

1 Aug 2005

Acta Cryst. (2004). C60, 000–000'*trans*-Dichloro(orthochloroaniline) (triphenylphosphine)palladium(II)'MALIHA ASMA,^a WERNER KAMINSKY^b AND AMIN BADSHAH^a^aDepartment of Chemistry Quaid-i-Azam University Islamabad, 45320 Pakistan, and^bDepartment of Chemistry Univ. of Washington Seattle, WA 98195 USA. E-mail:

kaminsky@chem.washington.edu

Abstract

The crystal structure of the title compound, $(\text{PdCl}_2(\text{C}_6\text{H}_5\text{NCl})(\text{C}_{18}\text{H}_{15}\text{P}))$ Pd(II) is a four coordinated PdII complex showing nearly square planar geometry, with bond distances of Pd–N = 2.170 (3) Å, Pd–P = 2.2322 (9) Å, Pd–Cl(1) = 2.3104 (9) Å, and Pd–Cl(2) = 2.2910 (9) Å and angles of the complexes between 86.53 to 93.58 Degrees.

Comment

Palladium (II) complexes are of current interest due to their antitumor (Faraglia *et al.*, 2001) and catalytic activity (Ali *et al.*, 1996) similar to Pt(II) complexes (Loehrer and Einhorn, 1984). For that reason, a variety of palladium(II) complexes containing nitrogen and sulfur donor ligands such as $\text{Pd}(2,3\text{diaminotoluene})\text{Cl}_2$, $\text{Pd}(4,5\text{-diaminoxylen})\text{Cl}_2$ (Cabre *et al.*, 2004), and $\text{Pd}(2\text{-benzoylpyridine thiosemicarbazone})$ have previously been extensively investigated (Rebolledo *et al.*, 2004). In addition, various palladium complexes coordinated to diaminocyclohexan containing ligands proved catalytically active in Heck type reactions (Bravo *et al.*, 2002). Pd(II)-phosphine complexes *cis*- $\text{Pd}(\text{H}_2\text{O})_2(\text{PPh}_3)(p\text{-CH}_3\text{C}_6\text{H}_4\text{SO}_3)\cdot 2\text{H}_2\text{O}$, and *cis*- $\text{Pd}(\text{H}_2\text{O})_2(\text{PPh}_3)(\text{CH}_3\text{SO}_3)_2\cdot 2\text{CH}_2\text{Cl}_2$ are efficient catalysts for carbonylation of olefins (Cavinato *et al.*, 2004). Here, in continuation of our previous work (Parvez *et al.*, 2004) we report a new convenient synthesis and the crystal structure of a palladium(II) complex containing phosphine and aniline ligands. Palladium(II) complexes are unique due to a strong preference of Pd(II) for square planar coordination in which the ligand framework is proven to be highly stable (Porai-Koshits, 1987). The planar environment is slightly distorted tetrahedral. The corresponding bond angles of N(1)–Pd(1)–Cl(2), P(1)–Pd(1)–Cl(2), N(1)–Pd(1)–Cl(1), and P(1)–Pd(1)–Cl(1) are 91.51 (9)°, 93.58 (4)°, 88.06 (9)°, and 86.85 (3)° respectively. Orthochloroaniline and triphenylphosphine are *trans* to each other with the bond angles of N(1)–Pd(1)–P(1), Cl(2)–Pd(1)–Cl(1) being 174.79 (9)° and 179.16 (4)° respectively. The metal-ligand bond distances are Pd(1)–N(1) = 2.170 (3) Å, Pd(1)–P(1) = 2.322 (9) Å, Pd(1)–Cl(2) = 2.2910 (9) Å, and Pd(1)–Cl(1) = 2.3104 (9) Å which are in good agreement with those found in $\text{Pd}(\text{PPh}_3)(\text{indoline-N})\text{Cl}_2$ (Chen *et al.* 1997).

