Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(±)-Di-μ-chlorido-(μ-*N*,*N*′-{[3,3′-methylenebis(2,4,6-trimethyl-3,1-phenylene)]dimethylene}bis(2-methylpropan-2-amine))bis[chloridopalladium(II)]

Ludovic Chahen, Bruno Therrien and Georg Süss-Fink*

Institut de Chimie, Université de Neuchâtel, Case postale 158, CH-2009 Neuchâtel, Switzerland
Correspondence e-mail: georg.suess-fink@unine.ch

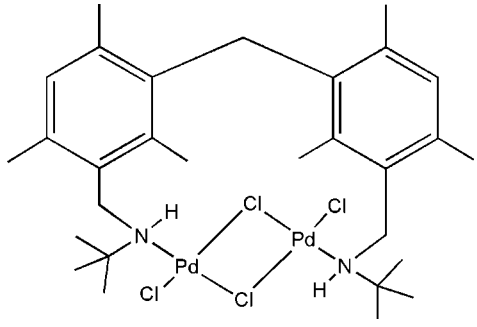
Received 24 September 2007; accepted 28 September 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.105; data-to-parameter ratio = 18.0.

In the title dinuclear palladium complex, $[Pd_2Cl_4(C_{29}H_{46}N_2)]$, the terminal ligands adopt an *anti* configuration, with an intramolecular metal–metal distance of 3.3625 (5) Å. The dinuclear palladium complex adopts a V-shaped conformation, with a dihedral angle of 152.67 (3)° between the two chloride-bridged $PdNCl_3$ square-planar systems. The benzene rings in the chelating amine ligand are at an angle of 74.9 (1)° with respect to each other. The complex is the first example of chloride-bridged dinuclear palladium complex with a bidentate secondary amine ligand.

Related literature

For similar dinuclear chlorido-bridged palladium complexes, see: Guzei *et al.* (2003). For the synthesis of NH^{t}Bu-CH_2-2,4,6-C_6HMe_3-CH_2-2,4,6-C_6HMe_3-CH_2-NH^{t}Bu, see: Chahen *et al.* (2007). For structural information, see: Barnes *et al.* (1981).



Experimental

Crystal data

$[Pd_2Cl_4(C_{29}H_{46}N_2)]$
M_r = 777.28
Orthorhombic, *Pbca*
a = 18.7173 (11) Å
b = 14.7968 (8) Å
c = 23.1967 (18) Å
V = 6424.5 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 173 (2) K
0.22 × 0.19 × 0.16 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: none
47318 measured reflections
6218 independent reflections
4450 reflections with $I > 2\sigma(I)$
R_{int} = 0.106

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.105
S = 0.92
6218 reflections
346 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −1.24 e Å^{-3}

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Swiss National Science Foundation (grant No. 20-61227-00).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2236).

References

Barnes, J. C., Paton, J. D., Damewood, J. R. Jr & Mislow, K. (1981). *J. Org. Chem.* **46**, 4975–4979.
Chahen, L., Therrien, B. & Süss-Fink, G. (2007). *Eur. J. Inorg. Chem.* doi:10.1002/ejic.200700518.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Guzei, I. A., Li, K., Bikzhanova, G. A., Darkwa, J. & Mapolie, S. F. (2003). *Dalton Trans.* pp. 715–722.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2000). *IPDS Software*. Stoe & Cie GmbH, Darmstadt, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m2687 [**doi:10.1107/S1600536807047745**]

(±)-Di-μ-chlorido-(μ-*N*,*N*'-{[3,3'-methylenebis(2,4,6-trimethyl-3,1-phenylene)]dimethylene}bis(2-methylpropan-2-amine))bis[chloridopalladium(II)]

