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# [1,2-Bis(diphenylphosphanyl)ethane-$\kappa^2P,P'$]{2-[(4-nitrobenzoylmethyl)-diphenylphosphanyl]phenyl-$\kappa^2C,C'$}-palladium(II) trifluoromethanesulfonate–dichloromethane–*n*-hexane (1/1/0.5)

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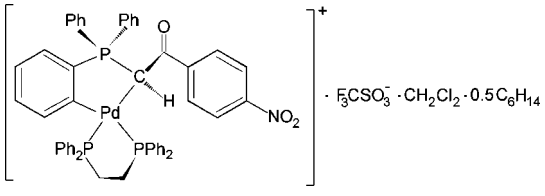
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.004 Å; disorder in solvent or counterion; $R$ factor = 0.029; $wR$ factor = 0.076; data-to-parameter ratio = 15.2.

In the cation of the title compound, $[Pd(C_{26}H_{19}NO_3P)(C_{26}H_{24}P_2)]CF_3O_3S\cdot CH_2Cl_2\cdot 0.5C_6H_{14}$, the $Pd^{II}$ atom has a slightly tetrahedrally distorted square-planar coordination geometry. The $PdC_3P$ and $PdC_2P_2$ five-membered metallacycles adopt envelope and twist conformations, respectively. In the crystal, intermolecular C—H···O hydrogen bonds link cations and anions into a three-dimensional network. The dichloromethane solvent molecule is disordered over three orientations with a site-occupancy ratio of 0.5/0.3/0.2. The *n*-hexane solvent molecule has a crystallographically imposed centre of symmetry.

## Related literature

For the synthesis and applications as catalysts of cyclopalladated metal complexes, see: Rietling *et al.* (2002); Aguilar *et al.* (2008); Dupont *et al.* (2001); Chen *et al.* (2009). For *ortho*-palladated $\alpha$-ketophosphorus ylides complexes reported by our group, see: Karami *et al.* (2010); Karami, Rizzoli & Salah (2011); Karami, Rizzoli & Borzooie (2011). For related structures, see: Falvello *et al.* (1998, 1999); Shao *et al.* (1982).




## Experimental

### Crystal data

$[Pd(C_{26}H_{19}NO_3P)(C_{26}H_{24}P_2)]CF_3O_3S\cdot CH_2Cl_2\cdot 0.5C_6H_{14}$
$M_r$ = 1206.27
Monoclinic, $P2_1/n$
$a$ = 12.4063 (7) Å
$b$ = 14.2445 (8) Å
$c$ = 31.3633 (17) Å
$\beta$ = 91.6675 (9)°
$V$ = 5540.2 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.62 mm$^{-1}$
$T$ = 294 K
0.19 × 0.16 × 0.10 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.872, $T_{max}$ = 0.955
62924 measured reflections
10529 independent reflections
8106 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
$S$ = 1.04
10529 reflections
691 parameters
14 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C19—H19···O1$^{i}$ | 0.93 | 2.54 | 3.284 (3) | 138 |
| C30—H30···O6$^{ii}$ | 0.93 | 2.55 | 3.372 (4) | 148 |
| C39—H39$B$···O6$^{iii}$ | 0.97 | 2.59 | 3.309 (4) | 131 |

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $x, y-1, z$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *SCHAKAL97* (Keller, 1997); software used to prepare material for publication: *SHELXL97* and *PARST95* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2004).

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# supporting information

*Acta Cryst.* (2011). E**67**, m416–m417 [doi:10.1107/S1600536811008075]

# [1,2-Bis(diphenylphosphanyl)ethane-$\kappa^2P,P'$]{2-[(4-nitrobenzoylmethyl)diphenylphosphanyl]phenyl-$\kappa^2C,C'$}palladium(II) trifluoromethanesulfonate–dichloromethane–*n*-hexane (1/1/0.5)

**Corrado Rizzoli, Kazem Karami and Farzaneh Borzooie**

## S1. Comment

The synthesis and characterization of cyclopalladated metal complexes (Rietling *et al.*, 2002) has attracted considerable attention due to their potential applications in organic synthesis and homogenous catalysis (Aguilar *et al.*, 2008; Dupont *et al.*, 2001; Chen *et al.*, 2009). As a continuation of our ongoing project devoted to the development of new catalysts based on *ortho*-palladated *α*-ketophosphorus ylides complexes (Karami *et al.*, 2010; Karami, Rizzoli & Salah, 2011; Karami, Rizzoli & Borzooie, 2011), we report herein the synthesis and crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) consists of one mononuclear complex cation, one trifluoromethanesulfonate anion, one disordered dichloromethane molecule and half an *n*-hexane lying on a centre of symmetry. In the cation (Fig. 2), the palladium(II) atom displays a slightly but not negligibly tetrahedrally distorted square planar coordination geometry, with atoms P2, P3, C1 and C9 displaced from the mean plane through the $P_2C_2$ core by -0.0061 (6), 0.0055 (6), -0.070 (2) and 0.069 (2) Å, respectively. The distortion from the regular square planar geometry is also indicated by the values of the *cis* and *trans* angles subtended at the metal, which range from 83.17 (8) to 100.49 (5)°, and from 175.31 (5) to 175.68 (5)°, respectively. The Pd–C bond lengths involving the aromatic and ylidic carbon atoms (Pd1–C9 = 2.0783 (19) Å; Pd–C1 = 2.1711 (19) Å) are in agreement with those observed in related cyclopalladated complexes (Falvello *et al.*, 1998; Falvello *et al.*, 1999; Karami *et al.*, 2010; Karami, Rizzoli & Salah, 2011; Karami, Rizzoli & Borzooie, 2011). The P1–C1 bond length (1.768 (2) Å) is significantly longer than that observed in the related free ylide (1.711 Å) of formula $PPh_3C(H)COPh$ (Shao *et al.*, 1982). The Pd1···P1 separation is 3.0241 (9) Å. The $PdC_3P$ five-membered metallacycle (Pd1/C9/C14/P1/C1) assumes an envelope conformation, with atom C1 displaced by 1.006 (2) Å from the mean planes of the remaining four atoms, whereas the $PdC_2P_2$ metallacycle (Pd1/P2/C39/C40/P3) adopts a twist conformation with the local twofold axis passing through the C39–C40 bond and the Pd atom. In the crystal structure (Fig. 3), cations and anions are linked into a three-dimensional network by intermolecular C—H···O hydrogen bonds (Table 1).

## S2. Experimental

The title compound was obtained according to the procedure recently reported elsewhere (Karami, Rizzoli & Borzooie, 2011). Crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane/*n*-hexane (1:1 *v*/*v*) solution at room temperature.

### S3. Refinement

All H atoms were placed in calculated positions and refined using a riding model, with C–H = 0.93–0.98 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(C) for methyl H atoms. The dichloromethane solvent molecule was found to be disordered over three orientations (called *A*, *B*, and *C*) with site-occupancy factors of 1/2, 0.3 and 1/5, respectively. During the refinement, the C–Cl and Cl···Cl distances were constrained to 1.75 (1) and 2.75 (2) Å, respectively, and only the major component of disorder was refined anisotropically. The *n*-hexane molecule, which has crystallographically imposed centre of symmetry, showed rather high displacement ellipsoids, suggesting the presence of disorder. Attempts to model the molecule in terms of disordered contributors were unsuccessful, however. The molecule was therefore anisotropically refined by constraining the C–C bond lengths to 1.54 (1) Å, and the 1–3 C···C separations to 2.52 (2) Å.