Experimental

Palladium(II) chloride (0.5g, 2.82mmol from E-Merck) was dissolved completely in 20ml distilled water by adding 2–3 drops of dil. HCl. A solution of triphenylphosphine (0.74g, 2.82mmol) in acetone was added dropwise alongwith constant stirring. The reaction mixture was stirred overnight at room temperature. The resulting yellow precipitates of ($\text{PdCl}_2(\text{PPh}_3)(\text{H}_2\text{O})$) were filtered, washed with diethyl ether and dried under vacuum.(0.23 ml, 2.20mmol) 2-chloroaniline was added dropwise into suspension of ($\text{PdCl}_2(\text{PPh}_3)(\text{H}_2\text{O})$) (0.97g, 2.20mmol) in 20 ml of CH_2Cl_2 and refluxed for 1 hr resulting in a clear solution. Dark orange crystals were obtained after slow evaporation of the solvent at room temperature.

Crystal data

$\text{C}_{24}\text{H}_{21}\text{Cl}_3\text{NPPd} \cdot \text{CH}_2\text{Cl}_2$	Mo $K\alpha$ radiation
$M_r = 652.06$	$\lambda = 0.71073 \text{ \AA}$
Triclinic	Cell parameters from 621 reflections
$P\bar{1}$	$\theta = 2.21\text{--}29.99^\circ$
$a = 10.0120 (2) \text{ \AA}$	$\mu = 1.293 \text{ mm}^{-1}$
$b = 10.3890 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 14.2220 (4) \text{ \AA}$	Prism
$\alpha = 104.6190 (10)^\circ$	Orange
$\beta = 89.9230 (10)^\circ$	$0.32 \times 0.29 \times 0.24 \text{ mm}$
$\gamma = 112.7541 (12)^\circ$	
$V = 1312.30 (5) \text{ \AA}^3$	
$Z = 2$	
$D_x = 1.650 \text{ Mg m}^{-3}$	
D_m not measured	

Data collection

Nonius KappaCCD diffractometer	4057 reflections with
φ and ω scans	$>2\sigma(I)$
Absorption correction:	$R_{\text{int}} = 0.0350$
multi-scan HKL2000 (Otwinowski & Minor 1997)	$\theta_{\text{max}} = 29.99^\circ$
$T_{\text{min}} = 0.6800, T_{\text{max}} = 0.7400$	$h = -13 \rightarrow 12$
10268 measured reflections	$k = -12 \rightarrow 14$
6247 independent reflections	$l = -19 \rightarrow 18$
	0. standard reflections
	every 0. reflections
	intensity decay: none

*Refinement*Refinement on F^2

$$w=1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.0000P]$$

$$R[F^2 > 2\sigma(F^2)] = 0.0441$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$wR(F^2) = 0.1164$$

$$(\Delta/\sigma)_{\max} = 0.000$$

$$S = 1.014$$

$$\Delta\rho_{\max} = 0.670 \text{ e \AA}^{-3}$$

$$6247 \text{ reflections}$$

$$\Delta\rho_{\min} = -0.900 \text{ e \AA}^{-3}$$

$$298 \text{ parameters}$$

Extinction correction: none

$$\text{H-atom parameters constrained}$$

Scattering factors from *International Tables
for Crystallography* (Vol. C)

All H atoms were initially located in a difference Fourier map and were refined with a riding model. U_{iso} values were fixed such that they were $1.2 U_{\text{eq}}$ of their parent atom U_{eq} for CH's and $1.5 U_{\text{eq}}$ of their parent atom U_{eq} in case of methyl groups.

Data collection: KappaCCD. Cell refinement: HKL Scale pack (Otwinowski & Minor 1997).

Data reduction: HKL Scale pack (Otwinowski & Minor 1997). Program(s) used to solve structure: DIRDIFF. Program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997). Molecular graphics: maXus, Zortep. Software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: PREVIEW). Services for accessing these data are described at the back of the journal.

