

[*N,N*-Bis(diphenylphosphanyl)-propanamine- κ^2P,P']dichloridonickel(II)

Bang-Shao Yin,* Tian-Bao Li and Ming-Sheng Yang

 College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha, Hunan 410081, People's Republic of China
 Correspondence e-mail: yinbangshao@yahoo.cn

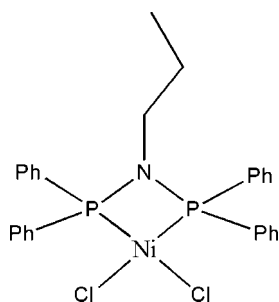
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 Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.068; wR factor = 0.175; data-to-parameter ratio = 15.2.

In the title complex, $[\text{NiCl}_2(\text{C}_{27}\text{H}_{27}\text{NP}_2)]$, the Ni^{2+} ion is coordinated by two chloride ions and two P atoms of the bidentate *N,N*-bis(diphenylphosphanyl)propyl ligand to generate a strongly distorted *cis*- NiCl_2P_2 square-planar geometry for the metal ion. A NiP_2N rhombus occurs within the chelating ligand.

Related literature

For details of the synthesis, see: Sun *et al.* (2006). For a related structure, see: Yin *et al.* (2011).



Experimental

Crystal data

 $[\text{NiCl}_2(\text{C}_{27}\text{H}_{27}\text{NP}_2)]$
 $M_r = 557.05$

 Monoclinic, $P2_1/c$
 $a = 10.210$ (4) Å
 $b = 19.308$ (7) Å
 $c = 15.538$ (4) Å
 $\beta = 122.669$ (18)°
 $V = 2578.5$ (15) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.10$ mm⁻¹
 $T = 113$ K
 $0.08 \times 0.08 \times 0.04$ mm

Data collection

 Rigaku Saturn724 CCD
 diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2005)
 $T_{\min} = 0.917$, $T_{\max} = 0.957$

 21461 measured reflections
 4550 independent reflections
 3978 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.076$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.175$
 $S = 1.15$
 4550 reflections

 299 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 1.66$ e Å⁻³
 $\Delta\rho_{\min} = -0.57$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|-------------|-------------|-------------|
| Ni1—P2 | 2.1244 (16) | Ni1—Cl2 | 2.1964 (17) |
| Ni1—P1 | 2.1274 (16) | Ni1—Cl1 | 2.1977 (16) |
| P2—Ni1—P1 | 73.41 (5) | P2—Ni1—Cl1 | 163.08 (6) |
| P2—Ni1—Cl2 | 96.11 (5) | P1—Ni1—Cl1 | 91.96 (6) |
| P1—Ni1—Cl2 | 168.01 (6) | Cl2—Ni1—Cl1 | 99.22 (6) |

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MS, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6453).

References

- Rigaku/MS (2005). *CrystalClear* and *CrystalStructure*. Rigaku/MS Inc., The Woodlands, Texas, USA.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Sun, Z., Zhu, F. & Lin, S. (2006). *Appl. Organomet. Chem.* **20**, 175–180.
 Yin, B.-S., Li, T.-B. & Yang, M.-S. (2011). *Acta Cryst.* **E67**, m1571.

supplementary materials

Acta Cryst. (2011). E67, m1572 [doi:10.1107/S1600536811042760]

[*N,N*-Bis(diphenylphosphanyl)propanamine- κ^2P,P']dichloridonickel(II)

B.-S. Yin, T.-B. Li and M.-S. Yang

Experimental

The title complex, (I), was prepared according to the literature procedures (Sun *et al.*, 2006). Red prisms of (I) were grown from slow evaporation of a dichloromethane and hexane solution at room temperature.

Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

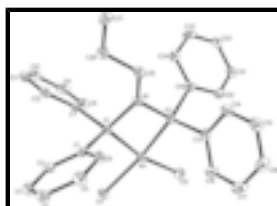


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

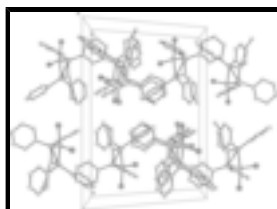


Fig. 2. The packing for (I).