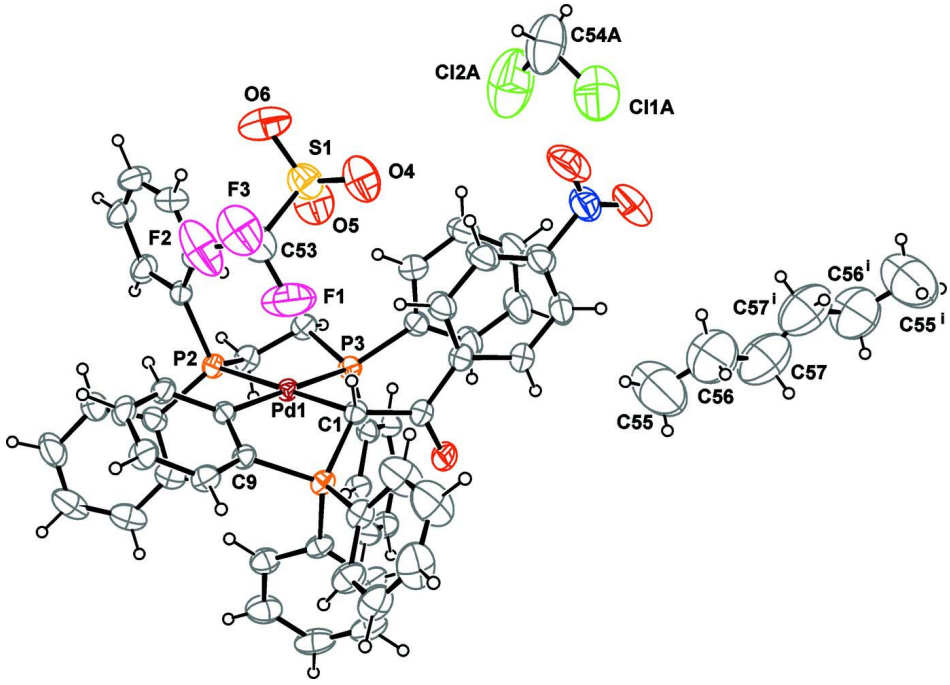


**Figure 1**

The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 30% probability level. Only the major component of the disordered dichloromethane molecule is shown. Symmetry code: (i) -*x*, 1 - *y*, -*z*.

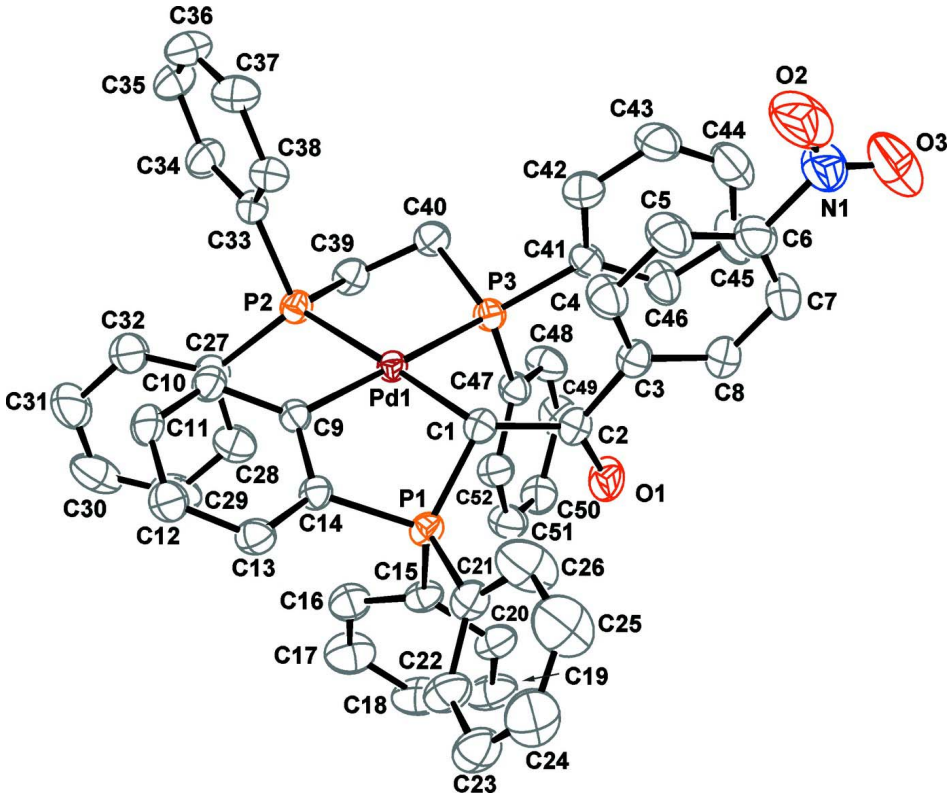


**Figure 2**

The cation of the title compound, showing the labelling scheme adopted. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are omitted for clarity.

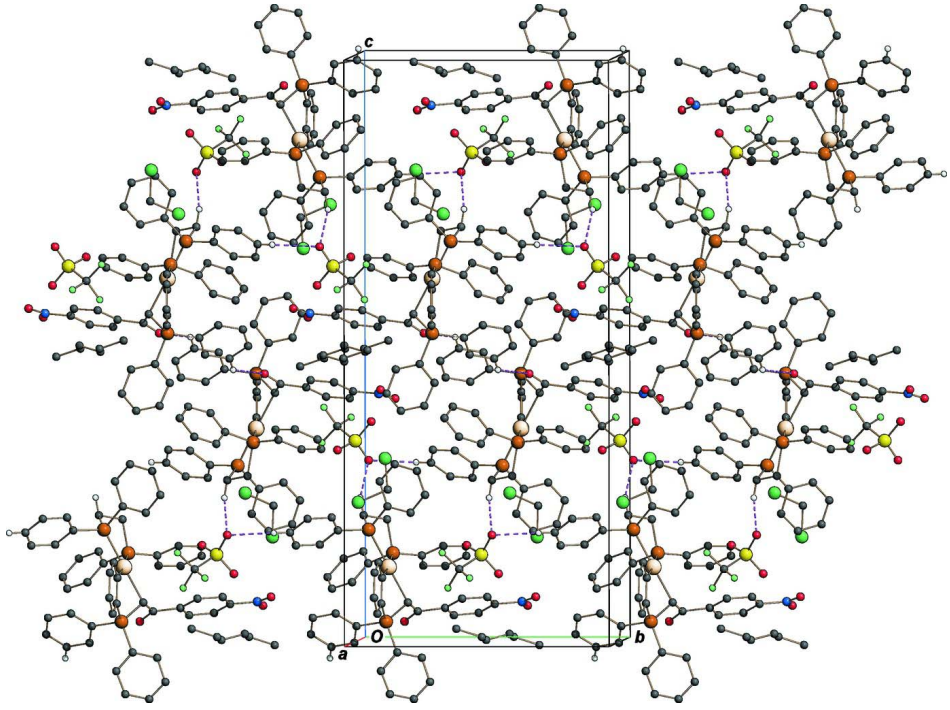


**Figure 3**

Crystal packing of the title compound approximately viewed along the *a* axis. Only the major component of the disordered dichloromethane molecule is shown. Hydrogen atoms not involved in intermolecular C—H···O hydrogen bonds (dashed lines) are omitted for clarity.