References

- Faraglia, G., Fregona, D., Sitran, S., Giovagnini, L., Marzano, C., Baccichetti, F., Casellato, U. & Graziani, R. (2001). *J. Inorg. Biochem.* **83**, 31.
- Ali, B. E., Okuro, K., Vasapollo, G. & Alper, H. (1996). *J. Am. Chem. Soc.* **118**, 4264.
- Loehrer, P. & Einhorn, L. (1984). *Ann. Intern. Med.* **100**, 104.
- Cabre, M. P., Cervantes, G., Moreno, V., Prieto, M. J., Perez, M. J., Bardia, M. F. & Solans, X. (2004). *J. Inorg. Biochem.* **98**, 510.
- Rebolledo, A. P., Vieites, M., Gambino, D., Piro, O. E., Castellano, E. E., Zani, C. L., Souza-Fagundes, E. M., Teixeira, L. R., Batista, A. A. & Beraldo, H. (2005). *J. Inorg. Biochem.* **99**, 698.
- Bravo, J., Cativiela, C., Esteban, R. N. & Urriolabeitia, P. (2002). *J. Organomett. Chem.* **650**, 157–172.
- Cavinato, G., Vavasori, A., Toniolo, L. & Dolmella, A. (2004). *Inorg. Chim. Acta* **357**, 2737–2747.
- Parvez, M., Badshah, A., Asma, M., Ali, S., Ahmed, S., Malik, A., and Ahmed, F. (2004). *Acta Cryst. E60*, 1602–1604.
- Porai-Koshits, M. A. (1987). *Sov. Sci. Rev. B* **10**, 91.
- Chen, S., Vasquez, L., Noll, B. C. & Dubois, M. R. (1997). *Organomett.* **16**, 1757.
- Altomare, A.; Cascarano, G.; Giacovazzo, C.; Burla, M. C.; Polidori, G.; Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–442.
- MacKay, S.; Gilmore, C. J.; Edwards, C.; Tremayne, M.; Stewart, N.; Shankland, K. (1998). "maXus: a computer program for the solution and refinement of crystal structures from diffraction data" University of Glasgow, Scotland, UK, Nonius BV, Delft, The Netherlands and MacScience Co. Ltd, Yokohama, Japan.
- Otwinowski, Z.; Minor, W. (1996). *Methods in Enzymology*, **276**, 307–326.
- Sheldrick, G. M. (1997). *SHELXL97* University of Göttingen, Germany.

Fig. 1. View of the molecule showing the atom-labeling scheme for atoms discussed in the text. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

Supplementary data

The tables of data shown below are not normally printed in *Acta Cryst. Section C* but the data will be available electronically *via* the online contents pages at