L. Chahen, B. Therrien and G. Süss-Fink

Comment

The title compound [PdCl(μ-Cl) (NH^tBu—CH_2-2,4,6-C_6HMe_3—CH_2-2,4,6-C_6HMe_3—CH_2—NH^tBu)]$_2$ (**1**) is prepared from *N*,*N*'-{3,3'-methylenebis(2,4,6-trimethyl-3,1-phenylene)}bis(methylene)bis (2-methylpropan-2-amine) (Chahen *et al.*, 2007) and 2 eq. of [$PdCl_2(C_6H_5CN)_2$]. The molecular structure of **1** shows the palladium atoms to be surrounded by a terminal chloro ligand, a nitrogen atom of the bidentate amine ligand, NH^tBu—CH_2-2,4,6-C_6HMe_3—CH_2-2,4,6-C_6HMe_3—CH_2—NH^tBu, and two bridging chloro ligands. Each Pd atom and the four atoms comprising its square-planar coordination sphere are planar with a mean deviation of the fitted atoms of 0.009Å for Pd1 and 0.03Å for Pd2. The angle between these two planes is 152.67 (3)°. The intramolecular Pd—Pd distance of 3.3625 (5) Å is slightly longer then those observed for the pyrazolyl analogues [3.2004 (6) to 3.2569 (6) Å] (Guzei *et al.*, 2003).

A characteristic helical conformation of the diphenyl methane moiety (Barnes *et al.*, 1981), which occurs as enantiomeric pairs, is observed in the bis-amine ligand. The two C_6HMe_3 planes are inclined at an angle of 74.9 (1)° to each other.

Experimental

A solution of di(^{t}tbutylamino-methyl-mesityl)methane (178 mg, 0.42 mmol) and [$PdCl_2(C_6H_5CN)_2$] (322 mg, 0.84 mmol) in dichloromethane (80 ml) was stirred during 18 h. After that period the solvent was evaporated and the residue filtered through a short silicagel column using dichloromethane as eluent. The filtrate was evaporated to dryness and the orange product was washed with diethylether (10 ml) (78% yield).

Complex **1** was disolved in chloroform, and crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the chloroform solution.

^{1}H NMR (400 MHz, $CDCl_3$): 7.09 (s, 2H), 4.59 (d, ^{3}J = 11.4 Hz, 2H), 4.38 (s, 2H), 3.81 (dd, ^{2}J = 12.7 Hz, 2H), 3.14 (d, ^{2}J = 12.7 Hz, 2H), 2.60 (s, 6H), 2.49 (s, 6H), 2.37 (s, 6H), 1.57 (s, 18H) p.p.m.. ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): 138.23, 137.67, 137.42, 135.05, 132.27, 130.18, 60.83, 47.11, 33.94, 29.35, 22.68, 20.72, 19.24 p.p.m.. Calcd. for $C_{29}H_{46}Cl_4N_2Pd_2$: C 44.81 H 5.96 N 3.60 Found: C 44.56 H 5.92 N 3.57.

Refinement

The H atoms were included in calculated positions and refined using a riding model, with C—H (N—H)= 0.93–0.96 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Figures

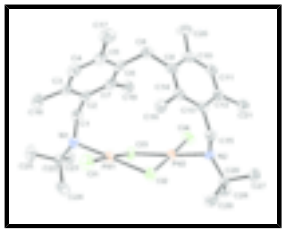


Fig. 1. The molecular structure of [PdCl(μ-Cl) (NH^tBu—CH_2-2,4,6-C_6HMe_3—CH_2-2,4,6-C_6HMe_3—CH_2—NH^tBu)]$_2$. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity

(±)-Di-μ-chlorido-[μ-*N*,*N*'-{[3,3'-methylenebis(2,4,6-trimethyl- 3,1-phenylene)]dimethylene}bis(2-methylpropan-2- amine)]bis[chloridopalladium(II)]