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*Crystal data*

| | |
|---|---|
| $[Pd(C_{26}H_{19}NO_3P)(C_{26}H_{24}P_2)]CF_3O_3S\cdot CH_2Cl_2\cdot 0.5C_6H_{14}$ | $Z = 4$ |
| $M_r = 1206.27$ | $F(000) = 2468$ |
| Monoclinic, $P2_1/n$ | $D_x = 1.446$ Mg m$^{-3}$ |
| Hall symbol: -P 2yn | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 12.4063$ (7) Å | Cell parameters from 1226 reflections |
| $b = 14.2445$ (8) Å | $\theta = 6.3$–$23.4°$ |
| $c = 31.3633$ (17) Å | $\mu = 0.62$ mm$^{-1}$ |
| $\beta = 91.6675$ (9)° | $T = 294$ K |
| $V = 5540.2$ (5) Å$^3$ | Irregular block, yellow |
| | 0.19 × 0.16 × 0.10 mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 62924 measured reflections |
| Radiation source: fine-focus sealed tube | 10529 independent reflections |
| Graphite monochromator | 8106 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.036$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | $\theta_{max} = 25.7°$, $\theta_{min} = 1.6°$ |
| $T_{min} = 0.872$, $T_{max} = 0.955$ | $h = -15\rightarrow15$ |
| | $k = -17\rightarrow17$ |
| | $l = -38\rightarrow38$ |

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.076$
$S = 1.04$
10529 reflections
691 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*Special details*

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pd1 | 0.756229 (11) | 0.147230 (10) | 0.131977 (5) | 0.03814 (6) | |
| S1 | 0.90642 (7) | 0.50943 (6) | 0.15555 (3) | 0.0883 (2) | |
| P1 | 0.81951 (4) | 0.14269 (4) | 0.039724 (17) | 0.04289 (13) | |
| P3 | 0.57524 (4) | 0.14972 (4) | 0.152637 (18) | 0.04526 (13) | |
| P2 | 0.78566 (4) | 0.07474 (4) | 0.196011 (17) | 0.04514 (14) | |
| O1 | 0.57447 (13) | 0.19304 (12) | 0.03587 (6) | 0.0709 (5) | |
| O2 | 0.5578 (3) | 0.68752 (18) | 0.07768 (10) | 0.1340 (10) | |
| O3 | 0.4015 (3) | 0.6445 (2) | 0.06026 (13) | 0.1685 (14) | |
| O4 | 0.8765 (2) | 0.57210 (17) | 0.12237 (9) | 0.1226 (8) | |
| O5 | 0.82523 (18) | 0.44856 (18) | 0.17003 (8) | 0.1183 (8) | |
| O6 | 0.9700 (3) | 0.5548 (2) | 0.18984 (9) | 0.1499 (11) | |
| F1 | 0.9555 (2) | 0.3873 (2) | 0.09940 (9) | 0.1675 (11) | |
| F2 | 1.0418 (2) | 0.37281 (17) | 0.16085 (10) | 0.1651 (11) | |
| F3 | 1.08767 (16) | 0.47955 (15) | 0.11854 (7) | 0.1293 (7) | |
| N1 | 0.4919 (3) | 0.6307 (2) | 0.06826 (9) | 0.0947 (9) | |
| C1 | 0.74213 (16) | 0.21915 (14) | 0.07104 (6) | 0.0428 (5) | |
| H1 | 0.7844 | 0.2770 | 0.0742 | 0.051* | |
| C2 | 0.63523 (17) | 0.24779 (16) | 0.05422 (7) | 0.0487 (5) | |
| C3 | 0.60121 (18) | 0.34836 (15) | 0.05941 (7) | 0.0524 (5) | |
| C4 | 0.6672 (2) | 0.41801 (17) | 0.07639 (9) | 0.0697 (7) | |
| H4 | 0.7363 | 0.4030 | 0.0865 | 0.084* | |
| C5 | 0.6311 (3) | 0.51037 (18) | 0.07854 (10) | 0.0794 (8) | |
| H5 | 0.6762 | 0.5574 | 0.0893 | 0.095* | |
| C6 | 0.5308 (3) | 0.53044 (19) | 0.06495 (9) | 0.0731 (7) | |
| C7 | 0.4620 (2) | 0.4644 (2) | 0.04858 (9) | 0.0828 (9) | |
| H7 | 0.3923 | 0.4807 | 0.0397 | 0.099* | |
| C8 | 0.4971 (2) | 0.37316 (19) | 0.04537 (8) | 0.0694 (7) | |
| H8 | 0.4513 | 0.3276 | 0.0338 | 0.083* | |

| | | | | |
|---|---|---|---|---|
| C9 | 0.91717 (15) | 0.13543 (13) | 0.11614 (6) | 0.0398 (5) |
| C10 | 1.00786 (17) | 0.12915 (15) | 0.14348 (7) | 0.0502 (5) |
| H10 | 0.9988 | 0.1295 | 0.1728 | 0.060* |
| C11 | 1.11043 (17) | 0.12245 (18) | 0.12802 (8) | 0.0608 (6) |
| H11 | 1.1689 | 0.1186 | 0.1472 | 0.073* |
| C12 | 1.12825 (18) | 0.12141 (18) | 0.08535 (8) | 0.0641 (7) |
| H12 | 1.1981 | 0.1167 | 0.0755 | 0.077* |
| C13 | 1.04155 (18) | 0.12737 (16) | 0.05688 (7) | 0.0545 (6) |
| H13 | 1.0521 | 0.1268 | 0.0276 | 0.065* |
| C14 | 0.93907 (16) | 0.13423 (14) | 0.07244 (6) | 0.0424 (5) |
| C15 | 0.76628 (17) | 0.02642 (16) | 0.03113 (6) | 0.0490 (5) |
| C16 | 0.8100 (2) | −0.04862 (17) | 0.05335 (8) | 0.0621 (6) |
| H16 | 0.8659 | −0.0395 | 0.0733 | 0.074* |
| C17 | 0.7694 (3) | −0.13839 (18) | 0.04549 (10) | 0.0845 (9) |
| H17 | 0.7980 | −0.1894 | 0.0604 | 0.101* |
| C18 | 0.6875 (3) | −0.1518 (2) | 0.01586 (11) | 0.0873 (10) |
| H18 | 0.6610 | −0.2120 | 0.0108 | 0.105* |
| C19 | 0.6445 (2) | −0.0779 (2) | −0.00625 (9) | 0.0789 (8) |
| H19 | 0.5893 | −0.0877 | −0.0264 | 0.095* |
| C20 | 0.68299 (19) | 0.01173 (19) | 0.00130 (7) | 0.0618 (6) |
| H20 | 0.6531 | 0.0623 | −0.0136 | 0.074* |
| C21 | 0.84920 (18) | 0.18697 (18) | −0.01227 (7) | 0.0545 (6) |
| C22 | 0.8883 (2) | 0.1285 (2) | −0.04356 (8) | 0.0712 (7) |
| H22 | 0.8942 | 0.0643 | −0.0384 | 0.085* |
| C23 | 0.9187 (2) | 0.1647 (3) | −0.08236 (9) | 0.0815 (9) |
| H23 | 0.9486 | 0.1252 | −0.1025 | 0.098* |
| C24 | 0.9057 (3) | 0.2541 (3) | −0.09099 (11) | 0.1113 (12) |
| H24 | 0.9286 | 0.2781 | −0.1168 | 0.134* |
| C25 | 0.8589 (3) | 0.3115 (3) | −0.06240 (12) | 0.1215 (13) |
| H25 | 0.8428 | 0.3732 | −0.0699 | 0.146* |
| C26 | 0.8347 (3) | 0.2789 (2) | −0.02164 (10) | 0.1082 (12) |
| H26 | 0.8090 | 0.3199 | −0.0013 | 0.130* |
| C27 | 0.85865 (19) | −0.03586 (15) | 0.19613 (7) | 0.0533 (6) |
| C28 | 0.8165 (2) | −0.10762 (19) | 0.17098 (9) | 0.0715 (7) |
| H28 | 0.7543 | −0.0974 | 0.1544 | 0.086* |
| C29 | 0.8663 (3) | −0.1941 (2) | 0.17036 (11) | 0.0857 (9) |
| H29 | 0.8370 | −0.2422 | 0.1537 | 0.103* |
| C30 | 0.9574 (3) | −0.2089 (2) | 0.19399 (11) | 0.0962 (11) |
| H30 | 0.9903 | −0.2675 | 0.1937 | 0.115* |
| C31 | 1.0012 (3) | −0.1393 (3) | 0.21797 (11) | 0.1123 (13) |
| H31 | 1.0649 | −0.1501 | 0.2336 | 0.135* |
| C32 | 0.9523 (2) | −0.0517 (2) | 0.21953 (9) | 0.0830 (8) |
| H32 | 0.9827 | −0.0042 | 0.2363 | 0.100* |
| C33 | 0.84562 (17) | 0.15069 (15) | 0.23661 (7) | 0.0498 (5) |
| C34 | 0.8534 (2) | 0.1220 (2) | 0.27935 (8) | 0.0698 (7) |
| H34 | 0.8303 | 0.0625 | 0.2871 | 0.084* |
| C35 | 0.8953 (2) | 0.1821 (3) | 0.30950 (9) | 0.0839 (9) |
| H35 | 0.8999 | 0.1634 | 0.3379 | 0.101* |