[*N,N*-Bis(diphenylphosphanyl)propanamine- κ^2P,P']dichloridonickel(II)

Crystal data

[NiCl₂(C₂₇H₂₇NP₂)]

$M_r = 557.05$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.210$ (4) Å

$b = 19.308$ (7) Å

$c = 15.538$ (4) Å

$\beta = 122.669$ (18)°

$V = 2578.5$ (15) Å³

$F(000) = 1152$

$D_x = 1.435$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7237 reflections

$\theta = 1.9$ – 26.1 °

$\mu = 1.10$ mm⁻¹

$T = 113$ K

Prism, red

$0.08 \times 0.08 \times 0.04$ mm

supplementary materials

Z = 4

Data collection

| | |
|---|--|
| Rigaku Saturn724 CCD diffractometer | 4550 independent reflections |
| Radiation source: rotating anode multilayer | 3978 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 14.22 pixels mm^{-1} | $R_{\text{int}} = 0.076$ |
| ω and φ scans | $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.9^\circ$ |
| Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MSO, 2005) | $h = -12 \rightarrow 12$ |
| $T_{\text{min}} = 0.917$, $T_{\text{max}} = 0.957$ | $k = -22 \rightarrow 22$ |
| 21461 measured reflections | $l = -17 \rightarrow 18$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.068$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.175$ | H-atom parameters constrained |
| $S = 1.15$ | $w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 3.0298P]$ |
| 4550 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 299 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 1.66 \text{ e } \text{\AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.57 \text{ e } \text{\AA}^{-3}$ |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|--------------|----------------------------------|
| Ni1 | 0.68919 (7) | 0.31831 (3) | 0.21970 (5) | 0.0212 (2) |
| Cl1 | 0.44166 (14) | 0.29800 (7) | 0.10697 (10) | 0.0306 (3) |
| Cl2 | 0.67979 (15) | 0.43135 (7) | 0.23126 (10) | 0.0330 (3) |
| P1 | 0.74240 (14) | 0.21070 (7) | 0.23889 (10) | 0.0211 (3) |