Crystal data

$[Pd_2Cl_4(C_{29}H_{46}N_2)]$	F_{000} = 3152
M_r = 777.28	D_x = 1.607 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 8003 reflections
a = 18.7173 (11) Å	θ = 2.1–26.0º
b = 14.7968 (8) Å	μ = 1.47 mm^{-1}
c = 23.1967 (18) Å	*T* = 173 (2) K
V = 6424.5 (7) Å^3	Plate, yellow
Z = 8	0.22 × 0.19 × 0.16 mm

Data collection

Stoe IPDS diffractometer	4450 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.106
Monochromator: graphite	θ_{max} = 25.9º
T = 173(2) K	θ_{min} = 2.2º
φ oscillation scans	*h* = −23→22
Absorption correction: none	*k* = −17→17
47318 measured reflections	*l* = −28→28
6218 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H-atom parameters constrained
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.92	$(\Delta/\sigma)_{max}$ = 0.001

6218 reflections	$\Delta\rho_{max} = 0.83$ e Å^{-3}
346 parameters	$\Delta\rho_{min} = -1.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. A crystal was mounted at 173 K on a Stoe Image Plate Diffraction System (Stoe & Cie, 2000) using Mo *K*α graphite monochromated radiation. Image plate distance 70 mm, φ oscillation scans 0 − 100°, step Δφ = 0.8°, 5 minutes per frame.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5736 (2)	0.4144 (3)	0.31830 (17)	0.0296 (9)
H1A	0.6244	0.4184	0.3103	0.036*
H1B	0.5554	0.4753	0.3230	0.036*
C2	0.5361 (2)	0.3695 (3)	0.26755 (17)	0.0271 (9)
C3	0.5634 (2)	0.2868 (3)	0.24702 (17)	0.0288 (9)
C4	0.5300 (2)	0.2459 (3)	0.20064 (18)	0.0328 (10)
H4	0.5491	0.1923	0.1864	0.039*
C5	0.4696 (2)	0.2807 (3)	0.17434 (18)	0.0316 (9)
C6	0.4423 (2)	0.3634 (3)	0.19445 (17)	0.0303 (9)
C7	0.4773 (2)	0.4101 (3)	0.23907 (17)	0.0289 (9)
C8	0.3776 (2)	0.4033 (4)	0.16409 (18)	0.0389 (11)
H8A	0.3563	0.3549	0.1416	0.047*
H8B	0.3954	0.4474	0.1368	0.047*
C9	0.3170 (2)	0.4485 (3)	0.19724 (17)	0.0293 (9)
C10	0.2895 (2)	0.5295 (3)	0.17559 (17)	0.0319 (9)
C11	0.2326 (2)	0.5708 (3)	0.20403 (16)	0.0286 (9)
H11	0.2149	0.6249	0.1895	0.034*
C12	0.2015 (2)	0.5345 (3)	0.25317 (17)	0.0271 (9)
C13	0.2288 (2)	0.4529 (3)	0.27535 (16)	0.0274 (9)
C14	0.2851 (2)	0.4084 (3)	0.24643 (17)	0.0268 (9)
C15	0.1935 (2)	0.4135 (3)	0.32872 (17)	0.0283 (9)
H15A	0.1427	0.4060	0.3218	0.034*
H15B	0.2136	0.3545	0.3368	0.034*
C16	0.6282 (2)	0.2403 (3)	0.2727 (2)	0.0360 (10)
H16A	0.6139	0.2050	0.3054	0.054*
H16B	0.6624	0.2849	0.2846	0.054*