| | | | | | |
|---|---|---|---|---|---|
| C36 | 0.9302 (2) | 0.2687 (3) | 0.29844 (10) | 0.0884 (9) | |
| H36 | 0.9601 | 0.3082 | 0.3192 | 0.106* | |
| C37 | 0.9221 (2) | 0.2985 (2) | 0.25752 (10) | 0.0777 (8) | |
| H37 | 0.9457 | 0.3583 | 0.2504 | 0.093* | |
| C38 | 0.87898 (18) | 0.24007 (17) | 0.22645 (8) | 0.0581 (6) | |
| H38 | 0.8723 | 0.2611 | 0.1984 | 0.070* | |
| C39 | 0.65511 (18) | 0.04531 (17) | 0.21851 (7) | 0.0572 (6) | |
| H39A | 0.6257 | −0.0108 | 0.2050 | 0.069* | |
| H39B | 0.6635 | 0.0338 | 0.2489 | 0.069* | |
| C40 | 0.58024 (18) | 0.12801 (17) | 0.21030 (7) | 0.0556 (6) | |
| H40A | 0.6071 | 0.1831 | 0.2254 | 0.067* | |
| H40B | 0.5087 | 0.1138 | 0.2202 | 0.067* | |
| C41 | 0.48826 (17) | 0.25194 (16) | 0.14711 (7) | 0.0513 (5) | |
| C42 | 0.5253 (2) | 0.33604 (18) | 0.16386 (9) | 0.0713 (7) | |
| H42 | 0.5942 | 0.3398 | 0.1762 | 0.086* | |
| C43 | 0.4591 (3) | 0.4154 (2) | 0.16227 (9) | 0.0848 (9) | |
| H43 | 0.4840 | 0.4720 | 0.1736 | 0.102* | |
| C44 | 0.3585 (3) | 0.4099 (2) | 0.14422 (11) | 0.0940 (10) | |
| H44 | 0.3141 | 0.4625 | 0.1439 | 0.113* | |
| C45 | 0.3215 (2) | 0.3273 (2) | 0.12634 (12) | 0.0943 (10) | |
| H45 | 0.2533 | 0.3243 | 0.1133 | 0.113* | |
| C46 | 0.38683 (19) | 0.24915 (19) | 0.12800 (9) | 0.0733 (7) | |
| H46 | 0.3620 | 0.1932 | 0.1160 | 0.088* | |
| C47 | 0.49623 (16) | 0.04970 (15) | 0.13374 (7) | 0.0484 (5) | |
| C48 | 0.40033 (18) | 0.02404 (18) | 0.15241 (9) | 0.0669 (7) | |
| H48 | 0.3732 | 0.0610 | 0.1741 | 0.080* | |
| C49 | 0.3453 (2) | −0.05461 (19) | 0.13946 (9) | 0.0732 (7) | |
| H49 | 0.2799 | −0.0693 | 0.1516 | 0.088* | |
| C50 | 0.3860 (2) | −0.11248 (18) | 0.10840 (9) | 0.0661 (7) | |
| H50 | 0.3497 | −0.1669 | 0.1001 | 0.079* | |
| C51 | 0.4797 (2) | −0.08836 (18) | 0.09037 (8) | 0.0662 (7) | |
| H51 | 0.5077 | −0.1269 | 0.0694 | 0.079* | |
| C52 | 0.53468 (18) | −0.00806 (16) | 0.10225 (7) | 0.0554 (6) | |
| H52 | 0.5983 | 0.0074 | 0.0889 | 0.067* | |
| C53 | 1.0025 (3) | 0.4339 (3) | 0.13228 (13) | 0.1008 (10) | |
| C54A | 0.3163 (9) | 0.6781 (8) | 0.2291 (3) | 0.194 (5) | 0.50 |
| H54A | 0.2741 | 0.7264 | 0.2427 | 0.232* | 0.50 |
| H54B | 0.3922 | 0.6927 | 0.2334 | 0.232* | 0.50 |
| Cl1A | 0.2831 (3) | 0.6713 (2) | 0.17539 (14) | 0.1998 (15) | 0.50 |
| Cl2A | 0.2875 (4) | 0.5690 (5) | 0.25025 (15) | 0.288 (3) | 0.50 |
| C54B | 0.2090 (16) | 0.6089 (8) | 0.2196 (4) | 0.141 (6)* | 0.30 |
| H54C | 0.2623 | 0.6138 | 0.1977 | 0.170* | 0.30 |
| H54D | 0.1382 | 0.6202 | 0.2067 | 0.170* | 0.30 |
| Cl1B | 0.2144 (9) | 0.4956 (6) | 0.2440 (3) | 0.295 (5)* | 0.30 |
| Cl2B | 0.2361 (6) | 0.6898 (5) | 0.2604 (2) | 0.198 (2)* | 0.30 |
| C54C | 0.2675 (17) | 0.7357 (9) | 0.2117 (4) | 0.107 (6)* | 0.20 |
| H54E | 0.3340 | 0.7619 | 0.2013 | 0.129* | 0.20 |
| H54F | 0.2060 | 0.7657 | 0.1976 | 0.129* | 0.20 |