<http://journals.iucr.org/c/journalhomepage.html>

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U^{ij} a^i a^j \mathbf{a}_i \cdot \mathbf{a}_j.$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Pd1	0.03793 (3)	0.02779 (3)	0.21760 (2)	0.03847 (11)
Cl1	-0.09129 (12)	0.10275 (11)	0.12449 (7)	0.0528 (3)
Cl2	0.16849 (11)	-0.04633 (11)	0.30827 (7)	0.0501 (2)
Cl3	-0.32775 (15)	-0.28149 (15)	0.06572 (13)	0.0957 (5)
Cl4	0.58409 (18)	-0.15758 (18)	0.85652 (15)	0.1068 (6)
Cl5	0.62230 (16)	0.14137 (16)	0.93286 (11)	0.0915 (4)
P1	0.06090 (10)	0.22256 (10)	0.33833 (7)	0.0364 (2)
N1	0.0009 (4)	-0.1579 (3)	0.0933 (2)	0.0456 (7)
H1A	-0.0486	-0.1489	0.0443	0.055
H1B	0.0885	-0.1509	0.0740	0.055
C1	-0.0742 (4)	-0.3014 (4)	0.1026 (3)	0.0441 (9)
C2	0.0064 (5)	-0.3755 (4)	0.1256 (3)	0.0509 (10)
H2	0.1076	-0.3317	0.1330	0.061
C3	-0.0624 (5)	-0.5117 (5)	0.1371 (3)	0.0599 (11)
H3	-0.0076	-0.5607	0.1508	0.072
C4	-0.2119 (5)	-0.5769 (5)	0.1287 (3)	0.0632 (12)
H4	-0.2577	-0.6689	0.1379	0.076
C5	-0.2931 (5)	-0.5065 (5)	0.1067 (3)	0.0627 (12)
H5	-0.3943	-0.5511	0.1000	0.075
C6	-0.2242 (5)	-0.3685 (4)	0.0945 (3)	0.0535 (10)
C7	-0.1230 (4)	0.2015 (4)	0.3637 (3)	0.0399 (8)
C8	-0.1815 (4)	0.3011 (4)	0.3579 (3)	0.0486 (10)
H8	-0.1251	0.3866	0.3426	0.058
C9	-0.3253 (5)	0.2707 (5)	0.3753 (3)	0.0616 (12)
H9	-0.3654	0.3367	0.3716	0.074
C10	-0.4096 (5)	0.1447 (5)	0.3979 (3)	0.0638 (13)
H10	-0.5056	0.1266	0.4100	0.077
C11	-0.3529 (4)	0.0461 (5)	0.4027 (3)	0.0590 (11)
H11	-0.4105	-0.0399	0.4170	0.071
C12	-0.2092 (4)	0.0746 (4)	0.3861 (3)	0.0504 (10)
H12	-0.1702	0.0079	0.3901	0.061
C13	0.1558 (4)	0.3921 (4)	0.3069 (3)	0.0385 (8)
C14	0.2254 (4)	0.3953 (4)	0.2234 (3)	0.0491 (10)
H14	0.2180	0.3089	0.1798	0.059
C15	0.3060 (5)	0.5256 (5)	0.2038 (3)	0.0598 (11)
H15	0.3536	0.5271	0.1477	0.072
C16	0.3152 (5)	0.6522 (5)	0.2676 (4)	0.0640 (13)
H16	0.3690	0.7399	0.2542	0.077
C17	0.2476 (5)	0.6519 (4)	0.3497 (3)	0.0581 (11)
H17	0.2535	0.7390	0.3918	0.070
C18	0.1699 (4)	0.5230 (4)	0.3712 (3)	0.0507 (10)
H18	0.1265	0.5235	0.4291	0.061
C19	0.1611 (4)	0.2597 (4)	0.4559 (3)	0.0373 (8)
C20	0.3100 (4)	0.3037 (4)	0.4610 (3)	0.0479 (9)
H20	0.3559	0.3074	0.4042	0.058
C21	0.3921 (4)	0.3423 (5)	0.5493 (3)	0.0565 (11)
H21	0.4928	0.3724	0.5518	0.068
C22	0.3261 (5)	0.3362 (5)	0.6323 (3)	0.0592 (11)
H22	0.3817	0.3620	0.6916	0.071
C23	0.1771 (5)	0.2922 (5)	0.6294 (3)	0.0588 (11)
H23	0.1322	0.2882	0.6865	0.071

C24	0.0946 (4)	0.2539 (4)	0.5408 (3)	0.0493 (10)
H24	-0.0060	0.2241	0.5386	0.059
C25	0.5296 (6)	-0.0231 (5)	0.8473 (4)	0.0818 (15)
H25A	0.4263	-0.0546	0.8545	0.098
H25B	0.5431	-0.0092	0.7825	0.098