| | | | | |
|------|--------------|-------------|--------------|-------------|
| P2 | 0.93563 (14) | 0.31029 (7) | 0.31062 (10) | 0.0209 (3) |
| N1 | 0.9378 (4) | 0.2224 (2) | 0.3110 (3) | 0.0218 (9) |
| C1 | 0.6902 (5) | 0.1587 (3) | 0.1285 (4) | 0.0214 (10) |
| C2 | 0.5479 (6) | 0.1242 (3) | 0.0752 (4) | 0.0268 (12) |
| H2 | 0.4800 | 0.1259 | 0.0993 | 0.032* |
| C3 | 0.5054 (6) | 0.0877 (3) | -0.0125 (4) | 0.0307 (12) |
| H3 | 0.4084 | 0.0642 | -0.0485 | 0.037* |
| C4 | 0.6052 (6) | 0.0851 (3) | -0.0485 (4) | 0.0315 (13) |
| H4 | 0.5766 | 0.0594 | -0.1083 | 0.038* |
| C5 | 0.7447 (6) | 0.1200 (3) | 0.0033 (4) | 0.0327 (13) |
| H5 | 0.8123 | 0.1184 | -0.0211 | 0.039* |
| C6 | 0.7874 (6) | 0.1573 (3) | 0.0906 (4) | 0.0262 (11) |
| H6 | 0.8829 | 0.1821 | 0.1250 | 0.031* |
| C7 | 0.6744 (5) | 0.1657 (3) | 0.3101 (4) | 0.0248 (11) |
| C8 | 0.6334 (6) | 0.2064 (3) | 0.3666 (4) | 0.0333 (13) |
| H8 | 0.6415 | 0.2554 | 0.3666 | 0.040* |
| C9 | 0.5809 (7) | 0.1747 (4) | 0.4225 (4) | 0.0415 (16) |
| H9 | 0.5494 | 0.2024 | 0.4588 | 0.050* |
| C10 | 0.5737 (6) | 0.1036 (4) | 0.4260 (5) | 0.0435 (16) |
| H10 | 0.5413 | 0.0825 | 0.4667 | 0.052* |
| C11 | 0.6136 (6) | 0.0627 (3) | 0.3701 (4) | 0.0391 (15) |
| H11 | 0.6056 | 0.0137 | 0.3711 | 0.047* |
| C12 | 0.6652 (6) | 0.0932 (3) | 0.3127 (4) | 0.0295 (12) |
| H12 | 0.6941 | 0.0652 | 0.2753 | 0.035* |
| C13 | 1.0345 (6) | 0.3415 (3) | 0.2503 (4) | 0.0247 (11) |
| C14 | 1.1920 (6) | 0.3300 (3) | 0.2929 (4) | 0.0317 (13) |
| H14 | 1.2522 | 0.3079 | 0.3576 | 0.038* |
| C15 | 1.2620 (6) | 0.3506 (3) | 0.2417 (4) | 0.0343 (13) |
| H15 | 1.3699 | 0.3424 | 0.2713 | 0.041* |
| C16 | 1.1762 (7) | 0.3828 (3) | 0.1482 (4) | 0.0364 (14) |
| H16 | 1.2242 | 0.3960 | 0.1126 | 0.044* |
| C17 | 1.0194 (7) | 0.3960 (3) | 0.1059 (5) | 0.0410 (15) |
| H17 | 0.9608 | 0.4197 | 0.0425 | 0.049* |
| C18 | 0.9484 (6) | 0.3747 (3) | 0.1559 (4) | 0.0321 (13) |
| H18 | 0.8404 | 0.3828 | 0.1258 | 0.039* |
| C19 | 1.0500 (5) | 0.3412 (3) | 0.4406 (4) | 0.0239 (11) |
| C20 | 1.0872 (6) | 0.4110 (3) | 0.4589 (4) | 0.0265 (11) |
| H20 | 1.0581 | 0.4413 | 0.4031 | 0.032* |
| C21 | 1.1660 (6) | 0.4372 (3) | 0.5572 (4) | 0.0313 (12) |
| H21 | 1.1881 | 0.4853 | 0.5686 | 0.038* |
| C22 | 1.2134 (6) | 0.3926 (3) | 0.6401 (4) | 0.0291 (12) |
| H22 | 1.2697 | 0.4101 | 0.7079 | 0.035* |
| C23 | 1.1778 (6) | 0.3232 (3) | 0.6224 (4) | 0.0334 (13) |
| H23 | 1.2114 | 0.2930 | 0.6789 | 0.040* |
| C24 | 1.0937 (6) | 0.2961 (3) | 0.5239 (4) | 0.0283 (12) |
| H24 | 1.0662 | 0.2485 | 0.5128 | 0.034* |
| C25 | 1.0738 (6) | 0.1766 (3) | 0.3458 (4) | 0.0299 (12) |
| H25A | 1.1635 | 0.1957 | 0.4097 | 0.036* |
| H25B | 1.1010 | 0.1767 | 0.2936 | 0.036* |