| | | | | | |
|---|---|---|---|---|---|
| Cl1C | 0.2632 (13) | 0.6113 (9) | 0.2074 (5) | 0.245 (6)* | 0.20 |
| Cl2C | 0.2614 (9) | 0.7397 (8) | 0.2671 (3) | 0.207 (4)* | 0.20 |
| C55 | 0.1874 (6) | 0.3580 (5) | 0.0169 (3) | 0.281 (5) | |
| H55A | 0.2628 | 0.3594 | 0.0248 | 0.421* | |
| H55B | 0.1753 | 0.3134 | −0.0057 | 0.421* | |
| H55C | 0.1467 | 0.3400 | 0.0412 | 0.421* | |
| C56 | 0.1529 (5) | 0.4517 (5) | 0.0023 (2) | 0.220 (3) | |
| H56A | 0.1877 | 0.4664 | −0.0241 | 0.265* | |
| H56B | 0.1758 | 0.4980 | 0.0234 | 0.265* | |
| C57 | 0.0311 (5) | 0.4582 (4) | −0.0047 (3) | 0.221 (4) | |
| H57A | 0.0165 | 0.4437 | −0.0345 | 0.265* | |
| H57B | 0.0003 | 0.4074 | 0.0116 | 0.265* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.03380 (9) | 0.04284 (10) | 0.03775 (9) | −0.00153 (7) | 0.00029 (6) | −0.00164 (7) |
| S1 | 0.0898 (6) | 0.0880 (5) | 0.0879 (6) | 0.0087 (5) | 0.0177 (5) | 0.0037 (5) |
| P1 | 0.0401 (3) | 0.0506 (3) | 0.0378 (3) | −0.0059 (2) | 0.0005 (2) | 0.0001 (2) |
| P3 | 0.0354 (3) | 0.0529 (3) | 0.0476 (3) | −0.0014 (2) | 0.0040 (2) | −0.0047 (3) |
| P2 | 0.0459 (3) | 0.0482 (3) | 0.0414 (3) | −0.0009 (2) | 0.0010 (2) | 0.0032 (2) |
| O1 | 0.0542 (10) | 0.0624 (10) | 0.0944 (13) | −0.0030 (8) | −0.0271 (9) | −0.0110 (10) |
| O2 | 0.193 (3) | 0.0650 (16) | 0.145 (2) | 0.0284 (18) | 0.019 (2) | 0.0046 (16) |
| O3 | 0.173 (3) | 0.112 (2) | 0.220 (4) | 0.076 (2) | −0.017 (3) | −0.022 (2) |
| O4 | 0.1203 (19) | 0.1035 (18) | 0.144 (2) | 0.0192 (15) | 0.0099 (16) | 0.0336 (16) |
| O5 | 0.0866 (15) | 0.135 (2) | 0.135 (2) | −0.0087 (15) | 0.0315 (14) | 0.0224 (16) |
| O6 | 0.186 (3) | 0.153 (2) | 0.111 (2) | −0.027 (2) | 0.0091 (19) | −0.0592 (18) |
| F1 | 0.154 (2) | 0.170 (2) | 0.178 (3) | −0.0203 (18) | 0.0109 (19) | −0.098 (2) |
| F2 | 0.143 (2) | 0.1191 (17) | 0.236 (3) | 0.0479 (15) | 0.049 (2) | 0.0631 (19) |
| F3 | 0.0921 (13) | 0.1338 (17) | 0.165 (2) | −0.0059 (12) | 0.0491 (13) | 0.0272 (15) |
| N1 | 0.120 (3) | 0.079 (2) | 0.0850 (19) | 0.0314 (19) | 0.0008 (18) | 0.0077 (16) |
| C1 | 0.0426 (11) | 0.0408 (11) | 0.0448 (12) | −0.0048 (9) | −0.0013 (9) | 0.0020 (9) |
| C2 | 0.0447 (12) | 0.0530 (13) | 0.0482 (12) | −0.0034 (10) | −0.0035 (10) | 0.0043 (10) |
| C3 | 0.0539 (13) | 0.0559 (14) | 0.0472 (13) | 0.0003 (11) | −0.0010 (10) | 0.0044 (11) |
| C4 | 0.0569 (15) | 0.0557 (16) | 0.096 (2) | 0.0003 (12) | −0.0026 (14) | −0.0078 (14) |
| C5 | 0.089 (2) | 0.0500 (16) | 0.099 (2) | 0.0038 (15) | 0.0033 (17) | −0.0065 (14) |
| C6 | 0.099 (2) | 0.0605 (17) | 0.0601 (16) | 0.0193 (16) | 0.0048 (15) | 0.0053 (13) |
| C7 | 0.084 (2) | 0.088 (2) | 0.0758 (19) | 0.0364 (18) | −0.0124 (16) | 0.0035 (16) |
| C8 | 0.0663 (17) | 0.0726 (18) | 0.0681 (17) | 0.0130 (13) | −0.0174 (13) | −0.0053 (13) |
| C9 | 0.0360 (10) | 0.0371 (11) | 0.0462 (12) | −0.0018 (8) | −0.0006 (9) | −0.0015 (9) |
| C10 | 0.0427 (12) | 0.0605 (14) | 0.0470 (13) | −0.0016 (10) | −0.0025 (10) | −0.0043 (10) |
| C11 | 0.0347 (12) | 0.0830 (17) | 0.0642 (16) | 0.0008 (11) | −0.0079 (11) | −0.0086 (13) |
| C12 | 0.0335 (12) | 0.0918 (19) | 0.0674 (17) | −0.0053 (12) | 0.0092 (11) | −0.0139 (14) |
| C13 | 0.0476 (13) | 0.0662 (15) | 0.0500 (13) | −0.0069 (11) | 0.0083 (11) | −0.0080 (11) |
| C14 | 0.0360 (11) | 0.0476 (12) | 0.0435 (12) | −0.0046 (9) | 0.0004 (9) | −0.0022 (9) |
| C15 | 0.0489 (12) | 0.0590 (14) | 0.0394 (12) | −0.0133 (11) | 0.0069 (10) | −0.0066 (10) |
| C16 | 0.0681 (16) | 0.0558 (15) | 0.0622 (15) | −0.0101 (12) | 0.0007 (12) | −0.0043 (12) |
| C17 | 0.113 (3) | 0.0540 (17) | 0.086 (2) | −0.0182 (16) | 0.0076 (19) | −0.0043 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.092 (2) | 0.083 (2) | 0.088 (2) | −0.0443 (18) | 0.0201 (18) | −0.0323 (18) |
| C19 | 0.0768 (19) | 0.097 (2) | 0.0630 (17) | −0.0370 (17) | 0.0086 (14) | −0.0254 (16) |
| C20 | 0.0581 (14) | 0.0802 (17) | 0.0471 (13) | −0.0148 (13) | 0.0009 (11) | −0.0107 (12) |
| C21 | 0.0491 (13) | 0.0673 (15) | 0.0473 (13) | −0.0062 (12) | 0.0043 (10) | 0.0060 (12) |
| C22 | 0.0755 (18) | 0.091 (2) | 0.0469 (15) | −0.0106 (15) | 0.0085 (13) | −0.0012 (13) |
| C23 | 0.0714 (18) | 0.123 (3) | 0.0512 (16) | −0.0050 (18) | 0.0115 (13) | 0.0022 (17) |
| C24 | 0.114 (3) | 0.154 (4) | 0.067 (2) | 0.022 (3) | 0.0348 (19) | 0.042 (2) |
| C25 | 0.161 (4) | 0.100 (3) | 0.105 (3) | 0.024 (3) | 0.047 (3) | 0.047 (2) |
| C26 | 0.150 (3) | 0.088 (2) | 0.090 (2) | 0.019 (2) | 0.061 (2) | 0.0298 (18) |
| C27 | 0.0638 (15) | 0.0481 (13) | 0.0483 (13) | 0.0064 (11) | 0.0064 (11) | 0.0051 (10) |
| C28 | 0.0780 (18) | 0.0604 (16) | 0.0767 (18) | −0.0021 (14) | 0.0118 (14) | −0.0049 (14) |
| C29 | 0.111 (3) | 0.0569 (18) | 0.090 (2) | −0.0035 (18) | 0.029 (2) | −0.0093 (16) |
| C30 | 0.145 (3) | 0.069 (2) | 0.076 (2) | 0.039 (2) | 0.041 (2) | 0.0141 (17) |
| C31 | 0.138 (3) | 0.115 (3) | 0.084 (2) | 0.073 (3) | −0.012 (2) | 0.006 (2) |
| C32 | 0.104 (2) | 0.0723 (18) | 0.0711 (18) | 0.0271 (17) | −0.0163 (17) | −0.0026 (14) |
| C33 | 0.0479 (12) | 0.0562 (14) | 0.0450 (12) | 0.0088 (11) | −0.0031 (10) | −0.0020 (10) |
| C34 | 0.0757 (18) | 0.0842 (19) | 0.0491 (15) | 0.0040 (14) | −0.0061 (13) | 0.0033 (13) |
| C35 | 0.094 (2) | 0.111 (3) | 0.0451 (15) | 0.014 (2) | −0.0128 (14) | −0.0116 (16) |
| C36 | 0.092 (2) | 0.097 (2) | 0.075 (2) | 0.0012 (19) | −0.0113 (17) | −0.0382 (18) |
| C37 | 0.091 (2) | 0.0646 (17) | 0.077 (2) | −0.0046 (15) | 0.0014 (16) | −0.0201 (15) |
| C38 | 0.0625 (15) | 0.0575 (15) | 0.0546 (14) | 0.0037 (12) | 0.0040 (11) | −0.0075 (12) |
| C39 | 0.0560 (14) | 0.0681 (16) | 0.0477 (13) | −0.0055 (12) | 0.0069 (11) | 0.0069 (11) |
| C40 | 0.0454 (13) | 0.0728 (16) | 0.0492 (13) | −0.0041 (11) | 0.0100 (10) | −0.0038 (11) |
| C41 | 0.0444 (12) | 0.0579 (14) | 0.0522 (13) | 0.0032 (11) | 0.0103 (10) | −0.0022 (11) |
| C42 | 0.0787 (18) | 0.0628 (17) | 0.0718 (18) | −0.0018 (14) | −0.0072 (14) | −0.0117 (13) |
| C43 | 0.115 (3) | 0.0577 (17) | 0.082 (2) | 0.0130 (17) | 0.0013 (18) | −0.0129 (14) |
| C44 | 0.091 (2) | 0.083 (2) | 0.108 (3) | 0.0334 (19) | 0.018 (2) | 0.0008 (19) |
| C45 | 0.0572 (18) | 0.085 (2) | 0.141 (3) | 0.0117 (16) | 0.0014 (18) | 0.010 (2) |
| C46 | 0.0510 (15) | 0.0648 (17) | 0.104 (2) | 0.0061 (13) | −0.0028 (14) | −0.0014 (15) |
| C47 | 0.0409 (12) | 0.0489 (12) | 0.0554 (13) | −0.0004 (10) | 0.0021 (10) | −0.0018 (10) |
| C48 | 0.0484 (14) | 0.0686 (17) | 0.0848 (18) | −0.0083 (12) | 0.0186 (13) | −0.0168 (14) |
| C49 | 0.0475 (14) | 0.0739 (18) | 0.099 (2) | −0.0160 (13) | 0.0126 (14) | 0.0011 (16) |
| C50 | 0.0646 (16) | 0.0532 (14) | 0.0797 (18) | −0.0089 (13) | −0.0098 (14) | −0.0012 (13) |
| C51 | 0.0692 (17) | 0.0595 (16) | 0.0702 (17) | −0.0003 (13) | 0.0050 (14) | −0.0128 (13) |
| C52 | 0.0503 (13) | 0.0614 (15) | 0.0548 (14) | −0.0054 (11) | 0.0053 (11) | −0.0049 (11) |
| C53 | 0.095 (2) | 0.085 (2) | 0.124 (3) | −0.002 (2) | 0.023 (2) | 0.008 (2) |
| C54A | 0.122 (9) | 0.263 (15) | 0.195 (13) | −0.032 (9) | −0.013 (8) | 0.081 (13) |
| Cl1A | 0.159 (3) | 0.172 (3) | 0.267 (4) | −0.043 (2) | −0.016 (3) | 0.060 (3) |
| Cl2A | 0.207 (4) | 0.462 (9) | 0.195 (4) | 0.047 (6) | 0.012 (3) | 0.067 (5) |
| C55 | 0.230 (9) | 0.196 (8) | 0.416 (15) | 0.034 (6) | 0.002 (9) | −0.029 (8) |
| C56 | 0.175 (6) | 0.245 (8) | 0.241 (8) | −0.032 (6) | −0.006 (5) | −0.001 (6) |
| C57 | 0.217 (10) | 0.264 (11) | 0.179 (6) | −0.084 (8) | −0.020 (6) | 0.001 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—C9 | 2.0783 (19) | C27—C28 | 1.384 (3) |
| Pd1—C1 | 2.1711 (19) | C28—C29 | 1.378 (4) |
| Pd1—P2 | 2.2783 (6) | C28—H28 | 0.9300 |