Table S2. Anisotropic displacement parameters (\AA^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd1	0.04429 (18)	0.03443 (17)	0.03807 (18)	0.01632 (13)	0.00652 (12)	0.01126 (12)
Cl1	0.0692 (7)	0.0499 (6)	0.0443 (6)	0.0289 (5)	-0.0032 (5)	0.0129 (4)
Cl2	0.0567 (6)	0.0476 (6)	0.0533 (6)	0.0266 (5)	0.0031 (5)	0.0170 (5)
Cl3	0.0735 (8)	0.0687 (8)	0.1453 (14)	0.0312 (7)	-0.0294 (9)	0.0249 (9)
Cl4	0.0964 (11)	0.0969 (11)	0.1608 (16)	0.0512 (9)	0.0590 (11)	0.0720 (11)
Cl5	0.0890 (10)	0.0782 (9)	0.0782 (9)	0.0123 (8)	0.0228 (8)	0.0060 (7)
P1	0.0372 (5)	0.0354 (5)	0.0377 (5)	0.0156 (4)	0.0054 (4)	0.0102 (4)
N1	0.064 (2)	0.0352 (17)	0.0366 (17)	0.0171 (16)	0.0121 (15)	0.0121 (14)
C1	0.054 (2)	0.040 (2)	0.035 (2)	0.0156 (19)	0.0028 (17)	0.0093 (16)
C2	0.050 (2)	0.042 (2)	0.057 (3)	0.0157 (19)	0.0036 (19)	0.0104 (19)
C3	0.068 (3)	0.052 (3)	0.062 (3)	0.025 (2)	-0.006 (2)	0.018 (2)
C4	0.070 (3)	0.043 (2)	0.067 (3)	0.010 (2)	-0.007 (2)	0.019 (2)
C5	0.047 (2)	0.048 (3)	0.076 (3)	0.005 (2)	-0.008 (2)	0.014 (2)
C6	0.057 (3)	0.046 (2)	0.051 (2)	0.019 (2)	-0.003 (2)	0.0048 (19)
C7	0.0391 (19)	0.041 (2)	0.036 (2)	0.0154 (17)	0.0037 (16)	0.0057 (16)
C8	0.049 (2)	0.050 (2)	0.048 (2)	0.024 (2)	0.0002 (18)	0.0099 (19)
C9	0.053 (3)	0.077 (3)	0.061 (3)	0.040 (3)	0.002 (2)	0.008 (2)
C10	0.037 (2)	0.087 (4)	0.055 (3)	0.020 (2)	0.002 (2)	0.005 (3)
C11	0.044 (2)	0.059 (3)	0.063 (3)	0.012 (2)	0.007 (2)	0.012 (2)
C12	0.045 (2)	0.048 (2)	0.060 (3)	0.020 (2)	0.0131 (19)	0.015 (2)
C13	0.0369 (19)	0.036 (2)	0.044 (2)	0.0152 (16)	-0.0003 (16)	0.0114 (16)
C14	0.045 (2)	0.044 (2)	0.060 (3)	0.0172 (19)	0.0082 (19)	0.018 (2)
C15	0.050 (2)	0.066 (3)	0.065 (3)	0.016 (2)	0.012 (2)	0.030 (2)
C16	0.054 (3)	0.047 (3)	0.084 (4)	0.004 (2)	-0.009 (3)	0.031 (3)
C17	0.067 (3)	0.037 (2)	0.061 (3)	0.015 (2)	-0.013 (2)	0.007 (2)
C18	0.059 (2)	0.041 (2)	0.048 (2)	0.018 (2)	-0.0003 (19)	0.0087 (18)
C19	0.0394 (19)	0.0324 (19)	0.042 (2)	0.0162 (16)	0.0061 (16)	0.0102 (16)
C20	0.047 (2)	0.059 (3)	0.041 (2)	0.026 (2)	0.0044 (18)	0.0121 (19)
C21	0.036 (2)	0.066 (3)	0.062 (3)	0.017 (2)	-0.001 (2)	0.013 (2)
C22	0.062 (3)	0.065 (3)	0.044 (2)	0.023 (2)	-0.010 (2)	0.008 (2)
C23	0.057 (3)	0.071 (3)	0.042 (2)	0.019 (2)	0.005 (2)	0.016 (2)
C24	0.045 (2)	0.057 (3)	0.043 (2)	0.017 (2)	0.0035 (18)	0.0128 (19)
C25	0.088 (4)	0.065 (3)	0.080 (4)	0.018 (3)	-0.006 (3)	0.020 (3)

Table S3. Geometric parameters (\AA , $^\circ$)

