NO}_2$ (**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 τ_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 Ph₂Pqn complexes, the τ_4 values are 0.273 (1)° and 0.189 (2)°, respectively. By contrast, the τ_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 $[\text{Pt}(\text{Ph}_2\text{Pqn})_2](\text{BF}_4)_2$ 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 Me₂Pqn 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, φ_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 [C₉H₆N] 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 φ_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, $[\text{Pd}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2$, has a τ_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 $[\text{Ni}(\text{Me}_2\text{Pqn})_2]^{2+}$ complex cation in the asymmetric unit. The asymmetric unit of the Pt^{II} complex, **2**, contains a $[\text{Pt}(\text{Me}_2\text{Pqn})_2]^{2+}$ 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*- $[\text{Pd}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2$ (refcode ZIFPUZ in the CSD database, version 5.41, last update May 2020; Groom *et al.*, 2016) and $[\text{Pd}_2\text{Cl}_2(\text{Me}_2\text{Pqn})_2]$ (ZIFQAG; Suzuki *et al.*, 1995), $[\text{Cu}(\text{Me}_2\text{Pqn})_2]\text{PF}_6$ (OZILAL; Suzuki *et al.*, 2011), $[\text{Ru}(\text{bpy})_{3-n}(\text{Me}_2\text{Pqn})_n](\text{PF}_6)_2$ (bpy = 2,2'-bipyridine; HUTRIV, HUTPCB, HUTPUH and HUTQAO; Suzuki *et al.*, 2003), and $[\text{Pt}(\text{ppy})(\text{Me}_2\text{Pqn})]\text{BF}_4$ (ppy = 2-(2'-pyridyl)phenyl; Mori & Suzuki, 2020). Some of the related bis(8-quinolylphosphanes) complexes are: $[\text{Ni}(\text{Ph}_2\text{Pqn})_2](\text{BF}_4)_n$ ($n = 1$ or 2 ; BUGDAJ, BUGDEN and BUGDOX) and $[\text{Ni}(\text{MePhPqn})_2](\text{BF}_4)_2$ (BUGDIR; Hashimoto *et al.*, 2010), $[\text{Pd}(\text{Ph}_2\text{Pqn})_2]\text{X}_2$ ($\text{X}_2 = \text{Cl}_2, \text{Br}_2$ or ClBF_4 ; FERZOS, FERZUY and FESBAH; Suzuki, 2004), $[\text{Cu}(\text{Ph}_2\text{Pqn})_2]\text{BF}_4$ (OZILEP and OZILEP01; Suzuki *et al.*, 2011) and $[\text{Cu}(\text{Ph}_2\text{Pqn})_2]\text{PF}_6$ (NOPNIQ; Tsukuda *et al.*, 2009).

5. Synthesis and crystallization

The ligand, Me_2Pqn , and the nickel(II) complexes, $[\text{Ni}(\text{Me}_2\text{Pqn})_2](\text{ClO}_4)_2$, 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, $[\text{Pt}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2$, 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 $[\text{PtCl}_2(\text{EtCN})_2]$ (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 $[\text{Pt}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2 \cdot \text{CH}_3\text{CN}$ (**2**) were obtained by recrystallization from an acetonitrile solution by diffusion of diisopropyl ether. Yield: 0.126 g (61%). Analysis calculated for $\text{C}_{24}\text{H}_{27}\text{B}_2\text{F}_8\text{N}_3\text{Pt}$: C, 35.37; H, 3.24; N, 3.75%. Found (after completely drying): C, 35.39; H, 2.89; N, 3.74%.