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|------|------------|------------|------------|-------------|
| C26 | 1.0480 (6) | 0.1034 (3) | 0.3647 (5) | 0.0347 (13) |
| H26A | 0.9621 | 0.0829 | 0.3003 | 0.042* |
| H26B | 1.0172 | 0.1027 | 0.4152 | 0.042* |
| C27 | 1.1960 (6) | 0.0599 (3) | 0.4050 (4) | 0.0322 (13) |
| H27A | 1.2205 | 0.0566 | 0.3522 | 0.048* |
| H27B | 1.1791 | 0.0133 | 0.4224 | 0.048* |
| H27C | 1.2828 | 0.0819 | 0.4661 | 0.048* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|-------------|--------------|
| Ni1 | 0.0193 (4) | 0.0231 (4) | 0.0222 (4) | 0.0025 (3) | 0.0119 (3) | 0.0018 (3) |
| Cl1 | 0.0179 (6) | 0.0413 (8) | 0.0293 (7) | 0.0024 (5) | 0.0106 (5) | 0.0007 (6) |
| Cl2 | 0.0362 (8) | 0.0258 (7) | 0.0377 (8) | 0.0063 (5) | 0.0205 (6) | 0.0023 (6) |
| P1 | 0.0193 (7) | 0.0236 (7) | 0.0216 (7) | -0.0009 (5) | 0.0118 (5) | -0.0001 (5) |
| P2 | 0.0194 (7) | 0.0213 (7) | 0.0219 (7) | 0.0008 (5) | 0.0112 (5) | 0.0004 (5) |
| N1 | 0.018 (2) | 0.023 (2) | 0.024 (2) | 0.0008 (17) | 0.0112 (18) | -0.0022 (18) |
| C1 | 0.022 (3) | 0.017 (3) | 0.026 (3) | 0.003 (2) | 0.013 (2) | 0.001 (2) |
| C2 | 0.025 (3) | 0.029 (3) | 0.023 (3) | -0.002 (2) | 0.012 (2) | 0.001 (2) |
| C3 | 0.028 (3) | 0.033 (3) | 0.030 (3) | -0.003 (2) | 0.014 (2) | -0.002 (2) |
| C4 | 0.034 (3) | 0.033 (3) | 0.025 (3) | 0.005 (2) | 0.014 (2) | -0.001 (2) |
| C5 | 0.034 (3) | 0.039 (3) | 0.030 (3) | -0.002 (2) | 0.021 (3) | -0.004 (3) |
| C6 | 0.027 (3) | 0.027 (3) | 0.027 (3) | -0.003 (2) | 0.017 (2) | -0.001 (2) |
| C7 | 0.020 (3) | 0.033 (3) | 0.020 (3) | -0.001 (2) | 0.010 (2) | 0.004 (2) |
| C8 | 0.033 (3) | 0.041 (3) | 0.031 (3) | 0.003 (3) | 0.021 (3) | 0.001 (3) |
| C9 | 0.034 (3) | 0.071 (5) | 0.027 (3) | 0.008 (3) | 0.021 (3) | 0.008 (3) |
| C10 | 0.026 (3) | 0.073 (5) | 0.034 (3) | -0.001 (3) | 0.017 (3) | 0.017 (3) |
| C11 | 0.026 (3) | 0.047 (4) | 0.034 (3) | -0.009 (3) | 0.009 (3) | 0.012 (3) |
| C12 | 0.019 (3) | 0.038 (3) | 0.028 (3) | -0.002 (2) | 0.010 (2) | 0.003 (2) |
| C13 | 0.028 (3) | 0.023 (3) | 0.026 (3) | -0.005 (2) | 0.016 (2) | -0.003 (2) |
| C14 | 0.025 (3) | 0.043 (4) | 0.025 (3) | -0.002 (2) | 0.013 (2) | -0.003 (2) |
| C15 | 0.028 (3) | 0.048 (4) | 0.033 (3) | -0.005 (3) | 0.021 (3) | -0.006 (3) |
| C16 | 0.044 (3) | 0.044 (4) | 0.038 (3) | 0.003 (3) | 0.033 (3) | 0.002 (3) |
| C17 | 0.049 (4) | 0.047 (4) | 0.038 (3) | 0.020 (3) | 0.031 (3) | 0.018 (3) |
| C18 | 0.030 (3) | 0.041 (4) | 0.028 (3) | 0.009 (2) | 0.017 (2) | 0.006 (2) |
| C19 | 0.020 (3) | 0.028 (3) | 0.025 (3) | 0.004 (2) | 0.013 (2) | 0.002 (2) |
| C20 | 0.029 (3) | 0.027 (3) | 0.027 (3) | 0.000 (2) | 0.017 (2) | 0.002 (2) |
| C21 | 0.029 (3) | 0.032 (3) | 0.031 (3) | -0.008 (2) | 0.016 (2) | -0.010 (2) |
| C22 | 0.025 (3) | 0.040 (3) | 0.024 (3) | 0.000 (2) | 0.014 (2) | -0.005 (2) |
| C23 | 0.036 (3) | 0.047 (4) | 0.018 (3) | 0.012 (3) | 0.015 (2) | 0.012 (2) |
| C24 | 0.029 (3) | 0.026 (3) | 0.037 (3) | 0.001 (2) | 0.022 (3) | 0.001 (2) |
| C25 | 0.020 (3) | 0.025 (3) | 0.039 (3) | 0.003 (2) | 0.013 (2) | -0.002 (2) |
| C26 | 0.030 (3) | 0.024 (3) | 0.045 (3) | 0.000 (2) | 0.017 (3) | -0.002 (3) |
| C27 | 0.034 (3) | 0.028 (3) | 0.040 (3) | 0.008 (2) | 0.023 (3) | 0.006 (3) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-------------|---------|-----------|
| Ni1—P2 | 2.1244 (16) | C12—H12 | 0.9500 |
| Ni1—P1 | 2.1274 (16) | C13—C14 | 1.387 (7) |