H16C	0.6495	0.2014	0.2443	0.054*
C17	0.4378 (3)	0.2303 (4)	0.1237 (2)	0.0464 (12)
H17A	0.4664	0.1780	0.1154	0.070*
H17B	0.4369	0.2692	0.0906	0.070*
H17C	0.3901	0.2118	0.1330	0.070*
C18	0.4534 (2)	0.5050 (3)	0.25403 (19)	0.0334 (10)
H18A	0.4126	0.5021	0.2791	0.050*
H18B	0.4408	0.5367	0.2194	0.050*
H18C	0.4916	0.5363	0.2732	0.050*
C19	0.3112 (2)	0.3161 (3)	0.26521 (19)	0.0320 (10)
H19A	0.3529	0.3228	0.2889	0.048*
H19B	0.3229	0.2807	0.2318	0.048*
H19C	0.2743	0.2863	0.2868	0.048*
C20	0.3157 (3)	0.5732 (4)	0.12039 (19)	0.0431 (12)
H20A	0.3057	0.5341	0.0884	0.065*
H20B	0.3663	0.5831	0.1229	0.065*
H20C	0.2918	0.6299	0.1149	0.065*
C21	0.1385 (2)	0.5844 (3)	0.27893 (19)	0.0325 (9)
H21A	0.1548	0.6231	0.3095	0.049*
H21B	0.1048	0.5416	0.2940	0.049*
H21C	0.1159	0.6203	0.2496	0.049*
C22	0.6132 (2)	0.3860 (3)	0.42283 (18)	0.0307 (9)
C23	0.6175 (2)	0.4873 (3)	0.43222 (19)	0.0354 (10)
H23A	0.6345	0.5159	0.3977	0.053*
H23B	0.6497	0.4999	0.4634	0.053*
H23C	0.5709	0.5102	0.4415	0.053*
C24	0.5848 (3)	0.3393 (3)	0.47687 (19)	0.0397 (11)
H24A	0.6192	0.3448	0.5074	0.060*
H24B	0.5765	0.2766	0.4688	0.060*
H24C	0.5408	0.3673	0.4885	0.060*
C25	0.6874 (2)	0.3479 (4)	0.4085 (2)	0.0451 (13)
H25A	0.7063	0.3785	0.3754	0.068*
H25B	0.6835	0.2844	0.4004	0.068*
H25C	0.7187	0.3568	0.4408	0.068*
C26	0.1549 (2)	0.4595 (3)	0.43174 (16)	0.0291 (9)
C27	0.0767 (2)	0.4595 (4)	0.4113 (2)	0.0399 (11)
H27A	0.0694	0.4103	0.3849	0.060*
H27B	0.0664	0.5156	0.3922	0.060*
H27C	0.0456	0.4526	0.4439	0.060*
C28	0.1667 (3)	0.5402 (3)	0.47139 (19)	0.0390 (11)
H28A	0.1391	0.5326	0.5059	0.058*
H28B	0.1520	0.5945	0.4521	0.058*
H28C	0.2165	0.5444	0.4811	0.058*
C29	0.1720 (3)	0.3719 (3)	0.4619 (2)	0.0435 (12)
H29A	0.2197	0.3744	0.4770	0.065*
H29B	0.1684	0.3228	0.4350	0.065*
H29C	0.1388	0.3626	0.4929	0.065*
Cl1	0.47124 (6)	0.19910 (8)	0.38347 (5)	0.0417 (3)
Cl2	0.33518 (5)	0.33643 (8)	0.41655 (5)	0.0344 (2)