Pd1—N1	2.170 (3)	C10—C11	1.365 (6)
Pd1—P1	2.2322 (9)	C10—H10	0.9300
Pd1—Cl2	2.2910 (9)	C11—C12	1.385 (5)
Pd1—Cl1	2.3104 (9)	C11—H11	0.9300
Cl3—C6	1.724 (4)	C12—H12	0.9300
Cl4—C25	1.717 (5)	C13—C14	1.377 (5)
Cl5—C25	1.729 (5)	C13—C18	1.389 (5)
P1—C7	1.816 (4)	C14—C15	1.380 (6)
P1—C13	1.819 (4)	C14—H14	0.9300
P1—C19	1.825 (4)	C15—C16	1.366 (6)
N1—C1	1.427 (5)	C15—H15	0.9300
N1—H1A	0.9000	C16—C17	1.349 (6)
N1—H1B	0.9000	C16—H16	0.9300
C1—C6	1.381 (6)	C17—C18	1.376 (6)
C1—C2	1.399 (5)	C17—H17	0.9300
C2—C3	1.366 (6)	C18—H18	0.9300
C2—H2	0.9300	C19—C20	1.376 (5)
C3—C4	1.374 (6)	C19—C24	1.382 (5)
C3—H3	0.9300	C20—C21	1.381 (5)
C4—C5	1.368 (6)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.356 (6)
C5—C6	1.387 (6)	C21—H21	0.9300
C5—H5	0.9300	C22—C23	1.378 (6)
C7—C12	1.384 (5)	C22—H22	0.9300
C7—C8	1.389 (5)	C23—C24	1.386 (5)
C8—C9	1.386 (6)	C23—H23	0.9300
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.373 (7)	C25—H25A	0.9700
C9—H9	0.9300	C25—H25B	0.9700

N1—Pd1—P1	174.79 (9)	C10—C11—C12	119.7 (4)
N1—Pd1—Cl2	91.52 (9)	C10—C11—H11	120.2
P1—Pd1—Cl2	93.58 (4)	C12—C11—H11	120.2
N1—Pd1—Cl1	88.06 (9)	C7—C12—C11	120.6 (4)
P1—Pd1—Cl1	86.85 (3)	C7—C12—H12	119.7
Cl2—Pd1—Cl1	179.16 (4)	C11—C12—H12	119.7
C7—P1—C13	110.27 (16)	C14—C13—C18	118.4 (4)
C7—P1—C19	106.03 (16)	C14—C13—P1	121.1 (3)
C13—P1—C19	101.10 (16)	C18—C13—P1	120.2 (3)
C7—P1—Pd1	106.06 (12)	C13—C14—C15	120.7 (4)
C13—P1—Pd1	112.93 (12)	C13—C14—H14	119.7
C19—P1—Pd1	120.14 (11)	C15—C14—H14	119.7
C1—N1—Pd1	120.0 (2)	C16—C15—C14	119.4 (4)
C1—N1—H1A	107.3	C16—C15—H15	120.3
Pd1—N1—H1A	107.3	C14—C15—H15	120.3
C1—N1—H1B	107.3	C17—C16—C15	121.0 (4)
Pd1—N1—H1B	107.3	C17—C16—H16	119.5
H1A—N1—H1B	106.9	C15—C16—H16	119.5
C6—C1—C2	118.0 (4)	C16—C17—C18	120.0 (4)
C6—C1—N1	122.7 (3)	C16—C17—H17	120.0
C2—C1—N1	119.2 (4)	C18—C17—H17	120.0
C3—C2—C1	120.6 (4)	C17—C18—C13	120.3 (4)
C3—C2—H2	119.7	C17—C18—H18	119.8
C1—C2—H2	119.7	C13—C18—H18	119.8
C2—C3—C4	120.6 (4)	C20—C19—C24	118.8 (3)
C2—C3—H3	119.7	C20—C19—P1	118.4 (3)
C4—C3—H3	119.7	C19—C20—C21	122.6 (3)
C5—C4—C3	120.0 (4)	C19—C20—H20	120.8 (4)
C5—C4—H4	120.0	C21—C20—H20	119.6
C3—C4—H4	120.0	C22—C21—C20	119.6
C4—C5—C6	119.8 (4)	C22—C21—H21	120.0
C4—C5—H5	120.1	C20—C21—H21	120.0
C6—C5—H5	120.1	C21—C22—C23	120.4 (4)
C1—C6—C5	121.0 (4)	C21—C22—H22	119.8
C1—C6—Cl3	119.6 (3)	C23—C22—H22	119.8
C5—C6—Cl3	119.4 (3)	C22—C23—C24	119.6 (4)
C12—C7—C8	119.6 (3)	C22—C23—H23	120.2
C12—C7—P1	116.4 (3)	C24—C23—H23	120.2
C8—C7—P1	124.0 (3)	C19—C24—C23	120.3 (4)
C9—C8—C7	118.9 (4)	C19—C24—H24	119.9
C9—C8—H8	120.6	C23—C24—H24	119.9
C7—C8—H8	120.6	C14—C25—Cl5	114.0 (3)
C10—C9—C8	121.1 (4)	C14—C25—H25A	108.8
C10—C9—H9	119.5	Cl5—C25—H25A	108.8
C8—C9—H9	119.5	Cl4—C25—H25B	108.8
C11—C10—C9	120.2 (4)	Cl5—C25—H25B	108.8
C11—C10—H10	119.9	H25A—C25—H25B	107.7
C9—C10—H10	119.9		