| | | | |
|-------------|-------------|-------------|-----------|
| Ni1—C12 | 2.1964 (17) | C13—C18 | 1.395 (7) |
| Ni1—C11 | 2.1977 (16) | C14—C15 | 1.385 (7) |
| P1—N1 | 1.695 (4) | C14—H14 | 0.9500 |
| P1—C1 | 1.802 (5) | C15—C16 | 1.376 (8) |
| P1—C7 | 1.815 (5) | C15—H15 | 0.9500 |
| P1—P2 | 2.5413 (19) | C16—C17 | 1.387 (8) |
| P2—N1 | 1.697 (4) | C16—H16 | 0.9500 |
| P2—C19 | 1.803 (5) | C17—C18 | 1.380 (8) |
| P2—C13 | 1.811 (5) | C17—H17 | 0.9500 |
| N1—C25 | 1.480 (6) | C18—H18 | 0.9500 |
| C1—C2 | 1.393 (7) | C19—C20 | 1.389 (7) |
| C1—C6 | 1.401 (7) | C19—C24 | 1.418 (7) |
| C2—C3 | 1.380 (7) | C20—C21 | 1.381 (7) |
| C2—H2 | 0.9500 | C20—H20 | 0.9500 |
| C3—C4 | 1.403 (7) | C21—C22 | 1.400 (8) |
| C3—H3 | 0.9500 | C21—H21 | 0.9500 |
| C4—C5 | 1.376 (8) | C22—C23 | 1.377 (8) |
| C4—H4 | 0.9500 | C22—H22 | 0.9500 |
| C5—C6 | 1.382 (7) | C23—C24 | 1.390 (8) |
| C5—H5 | 0.9500 | C23—H23 | 0.9500 |
| C6—H6 | 0.9500 | C24—H24 | 0.9500 |
| C7—C8 | 1.401 (7) | C25—C26 | 1.495 (7) |
| C7—C12 | 1.404 (8) | C25—H25A | 0.9900 |
| C8—C9 | 1.385 (8) | C25—H25B | 0.9900 |
| C8—H8 | 0.9500 | C26—C27 | 1.536 (7) |
| C9—C10 | 1.379 (9) | C26—H26A | 0.9900 |
| C9—H9 | 0.9500 | C26—H26B | 0.9900 |
| C10—C11 | 1.387 (9) | C27—H27A | 0.9800 |
| C10—H10 | 0.9500 | C27—H27B | 0.9800 |
| C11—C12 | 1.390 (7) | C27—H27C | 0.9800 |
| C11—H11 | 0.9500 | | |
| P2—Ni1—P1 | 73.41 (5) | C7—C12—H12 | 120.1 |
| P2—Ni1—C12 | 96.11 (5) | C14—C13—C18 | 119.1 (5) |
| P1—Ni1—C12 | 168.01 (6) | C14—C13—P2 | 121.8 (4) |
| P2—Ni1—C11 | 163.08 (6) | C18—C13—P2 | 119.1 (4) |
| P1—Ni1—C11 | 91.96 (6) | C15—C14—C13 | 120.4 (5) |
| C12—Ni1—C11 | 99.22 (6) | C15—C14—H14 | 119.8 |
| N1—P1—Ni1 | 94.77 (15) | C13—C14—H14 | 119.8 |
| N1—P2—Ni1 | 94.82 (14) | C16—C15—C14 | 120.3 (5) |
| P1—N1—P2 | 97.0 (2) | C16—C15—H15 | 119.8 |
| N1—P1—C1 | 109.9 (2) | C14—C15—H15 | 119.8 |
| N1—P1—C7 | 111.2 (2) | C15—C16—C17 | 119.8 (5) |
| C1—P1—C7 | 107.5 (2) | C15—C16—H16 | 120.1 |
| C1—P1—Ni1 | 119.23 (17) | C17—C16—H16 | 120.1 |
| C7—P1—Ni1 | 113.62 (18) | C18—C17—C16 | 120.1 (5) |
| N1—P2—C19 | 109.1 (2) | C18—C17—H17 | 119.9 |
| N1—P2—C13 | 108.9 (2) | C16—C17—H17 | 119.9 |
| C19—P2—C13 | 105.3 (2) | C17—C18—C13 | 120.3 (5) |
| C19—P2—Ni1 | 122.63 (16) | C17—C18—H18 | 119.9 |