Cl3	0.43593 (5)	0.50561 (7)	0.40657 (5)	0.0319 (2)
Cl4	0.29904 (6)	0.63889 (8)	0.37556 (5)	0.0365 (3)
N1	0.56226 (17)	0.3624 (2)	0.37331 (15)	0.0285 (8)
H1	0.5749	0.3050	0.3637	0.034*
N2	0.20462 (17)	0.4748 (2)	0.37997 (14)	0.0265 (7)
H2	0.1914	0.5301	0.3666	0.032*
Pd1	0.455757 (16)	0.35125 (2)	0.393763 (13)	0.02669 (11)
Pd2	0.312726 (15)	0.48875 (2)	0.395103 (12)	0.02541 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.029 (2)	0.024 (2)	0.037 (2)	−0.0035 (17)	0.0036 (17)	−0.0001 (17)
C2	0.0269 (19)	0.025 (2)	0.030 (2)	−0.0020 (17)	0.0095 (16)	0.0003 (16)
C3	0.029 (2)	0.027 (3)	0.031 (2)	−0.0009 (17)	0.0086 (17)	0.0002 (17)
C4	0.039 (2)	0.023 (2)	0.037 (2)	−0.0015 (18)	0.0088 (19)	−0.0029 (18)
C5	0.035 (2)	0.027 (3)	0.033 (2)	−0.0056 (18)	0.0076 (17)	−0.0027 (18)
C6	0.032 (2)	0.032 (3)	0.027 (2)	0.0001 (17)	0.0074 (16)	−0.0002 (17)
C7	0.032 (2)	0.022 (2)	0.033 (2)	−0.0028 (17)	0.0105 (17)	0.0001 (17)
C8	0.046 (3)	0.045 (3)	0.025 (2)	0.011 (2)	0.0036 (19)	−0.0042 (19)
C9	0.034 (2)	0.030 (3)	0.024 (2)	0.0003 (18)	−0.0033 (16)	−0.0045 (16)
C10	0.040 (2)	0.032 (3)	0.025 (2)	−0.0011 (19)	−0.0018 (17)	0.0014 (17)
C11	0.038 (2)	0.020 (2)	0.027 (2)	0.0018 (17)	−0.0049 (17)	0.0009 (16)
C12	0.0267 (19)	0.027 (2)	0.028 (2)	−0.0006 (16)	−0.0058 (16)	−0.0071 (17)
C13	0.030 (2)	0.028 (2)	0.0247 (19)	−0.0050 (17)	−0.0073 (16)	−0.0009 (16)
C14	0.031 (2)	0.022 (2)	0.028 (2)	0.0027 (17)	−0.0051 (16)	−0.0025 (16)
C15	0.0285 (19)	0.027 (2)	0.030 (2)	−0.0012 (17)	−0.0032 (16)	−0.0023 (17)
C16	0.034 (2)	0.027 (3)	0.047 (3)	0.0050 (19)	0.0043 (19)	−0.002 (2)
C17	0.055 (3)	0.042 (3)	0.041 (3)	0.002 (2)	0.000 (2)	−0.012 (2)
C18	0.036 (2)	0.027 (3)	0.037 (2)	0.0058 (18)	−0.0002 (19)	−0.0044 (18)
C19	0.033 (2)	0.027 (3)	0.036 (2)	0.0016 (18)	0.0012 (17)	−0.0034 (18)
C20	0.062 (3)	0.042 (3)	0.025 (2)	0.003 (2)	0.006 (2)	0.002 (2)
C21	0.033 (2)	0.027 (3)	0.037 (2)	−0.0006 (18)	−0.0013 (18)	0.0038 (18)
C22	0.0252 (19)	0.029 (3)	0.038 (2)	−0.0021 (17)	−0.0070 (17)	−0.0061 (18)
C23	0.035 (2)	0.032 (3)	0.039 (2)	−0.0034 (19)	−0.0075 (19)	−0.0055 (19)
C24	0.043 (3)	0.034 (3)	0.043 (3)	−0.003 (2)	−0.014 (2)	0.001 (2)
C25	0.031 (2)	0.039 (3)	0.065 (3)	0.006 (2)	−0.009 (2)	−0.014 (2)
C26	0.030 (2)	0.033 (3)	0.024 (2)	−0.0016 (18)	0.0053 (16)	0.0028 (17)
C27	0.027 (2)	0.051 (3)	0.042 (2)	−0.004 (2)	0.0018 (18)	−0.002 (2)
C28	0.045 (3)	0.044 (3)	0.028 (2)	−0.003 (2)	0.0036 (19)	−0.005 (2)
C29	0.048 (3)	0.040 (3)	0.043 (3)	0.005 (2)	0.016 (2)	0.011 (2)
Cl1	0.0401 (6)	0.0243 (6)	0.0607 (7)	−0.0071 (5)	−0.0001 (5)	−0.0003 (5)
Cl2	0.0273 (5)	0.0312 (6)	0.0447 (6)	−0.0032 (4)	0.0012 (4)	0.0070 (5)
Cl3	0.0251 (5)	0.0291 (6)	0.0414 (6)	−0.0036 (4)	0.0009 (4)	−0.0043 (4)
Cl4	0.0377 (5)	0.0265 (6)	0.0453 (6)	−0.0051 (4)	−0.0040 (5)	0.0035 (4)
N1	0.0280 (17)	0.024 (2)	0.0331 (17)	−0.0002 (14)	−0.0008 (14)	−0.0036 (14)
N2	0.0269 (17)	0.025 (2)	0.0275 (17)	−0.0028 (14)	0.0029 (14)	0.0017 (14)
Pd1	0.02492 (17)	0.0251 (2)	0.03005 (17)	−0.00315 (12)	−0.00053 (12)	0.00089 (13)