Cl2—Pd1—P1—C7	-120.11 (13)	C8—C7—C12—C11	0.1 (6)
Cl1—Pd1—P1—C7	60.61 (13)	P1—C7—C12—C11	-177.4 (3)
Cl2—Pd1—P1—C13	119.01 (12)	C10—C11—C12—C7	-0.7 (7)
Cl1—Pd1—P1—C13	-60.27 (12)	C7—P1—C13—C14	-128.7 (3)
Cl2—Pd1—P1—C19	-0.15 (14)	C19—P1—C13—C14	119.5 (3)
Cl1—Pd1—P1—C19	-179.43 (14)	Pd1—P1—C13—C14	-10.2 (3)
Cl2—Pd1—N1—C1	59.9 (3)	C7—P1—C13—C18	56.8 (3)
Cl1—Pd1—N1—C1	-120.8 (3)	C19—P1—C13—C18	-55.0 (3)
Pd1—N1—C1—C6	82.4 (4)	Pd1—P1—C13—C18	175.3 (3)
Pd1—N1—C1—C2	-94.4 (4)	C18—C13—C14—C15	-0.6 (6)
C6—C1—C2—C3	1.6 (6)	P1—C13—C14—C15	-175.2 (3)
N1—C1—C2—C3	178.5 (4)	C13—C14—C15—C16	-0.7 (6)
C1—C2—C3—C4	-1.5 (7)	C14—C15—C16—C17	0.4 (7)
C2—C3—C4—C5	1.2 (7)	C15—C16—C17—C18	1.1 (7)
C3—C4—C5—C6	-1.0 (7)	C16—C17—C18—C13	-2.5 (6)
C2—C1—C6—C5	-1.4 (6)	C14—C13—C18—C17	2.2 (6)
N1—C1—C6—C5	-178.2 (4)	P1—C13—C18—C17	176.9 (3)
C2—C1—C6—Cl3	-179.7 (3)	C7—P1—C19—C20	-169.6 (3)
N1—C1—C6—Cl3	3.6 (6)	C13—P1—C19—C20	-54.5 (3)
C4—C5—C6—C1	1.1 (7)	Pd1—P1—C19—C20	70.4 (3)
C4—C5—C6—Cl3	179.4 (4)	C7—P1—C19—C24	6.4 (4)
C13—P1—C7—C12	178.3 (3)	C13—P1—C19—C24	121.5 (3)
C19—P1—C7—C12	-73.1 (3)	Pd1—P1—C19—C24	-113.6 (3)
Pd1—P1—C7—C12	55.7 (3)	C24—C19—C20—C21	-0.4 (6)
C13—P1—C7—C8	1.0 (4)	P1—C19—C20—C21	175.8 (3)
C19—P1—C7—C8	109.6 (3)	C19—C20—C21—C22	0.4 (7)
Pd1—P1—C7—C8	-121.6 (3)	C20—C21—C22—C23	-0.2 (7)
C12—C7—C8—C9	0.3 (6)	C21—C22—C23—C24	0.0 (7)
P1—C7—C8—C9	177.5 (3)	C20—C19—C24—C23	0.2 (6)
C7—C8—C9—C10	0.0 (6)	P1—C19—C24—C23	-175.8 (3)
C8—C9—C10—C11	-0.7 (7)	C22—C23—C24—C19	0.0 (7)
C9—C10—C11—C12	1.0 (7)		