| | | | |
|---|---|---|---|
| Pd1—P3 | 2.3554 (6) | C29—C30 | 1.351 (4) |
| S1—O4 | 1.413 (2) | C29—H29 | 0.9300 |
| S1—O5 | 1.414 (2) | C30—C31 | 1.348 (5) |
| S1—O6 | 1.466 (3) | C30—H30 | 0.9300 |
| S1—C53 | 1.777 (4) | C31—C32 | 1.389 (4) |
| P1—C1 | 1.768 (2) | C31—H31 | 0.9300 |
| P1—C14 | 1.783 (2) | C32—H32 | 0.9300 |
| P1—C21 | 1.797 (2) | C33—C38 | 1.379 (3) |
| P1—C15 | 1.800 (2) | C33—C34 | 1.402 (3) |
| P3—C41 | 1.818 (2) | C34—C35 | 1.367 (4) |
| P3—C47 | 1.819 (2) | C34—H34 | 0.9300 |
| P3—C40 | 1.834 (2) | C35—C36 | 1.356 (4) |
| P2—C33 | 1.814 (2) | C35—H35 | 0.9300 |
| P2—C27 | 1.817 (2) | C36—C37 | 1.352 (4) |
| P2—C39 | 1.834 (2) | C36—H36 | 0.9300 |
| O1—C2 | 1.218 (2) | C37—C38 | 1.378 (3) |
| O2—N1 | 1.182 (4) | C37—H37 | 0.9300 |
| O3—N1 | 1.159 (4) | C38—H38 | 0.9300 |
| F1—C53 | 1.346 (4) | C39—C40 | 1.517 (3) |
| F2—C53 | 1.332 (4) | C39—H39A | 0.9700 |
| F3—C53 | 1.324 (4) | C39—H39B | 0.9700 |
| N1—C6 | 1.512 (4) | C40—H40A | 0.9700 |
| C1—C2 | 1.471 (3) | C40—H40B | 0.9700 |
| C1—H1 | 0.9800 | C41—C46 | 1.378 (3) |
| C2—C3 | 1.504 (3) | C41—C42 | 1.381 (3) |
| C3—C4 | 1.383 (3) | C42—C43 | 1.397 (4) |
| C3—C8 | 1.397 (3) | C42—H42 | 0.9300 |
| C4—C5 | 1.392 (3) | C43—C44 | 1.358 (4) |
| C4—H4 | 0.9300 | C43—H43 | 0.9300 |
| C5—C6 | 1.334 (4) | C44—C45 | 1.376 (4) |
| C5—H5 | 0.9300 | C44—H44 | 0.9300 |
| C6—C7 | 1.361 (4) | C45—C46 | 1.377 (4) |
| C7—C8 | 1.375 (4) | C45—H45 | 0.9300 |
| C7—H7 | 0.9300 | C46—H46 | 0.9300 |
| C8—H8 | 0.9300 | C47—C52 | 1.381 (3) |
| C9—C10 | 1.397 (3) | C47—C48 | 1.390 (3) |
| C9—C14 | 1.405 (3) | C48—C49 | 1.368 (3) |
| C10—C11 | 1.378 (3) | C48—H48 | 0.9300 |
| C10—H10 | 0.9300 | C49—C50 | 1.383 (4) |
| C11—C12 | 1.363 (3) | C49—H49 | 0.9300 |
| C11—H11 | 0.9300 | C50—C51 | 1.352 (3) |
| C12—C13 | 1.380 (3) | C50—H50 | 0.9300 |
| C12—H12 | 0.9300 | C51—C52 | 1.378 (3) |
| C13—C14 | 1.378 (3) | C51—H51 | 0.9300 |
| C13—H13 | 0.9300 | C52—H52 | 0.9300 |
| C15—C16 | 1.379 (3) | C54A—Cl1A | 1.726 (8) |
| C15—C20 | 1.389 (3) | C54A—Cl2A | 1.730 (8) |
| C16—C17 | 1.394 (3) | C54A—H54A | 0.9700 |