Pd2	0.02467 (17)	0.0255 (2)	0.02605 (17)	−0.00274 (12)	−0.00058 (12)	0.00051 (12)

Geometric parameters (Å, °)

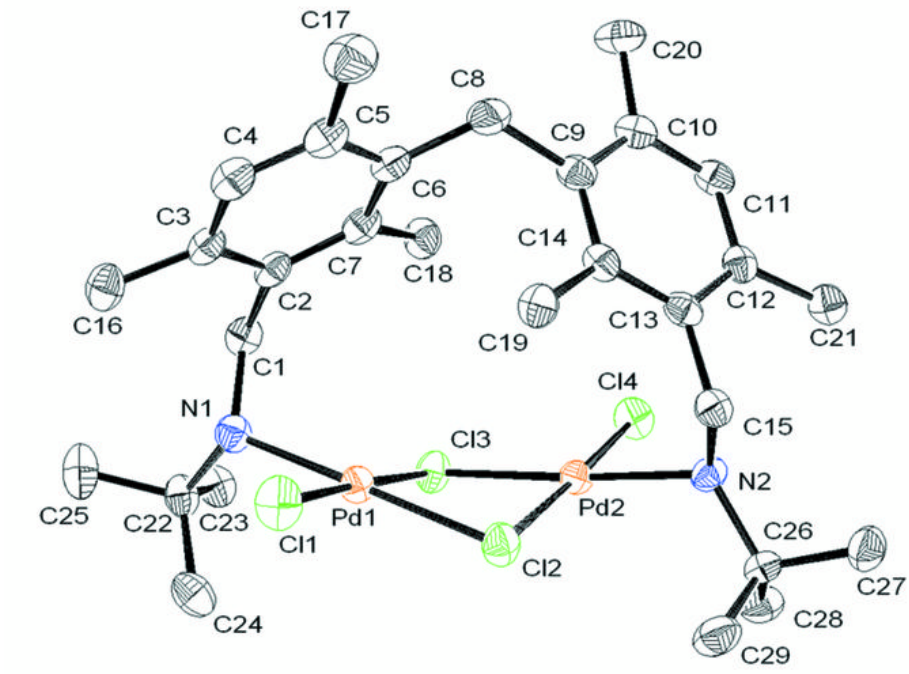
C1—N1	1.505 (5)	C19—H19C	0.9600
C1—C2	1.523 (6)	C20—H20A	0.9600
C1—H1A	0.9700	C20—H20B	0.9600
C1—H1B	0.9700	C20—H20C	0.9600
C2—C3	1.410 (6)	C21—H21A	0.9600
C2—C7	1.418 (6)	C21—H21B	0.9600
C3—C4	1.384 (6)	C21—H21C	0.9600
C3—C16	1.516 (6)	C22—C23	1.517 (6)
C4—C5	1.383 (6)	C22—C24	1.527 (6)
C4—H4	0.9300	C22—N1	1.533 (5)
C5—C6	1.407 (6)	C22—C25	1.535 (6)
C5—C17	1.513 (6)	C23—H23A	0.9600
C6—C7	1.407 (6)	C23—H23B	0.9600
C6—C8	1.520 (6)	C23—H23C	0.9600
C7—C18	1.513 (6)	C24—H24A	0.9600
C8—C9	1.525 (6)	C24—H24B	0.9600
C8—H8A	0.9700	C24—H24C	0.9600
C8—H8B	0.9700	C25—H25A	0.9600
C9—C10	1.397 (6)	C25—H25B	0.9600
C9—C14	1.418 (6)	C25—H25C	0.9600
C10—C11	1.394 (6)	C26—C29	1.508 (6)
C10—C20	1.516 (6)	C26—C28	1.523 (6)
C11—C12	1.388 (6)	C26—N2	1.536 (5)
C11—H11	0.9300	C26—C27	1.538 (6)
C12—C13	1.409 (6)	C27—H27A	0.9600
C12—C21	1.514 (6)	C27—H27B	0.9600
C13—C14	1.412 (6)	C27—H27C	0.9600
C13—C15	1.520 (6)	C28—H28A	0.9600
C14—C19	1.514 (6)	C28—H28B	0.9600
C15—N2	1.510 (5)	C28—H28C	0.9600
C15—H15A	0.9700	C29—H29A	0.9600
C15—H15B	0.9700	C29—H29B	0.9600
C16—H16A	0.9600	C29—H29C	0.9600
C16—H16B	0.9600	Cl1—Pd1	2.2825 (12)
C16—H16C	0.9600	Cl2—Pd1	2.3283 (10)
C17—H17A	0.9600	Cl2—Pd2	2.3460 (12)
C17—H17B	0.9600	Cl3—Pd1	2.3329 (11)
C17—H17C	0.9600	Cl3—Pd2	2.3347 (10)
C18—H18A	0.9600	Cl4—Pd2	2.2818 (12)
C18—H18B	0.9600	N1—Pd1	2.056 (3)
C18—H18C	0.9600	N1—H1	0.9100
C19—H19A	0.9600	N2—Pd2	2.064 (3)
C19—H19B	0.9600	N2—H2	0.9100
N1—C1—C2	111.6 (3)	H20A—C20—H20C	109.5
N1—C1—H1A	109.3	H20B—C20—H20C	109.5