supplementary materials

| | | | |
|---------------|--------------|---------------|------------|
| C13—P2—Ni1 | 115.01 (18) | C13—C18—H18 | 119.9 |
| C25—N1—P1 | 134.3 (3) | C20—C19—C24 | 119.5 (5) |
| C25—N1—P2 | 127.4 (3) | C20—C19—P2 | 119.4 (4) |
| C2—C1—C6 | 119.3 (5) | C24—C19—P2 | 121.0 (4) |
| C2—C1—P1 | 120.6 (4) | C21—C20—C19 | 120.9 (5) |
| C6—C1—P1 | 119.9 (4) | C21—C20—H20 | 119.6 |
| C3—C2—C1 | 120.1 (5) | C19—C20—H20 | 119.6 |
| C3—C2—H2 | 119.9 | C20—C21—C22 | 119.9 (5) |
| C1—C2—H2 | 119.9 | C20—C21—H21 | 120.1 |
| C2—C3—C4 | 120.2 (5) | C22—C21—H21 | 120.1 |
| C2—C3—H3 | 119.9 | C23—C22—C21 | 119.5 (5) |
| C4—C3—H3 | 119.9 | C23—C22—H22 | 120.3 |
| C5—C4—C3 | 119.6 (5) | C21—C22—H22 | 120.3 |
| C5—C4—H4 | 120.2 | C22—C23—C24 | 121.7 (5) |
| C3—C4—H4 | 120.2 | C22—C23—H23 | 119.2 |
| C4—C5—C6 | 120.5 (5) | C24—C23—H23 | 119.2 |
| C4—C5—H5 | 119.7 | C23—C24—C19 | 118.5 (5) |
| C6—C5—H5 | 119.7 | C23—C24—H24 | 120.7 |
| C5—C6—C1 | 120.2 (5) | C19—C24—H24 | 120.7 |
| C5—C6—H6 | 119.9 | N1—C25—C26 | 114.0 (4) |
| C1—C6—H6 | 119.9 | N1—C25—H25A | 108.7 |
| C8—C7—C12 | 119.7 (5) | C26—C25—H25A | 108.7 |
| C8—C7—P1 | 117.1 (4) | N1—C25—H25B | 108.7 |
| C12—C7—P1 | 123.2 (4) | C26—C25—H25B | 108.7 |
| C9—C8—C7 | 119.5 (6) | H25A—C25—H25B | 107.6 |
| C9—C8—H8 | 120.2 | C25—C26—C27 | 111.0 (4) |
| C7—C8—H8 | 120.2 | C25—C26—H26A | 109.4 |
| C10—C9—C8 | 120.7 (6) | C27—C26—H26A | 109.4 |
| C10—C9—H9 | 119.6 | C25—C26—H26B | 109.4 |
| C8—C9—H9 | 119.6 | C27—C26—H26B | 109.4 |
| C9—C10—C11 | 120.2 (5) | H26A—C26—H26B | 108.0 |
| C9—C10—H10 | 119.9 | C26—C27—H27A | 109.5 |
| C11—C10—H10 | 119.9 | C26—C27—H27B | 109.5 |
| C10—C11—C12 | 120.1 (6) | H27A—C27—H27B | 109.5 |
| C10—C11—H11 | 120.0 | C26—C27—H27C | 109.5 |
| C12—C11—H11 | 120.0 | H27A—C27—H27C | 109.5 |
| C11—C12—C7 | 119.7 (5) | H27B—C27—H27C | 109.5 |
| C11—C12—H12 | 120.1 | | |
| P2—Ni1—P1—N1 | -0.03 (14) | P1—C1—C2—C3 | 176.5 (4) |
| C12—Ni1—P1—N1 | -29.8 (3) | C1—C2—C3—C4 | -0.1 (8) |
| C11—Ni1—P1—N1 | 171.31 (15) | C2—C3—C4—C5 | -0.9 (8) |
| P2—Ni1—P1—C1 | -116.06 (19) | C3—C4—C5—C6 | 0.2 (9) |
| C12—Ni1—P1—C1 | -145.8 (3) | C4—C5—C6—C1 | 1.4 (8) |
| C11—Ni1—P1—C1 | 55.28 (19) | C2—C1—C6—C5 | -2.3 (8) |
| P2—Ni1—P1—C7 | 115.61 (19) | P1—C1—C6—C5 | -177.2 (4) |
| C12—Ni1—P1—C7 | 85.9 (3) | N1—P1—C7—C8 | 89.3 (4) |
| C11—Ni1—P1—C7 | -73.05 (18) | C1—P1—C7—C8 | -150.3 (4) |
| C12—Ni1—P1—P2 | -29.7 (3) | Ni1—P1—C7—C8 | -16.2 (5) |
| C11—Ni1—P1—P2 | 171.35 (6) | P2—P1—C7—C8 | 44.3 (5) |