| | | | |
|---|---|---|---|
| C16—H16 | 0.9300 | C54A—H54B | 0.9700 |
| C17—C18 | 1.370 (4) | C54B—Cl2B | 1.746 (9) |
| C17—H17 | 0.9300 | C54B—Cl1B | 1.787 (9) |
| C18—C19 | 1.361 (4) | C54B—H54C | 0.9700 |
| C18—H18 | 0.9300 | C54B—H54D | 0.9700 |
| C19—C20 | 1.381 (3) | C54C—Cl2C | 1.744 (10) |
| C19—H19 | 0.9300 | C54C—Cl1C | 1.778 (10) |
| C20—H20 | 0.9300 | C54C—H54E | 0.9700 |
| C21—C26 | 1.352 (4) | C54C—H54F | 0.9700 |
| C21—C22 | 1.386 (3) | C55—C56 | 1.472 (6) |
| C22—C23 | 1.384 (4) | C55—H55A | 0.9600 |
| C22—H22 | 0.9300 | C55—H55B | 0.9600 |
| C23—C24 | 1.310 (4) | C55—H55C | 0.9600 |
| C23—H23 | 0.9300 | C56—C57 | 1.523 (7) |
| C24—C25 | 1.357 (5) | C56—H56A | 0.9700 |
| C24—H24 | 0.9300 | C56—H56B | 0.9700 |
| C25—C26 | 1.401 (4) | C57—C57$^{i}$ | 1.455 (8) |
| C25—H25 | 0.9300 | C57—H57A | 0.9700 |
| C26—H26 | 0.9300 | C57—H57B | 0.9700 |
| C27—C32 | 1.375 (3) | | |

| | | | |
|---|---|---|---|
| C9—Pd1—C1 | 83.17 (8) | C30—C29—C28 | 120.0 (3) |
| C9—Pd1—P2 | 92.50 (6) | C30—C29—H29 | 120.0 |
| C1—Pd1—P2 | 175.31 (5) | C28—C29—H29 | 120.0 |
| C9—Pd1—P3 | 175.68 (5) | C31—C30—C29 | 120.6 (3) |
| C1—Pd1—P3 | 100.49 (5) | C31—C30—H30 | 119.7 |
| P2—Pd1—P3 | 83.91 (2) | C29—C30—H30 | 119.7 |
| O4—S1—O5 | 116.71 (16) | C30—C31—C32 | 120.7 (3) |
| O4—S1—O6 | 112.71 (18) | C30—C31—H31 | 119.7 |
| O5—S1—O6 | 114.10 (17) | C32—C31—H31 | 119.7 |
| O4—S1—C53 | 104.18 (18) | C27—C32—C31 | 119.5 (3) |
| O5—S1—C53 | 104.67 (17) | C27—C32—H32 | 120.3 |
| O6—S1—C53 | 102.43 (19) | C31—C32—H32 | 120.3 |
| C1—P1—C14 | 100.26 (9) | C38—C33—C34 | 118.5 (2) |
| C1—P1—C21 | 114.63 (11) | C38—C33—P2 | 120.54 (17) |
| C14—P1—C21 | 110.91 (10) | C34—C33—P2 | 120.85 (19) |
| C1—P1—C15 | 116.56 (10) | C35—C34—C33 | 119.5 (3) |
| C14—P1—C15 | 108.63 (10) | C35—C34—H34 | 120.2 |
| C21—P1—C15 | 105.72 (10) | C33—C34—H34 | 120.2 |
| C41—P3—C47 | 106.47 (10) | C36—C35—C34 | 120.7 (3) |
| C41—P3—C40 | 103.43 (10) | C36—C35—H35 | 119.6 |
| C47—P3—C40 | 101.05 (10) | C34—C35—H35 | 119.6 |
| C41—P3—Pd1 | 123.64 (7) | C37—C36—C35 | 120.8 (3) |
| C47—P3—Pd1 | 114.05 (7) | C37—C36—H36 | 119.6 |
| C40—P3—Pd1 | 105.28 (7) | C35—C36—H36 | 119.6 |
| C33—P2—C27 | 108.75 (10) | C36—C37—C38 | 119.9 (3) |
| C33—P2—C39 | 102.42 (11) | C36—C37—H37 | 120.0 |
| C27—P2—C39 | 104.28 (11) | C38—C37—H37 | 120.0 |