C2—C1—H1A	109.3	C12—C21—H21A	109.5
N1—C1—H1B	109.3	C12—C21—H21B	109.5
C2—C1—H1B	109.3	H21A—C21—H21B	109.5
H1A—C1—H1B	108.0	C12—C21—H21C	109.5
C3—C2—C7	119.5 (4)	H21A—C21—H21C	109.5
C3—C2—C1	118.2 (4)	H21B—C21—H21C	109.5
C7—C2—C1	122.2 (4)	C23—C22—C24	110.3 (4)
C4—C3—C2	118.6 (4)	C23—C22—N1	111.4 (3)
C4—C3—C16	118.0 (4)	C24—C22—N1	107.2 (3)
C2—C3—C16	123.5 (4)	C23—C22—C25	110.3 (4)
C5—C4—C3	123.4 (4)	C24—C22—C25	109.1 (4)
C5—C4—H4	118.3	N1—C22—C25	108.5 (3)
C3—C4—H4	118.3	C22—C23—H23A	109.5
C4—C5—C6	118.4 (4)	C22—C23—H23B	109.5
C4—C5—C17	118.7 (4)	H23A—C23—H23B	109.5
C6—C5—C17	122.9 (4)	C22—C23—H23C	109.5
C7—C6—C5	120.1 (4)	H23A—C23—H23C	109.5
C7—C6—C8	121.5 (4)	H23B—C23—H23C	109.5
C5—C6—C8	118.3 (4)	C22—C24—H24A	109.5
C6—C7—C2	119.8 (4)	C22—C24—H24B	109.5
C6—C7—C18	119.1 (4)	H24A—C24—H24B	109.5
C2—C7—C18	121.1 (4)	C22—C24—H24C	109.5
C6—C8—C9	121.9 (3)	H24A—C24—H24C	109.5
C6—C8—H8A	106.8	H24B—C24—H24C	109.5
C9—C8—H8A	106.8	C22—C25—H25A	109.5
C6—C8—H8B	106.8	C22—C25—H25B	109.5
C9—C8—H8B	106.8	H25A—C25—H25B	109.5
H8A—C8—H8B	106.7	C22—C25—H25C	109.5
C10—C9—C14	119.6 (4)	H25A—C25—H25C	109.5
C10—C9—C8	118.0 (4)	H25B—C25—H25C	109.5
C14—C9—C8	122.3 (4)	C29—C26—C28	111.3 (4)
C11—C10—C9	119.2 (4)	C29—C26—N2	111.1 (3)
C11—C10—C20	117.4 (4)	C28—C26—N2	105.6 (3)
C9—C10—C20	123.4 (4)	C29—C26—C27	110.2 (4)
C12—C11—C10	122.6 (4)	C28—C26—C27	109.0 (4)
C12—C11—H11	118.7	N2—C26—C27	109.6 (3)
C10—C11—H11	118.7	C26—C27—H27A	109.5
C11—C12—C13	118.6 (4)	C26—C27—H27B	109.5
C11—C12—C21	117.5 (4)	H27A—C27—H27B	109.5
C13—C12—C21	123.8 (4)	C26—C27—H27C	109.5
C12—C13—C14	119.8 (4)	H27A—C27—H27C	109.5
C12—C13—C15	117.9 (4)	H27B—C27—H27C	109.5
C14—C13—C15	122.2 (4)	C26—C28—H28A	109.5
C13—C14—C9	120.1 (4)	C26—C28—H28B	109.5
C13—C14—C19	121.6 (4)	H28A—C28—H28B	109.5
C9—C14—C19	118.3 (4)	C26—C28—H28C	109.5
N2—C15—C13	110.6 (3)	H28A—C28—H28C	109.5
N2—C15—H15A	109.5	H28B—C28—H28C	109.5
C13—C15—H15A	109.5	C26—C29—H29A	109.5