| | | | |
|----------------|-------------|-----------------|------------|
| P1—Ni1—P2—N1 | 0.03 (14) | N1—P1—C7—C12 | -89.2 (4) |
| C12—Ni1—P2—N1 | 174.09 (14) | C1—P1—C7—C12 | 31.2 (5) |
| C11—Ni1—P2—N1 | -31.1 (3) | Ni1—P1—C7—C12 | 165.4 (4) |
| P1—Ni1—P2—C19 | -116.3 (2) | P2—P1—C7—C12 | -134.2 (4) |
| C12—Ni1—P2—C19 | 57.7 (2) | C12—C7—C8—C9 | -1.4 (8) |
| C11—Ni1—P2—C19 | -147.4 (3) | P1—C7—C8—C9 | -180.0 (4) |
| P1—Ni1—P2—C13 | 113.49 (19) | C7—C8—C9—C10 | 2.3 (9) |
| C12—Ni1—P2—C13 | -72.46 (19) | C8—C9—C10—C11 | -2.5 (9) |
| C11—Ni1—P2—C13 | 82.4 (3) | C9—C10—C11—C12 | 1.8 (8) |
| C12—Ni1—P2—P1 | 174.05 (6) | C10—C11—C12—C7 | -1.0 (8) |
| C11—Ni1—P2—P1 | -31.1 (2) | C8—C7—C12—C11 | 0.8 (7) |
| C1—P1—P2—N1 | -78.3 (3) | P1—C7—C12—C11 | 179.2 (4) |
| C7—P1—P2—N1 | 84.2 (3) | N1—P2—C13—C14 | -64.9 (5) |
| Ni1—P1—P2—N1 | -179.9 (2) | C19—P2—C13—C14 | 52.0 (5) |
| N1—P1—P2—C19 | -74.5 (3) | Ni1—P2—C13—C14 | -169.8 (4) |
| C1—P1—P2—C19 | -152.8 (3) | P1—P2—C13—C14 | -108.7 (4) |
| C7—P1—P2—C19 | 9.7 (3) | N1—P2—C13—C18 | 111.7 (4) |
| Ni1—P1—P2—C19 | 105.5 (2) | C19—P2—C13—C18 | -131.3 (4) |
| N1—P1—P2—C13 | 81.5 (3) | Ni1—P2—C13—C18 | 6.8 (5) |
| C1—P1—P2—C13 | 3.2 (3) | P1—P2—C13—C18 | 67.9 (5) |
| C7—P1—P2—C13 | 165.7 (3) | C18—C13—C14—C15 | -0.8 (8) |
| Ni1—P1—P2—C13 | -98.5 (2) | P2—C13—C14—C15 | 175.8 (4) |
| N1—P1—P2—Ni1 | 179.9 (2) | C13—C14—C15—C16 | 0.2 (9) |
| C1—P1—P2—Ni1 | 101.7 (2) | C14—C15—C16—C17 | 1.3 (9) |
| C7—P1—P2—Ni1 | -95.8 (2) | C15—C16—C17—C18 | -2.2 (9) |
| C1—P1—N1—C25 | -43.7 (5) | C16—C17—C18—C13 | 1.7 (9) |
| C7—P1—N1—C25 | 75.2 (5) | C14—C13—C18—C17 | -0.1 (8) |
| Ni1—P1—N1—C25 | -167.2 (5) | P2—C13—C18—C17 | -176.9 (5) |
| P2—P1—N1—C25 | -167.2 (6) | N1—P2—C19—C20 | 169.1 (4) |
| C1—P1—N1—P2 | 123.5 (2) | C13—P2—C19—C20 | 52.3 (4) |
| C7—P1—N1—P2 | -117.6 (2) | Ni1—P2—C19—C20 | -81.8 (4) |
| Ni1—P1—N1—P2 | 0.04 (17) | P1—P2—C19—C20 | -148.4 (3) |
| C19—P2—N1—C25 | -64.5 (5) | N1—P2—C19—C24 | -15.1 (4) |
| C13—P2—N1—C25 | 50.0 (5) | C13—P2—C19—C24 | -131.9 (4) |
| Ni1—P2—N1—C25 | 168.5 (4) | Ni1—P2—C19—C24 | 94.0 (4) |
| P1—P2—N1—C25 | 168.5 (5) | P1—P2—C19—C24 | 27.4 (5) |
| C19—P2—N1—P1 | 127.0 (2) | C24—C19—C20—C21 | -0.1 (7) |
| C13—P2—N1—P1 | -118.5 (2) | P2—C19—C20—C21 | 175.8 (4) |
| Ni1—P2—N1—P1 | -0.04 (17) | C19—C20—C21—C22 | 1.9 (8) |
| N1—P1—C1—C2 | 160.0 (4) | C20—C21—C22—C23 | -1.4 (8) |
| C7—P1—C1—C2 | 38.9 (5) | C21—C22—C23—C24 | -0.9 (8) |
| Ni1—P1—C1—C2 | -92.2 (4) | C22—C23—C24—C19 | 2.7 (8) |
| P2—P1—C1—C2 | -156.3 (3) | C20—C19—C24—C23 | -2.2 (7) |
| N1—P1—C1—C6 | -25.2 (5) | P2—C19—C24—C23 | -178.0 (4) |
| C7—P1—C1—C6 | -146.3 (4) | P1—N1—C25—C26 | -32.8 (7) |
| Ni1—P1—C1—C6 | 82.6 (4) | P2—N1—C25—C26 | 163.3 (4) |
| P2—P1—C1—C6 | 18.5 (5) | N1—C25—C26—C27 | -177.5 (4) |
| C6—C1—C2—C3 | 1.6 (8) | | |