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| C33—P2—Pd1 | 113.60 (7) | C37—C38—C33 | 120.5 (2) |
| C27—P2—Pd1 | 117.51 (7) | C37—C38—H38 | 119.8 |
| C39—P2—Pd1 | 108.79 (8) | C33—C38—H38 | 119.8 |
| O3—N1—O2 | 126.6 (4) | C40—C39—P2 | 107.48 (15) |
| O3—N1—C6 | 117.0 (4) | C40—C39—H39A | 110.2 |
| O2—N1—C6 | 116.4 (3) | P2—C39—H39A | 110.2 |
| C2—C1—P1 | 118.04 (15) | C40—C39—H39B | 110.2 |
| C2—C1—Pd1 | 119.69 (14) | P2—C39—H39B | 110.2 |
| P1—C1—Pd1 | 99.62 (9) | H39A—C39—H39B | 108.5 |
| C2—C1—H1 | 106.1 | C39—C40—P3 | 107.53 (15) |
| P1—C1—H1 | 106.1 | C39—C40—H40A | 110.2 |
| Pd1—C1—H1 | 106.1 | P3—C40—H40A | 110.2 |
| O1—C2—C1 | 122.1 (2) | C39—C40—H40B | 110.2 |
| O1—C2—C3 | 119.31 (19) | P3—C40—H40B | 110.2 |
| C1—C2—C3 | 118.59 (19) | H40A—C40—H40B | 108.5 |
| C4—C3—C8 | 118.1 (2) | C46—C41—C42 | 118.7 (2) |
| C4—C3—C2 | 124.1 (2) | C46—C41—P3 | 123.39 (19) |
| C8—C3—C2 | 117.8 (2) | C42—C41—P3 | 117.94 (18) |
| C3—C4—C5 | 120.6 (2) | C41—C42—C43 | 120.0 (3) |
| C3—C4—H4 | 119.7 | C41—C42—H42 | 120.0 |
| C5—C4—H4 | 119.7 | C43—C42—H42 | 120.0 |
| C6—C5—C4 | 119.0 (3) | C44—C43—C42 | 120.0 (3) |
| C6—C5—H5 | 120.5 | C44—C43—H43 | 120.0 |
| C4—C5—H5 | 120.5 | C42—C43—H43 | 120.0 |
| C5—C6—C7 | 122.8 (3) | C43—C44—C45 | 120.7 (3) |
| C5—C6—N1 | 118.5 (3) | C43—C44—H44 | 119.6 |
| C7—C6—N1 | 118.7 (3) | C45—C44—H44 | 119.6 |
| C6—C7—C8 | 119.0 (3) | C44—C45—C46 | 119.1 (3) |
| C6—C7—H7 | 120.5 | C44—C45—H45 | 120.4 |
| C8—C7—H7 | 120.5 | C46—C45—H45 | 120.4 |
| C7—C8—C3 | 120.5 (3) | C45—C46—C41 | 121.5 (3) |
| C7—C8—H8 | 119.7 | C45—C46—H46 | 119.3 |
| C3—C8—H8 | 119.7 | C41—C46—H46 | 119.3 |
| C10—C9—C14 | 115.00 (18) | C52—C47—C48 | 117.5 (2) |
| C10—C9—Pd1 | 128.35 (16) | C52—C47—P3 | 120.37 (16) |
| C14—C9—Pd1 | 116.65 (14) | C48—C47—P3 | 121.90 (17) |
| C11—C10—C9 | 121.6 (2) | C49—C48—C47 | 121.1 (2) |
| C11—C10—H10 | 119.2 | C49—C48—H48 | 119.4 |
| C9—C10—H10 | 119.2 | C47—C48—H48 | 119.4 |
| C12—C11—C10 | 121.6 (2) | C48—C49—C50 | 120.5 (2) |
| C12—C11—H11 | 119.2 | C48—C49—H49 | 119.8 |
| C10—C11—H11 | 119.2 | C50—C49—H49 | 119.8 |
| C11—C12—C13 | 119.3 (2) | C51—C50—C49 | 118.7 (2) |
| C11—C12—H12 | 120.4 | C51—C50—H50 | 120.7 |
| C13—C12—H12 | 120.4 | C49—C50—H50 | 120.7 |
| C14—C13—C12 | 119.0 (2) | C50—C51—C52 | 121.5 (2) |
| C14—C13—H13 | 120.5 | C50—C51—H51 | 119.2 |
| C12—C13—H13 | 120.5 | C52—C51—H51 | 119.2 |

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| C13—C14—C9 | 123.56 (19) | C51—C52—C47 | 120.6 (2) |
| C13—C14—P1 | 124.16 (16) | C51—C52—H52 | 119.7 |
| C9—C14—P1 | 112.28 (14) | C47—C52—H52 | 119.7 |
| C16—C15—C20 | 119.9 (2) | F3—C53—F2 | 105.1 (3) |
| C16—C15—P1 | 120.01 (17) | F3—C53—F1 | 109.0 (3) |
| C20—C15—P1 | 120.12 (19) | F2—C53—F1 | 109.5 (3) |
| C15—C16—C17 | 119.1 (2) | F3—C53—S1 | 112.8 (3) |
| C15—C16—H16 | 120.4 | F2—C53—S1 | 110.9 (3) |
| C17—C16—H16 | 120.4 | F1—C53—S1 | 109.4 (3) |
| C18—C17—C16 | 120.3 (3) | Cl1A—C54A—Cl2A | 106.1 (6) |
| C18—C17—H17 | 119.8 | Cl1A—C54A—H54A | 110.5 |
| C16—C17—H17 | 119.8 | Cl2A—C54A—H54A | 110.5 |
| C19—C18—C17 | 120.6 (3) | Cl1A—C54A—H54B | 110.5 |
| C19—C18—H18 | 119.7 | Cl2A—C54A—H54B | 110.5 |
| C17—C18—H18 | 119.7 | H54A—C54A—H54B | 108.7 |
| C18—C19—C20 | 120.0 (3) | Cl2B—C54B—Cl1B | 106.2 (8) |
| C18—C19—H19 | 120.0 | Cl2B—C54B—H54C | 110.5 |
| C20—C19—H19 | 120.0 | Cl1B—C54B—H54C | 110.5 |
| C19—C20—C15 | 120.1 (3) | Cl2B—C54B—H54D | 110.5 |
| C19—C20—H20 | 120.0 | Cl1B—C54B—H54D | 110.5 |
| C15—C20—H20 | 120.0 | H54C—C54B—H54D | 108.7 |
| C26—C21—C22 | 118.4 (2) | Cl2C—C54C—Cl1C | 96.1 (7) |
| C26—C21—P1 | 120.5 (2) | Cl2C—C54C—H54E | 112.5 |
| C22—C21—P1 | 121.1 (2) | Cl1C—C54C—H54E | 112.5 |
| C23—C22—C21 | 120.6 (3) | Cl2C—C54C—H54F | 112.5 |
| C23—C22—H22 | 119.7 | Cl1C—C54C—H54F | 112.5 |
| C21—C22—H22 | 119.7 | H54E—C54C—H54F | 110.1 |
| C24—C23—C22 | 120.6 (3) | C56—C55—H55A | 109.5 |
| C24—C23—H23 | 119.7 | C56—C55—H55B | 109.5 |
| C22—C23—H23 | 119.7 | H55A—C55—H55B | 109.5 |
| C23—C24—C25 | 120.1 (3) | C56—C55—H55C | 109.5 |
| C23—C24—H24 | 119.9 | H55A—C55—H55C | 109.5 |
| C25—C24—H24 | 119.9 | H55B—C55—H55C | 109.5 |
| C24—C25—C26 | 120.6 (3) | C55—C56—C57 | 112.2 (6) |
| C24—C25—H25 | 119.7 | C55—C56—H56A | 109.2 |
| C26—C25—H25 | 119.7 | C57—C56—H56A | 109.2 |
| C21—C26—C25 | 119.3 (3) | C55—C56—H56B | 109.2 |
| C21—C26—H26 | 120.3 | C57—C56—H56B | 109.2 |
| C25—C26—H26 | 120.3 | H56A—C56—H56B | 107.9 |
| C32—C27—C28 | 118.8 (2) | C57$^{i}$—C57—C56 | 123.4 (9) |
| C32—C27—P2 | 123.8 (2) | C57$^{i}$—C57—H57A | 106.5 |
| C28—C27—P2 | 117.34 (19) | C56—C57—H57A | 106.5 |
| C29—C28—C27 | 120.4 (3) | C57$^{i}$—C57—H57B | 106.5 |
| C29—C28—H28 | 119.8 | C56—C57—H57B | 106.5 |
| C27—C28—H28 | 119.8 | H57A—C57—H57B | 106.5 |

Symmetry code: (i) $-x$, $-y+1$, $-z$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C19—H19···O1$^{ii}$ | 0.93 | 2.54 | 3.284 (3) | 138 |
| C30—H30···O6$^{iii}$ | 0.93 | 2.55 | 3.372 (4) | 148 |
| C39—H39*B*···O6$^{iv}$ | 0.97 | 2.59 | 3.309 (4) | 131 |

Symmetry codes: (ii) −*x*+1, −*y*, −*z*; (iii) *x*, *y*−1, *z*; (iv) −*x*+3/2, *y*−1/2, −*z*+1/2.