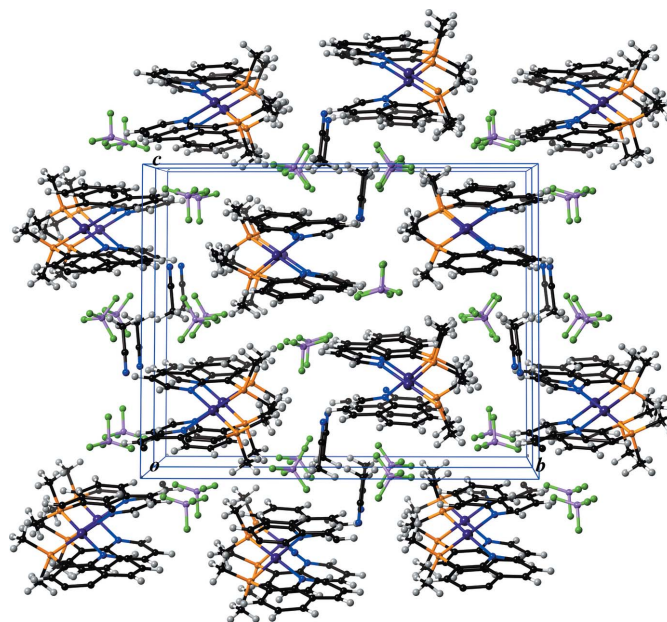


Figure 6

A packing drawing of $[\text{Pt}(\text{Me}_2\text{Pqn})_2](\text{BF}_4)_2 \cdot \text{CH}_3\text{CN}$ (**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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. 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 ·CH ₃ NO ₂	[Pt(C ₁₁ H ₁₂ NP) ₂](BF ₄) ₂ ·C ₂ H ₃ N
<i>M_r</i>	697.02	788.13
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	188	188
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.8114 (13), 8.9398 (6), 18.0245 (14)	7.9102 (3), 21.0833 (5), 16.7519 (4)
β (°)	100.524 (3)	95.3931 (11)
<i>V</i> (Å ³)	2821.8 (4)	2781.42 (15)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (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 (<i>ABSCOR</i> ; Rigaku, 1995)	Numerical (<i>NUMABS</i> ; Rigaku, 1999)
<i>T</i> _{min} , <i>T</i> _{max}	0.379, 0.811	0.338, 0.594
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	26671, 6459, 5440	43967, 6350, 5435
<i>R</i> _{int}	0.041	0.042
(sin θ/λ) _{max} (Å ⁻¹)	0.649	0.649
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	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
Δρ _{max} , Δρ _{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

Acta Cryst. (2020). E76, 1813-1817 [https://doi.org/10.1107/S2056989020014437]

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

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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- κ^2N,P]nickel(II) bis(perchlorate) nitromethane monosolvate (1)

Crystal data

[Ni(C₁₁H₁₂NP)₂](ClO₄)₂·CH₃NO₂

$M_r = 697.02$

Monoclinic, *P2₁/c*

$a = 17.8114$ (13) Å

$b = 8.9398$ (6) Å

$c = 18.0245$ (14) Å

$\beta = 100.524$ (3)°

$V = 2821.8$ (4) Å³

$Z = 4$

$F(000) = 1432$

$D_x = 1.641$ 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

$0.70 \times 0.50 \times 0.20$ mm

Data collection

Rigaku R-AXIS RAPID
diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 10.000 pixels mm⁻¹

ω 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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.2$ °

$h = -23$ → 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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.03 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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)

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, °)

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)

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
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—C11—O2	110.15 (13)	H10A—C10—H10B	109.5
O3—C11—O1	109.95 (14)	P1—C10—H10C	109.5
O2—C11—O1	109.60 (13)	H10A—C10—H10C	109.5
O3—C11—O4	109.09 (14)	H10B—C10—H10C	109.5
O2—C11—O4	109.61 (13)	P1—C11—H11A	109.5
O1—C11—O4	108.41 (14)	P1—C11—H11B	109.5
O7—C12—O5	111.9 (4)	H11A—C11—H11B	109.5
O7—C12—O6	106.6 (3)	P1—C11—H11C	109.5
O5—C12—O6	111.0 (2)	H11A—C11—H11C	109.5
O7—C12—O8	105.4 (3)	H11B—C11—H11C	109.5
O5—C12—O8	110.3 (2)	N2—C12—C13	123.4 (2)
O6—C12—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)

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- κ^2N,P]platinum(II) bis(tetrafluoroborate) acetonitrile monosolvate (2)

Crystal data

[Pt(C₁₁H₁₂NP)₂](BF₄)₂·C₂H₃N

M_r = 788.13

Monoclinic, *P*2₁/*n*

a = 7.9102 (3) Å

b = 21.0833 (5) Å

c = 16.7519 (4) Å

β = 95.3931 (11)°

V = 2781.42 (15) Å³

Z = 4

F(000) = 1528

D_x = 1.882 Mg m⁻³

Mo *K* α radiation, λ = 0.71075 Å

Cell parameters from 31045 reflections

θ = 3.1–27.5°

μ = 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

ω 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 σ (*I*)

R_{int} = 0.042

θ_{\max} = 27.5°, θ_{\min} = 3.1°

h = -10→10

k = -27→27

l = -21→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 $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 1.42 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -1.44 \text{ e } \text{Å}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	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, °)

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
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)

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)		
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)

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)