Fig. 1

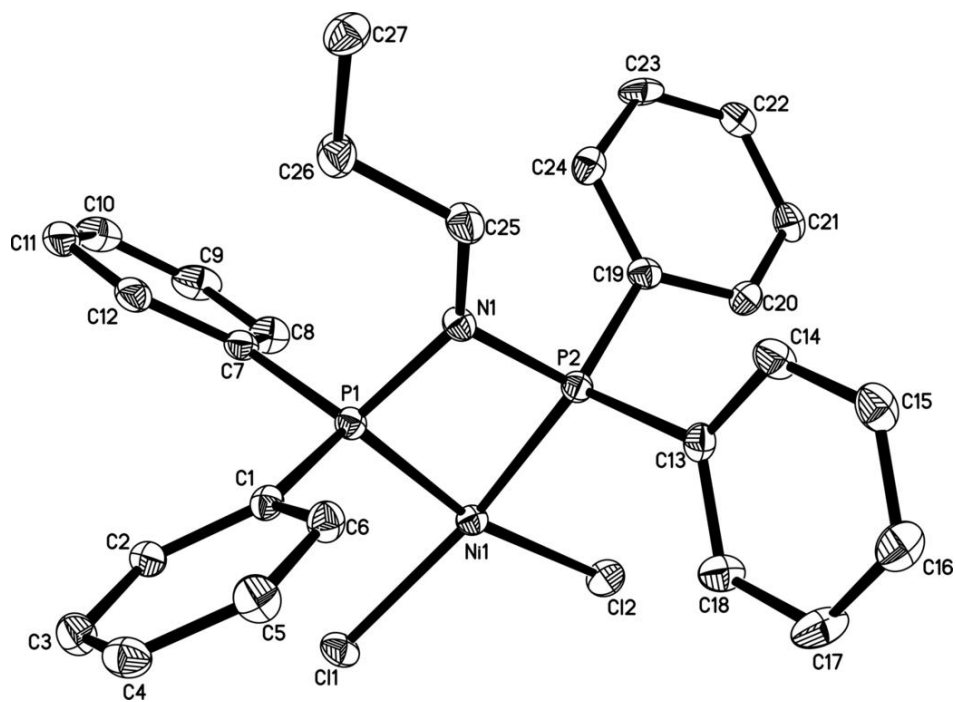


Fig. 2