N2—C15—H15B	109.5	C26—C29—H29B	109.5
C13—C15—H15B	109.5	H29A—C29—H29B	109.5
H15A—C15—H15B	108.1	C26—C29—H29C	109.5
C3—C16—H16A	109.5	H29A—C29—H29C	109.5
C3—C16—H16B	109.5	H29B—C29—H29C	109.5
H16A—C16—H16B	109.5	Pd1—Cl2—Pd2	92.01 (4)
C3—C16—H16C	109.5	Pd1—Cl3—Pd2	92.18 (4)
H16A—C16—H16C	109.5	C1—N1—C22	115.6 (3)
H16B—C16—H16C	109.5	C1—N1—Pd1	111.9 (2)
C5—C17—H17A	109.5	C22—N1—Pd1	116.6 (3)
C5—C17—H17B	109.5	C1—N1—H1	103.5
H17A—C17—H17B	109.5	C22—N1—H1	103.5
C5—C17—H17C	109.5	Pd1—N1—H1	103.5
H17A—C17—H17C	109.5	C15—N2—C26	116.3 (3)
H17B—C17—H17C	109.5	C15—N2—Pd2	109.2 (2)
C7—C18—H18A	109.5	C26—N2—Pd2	118.4 (2)
C7—C18—H18B	109.5	C15—N2—H2	103.6
H18A—C18—H18B	109.5	C26—N2—H2	103.6
C7—C18—H18C	109.5	Pd2—N2—H2	103.6
H18A—C18—H18C	109.5	N1—Pd1—Cl1	86.11 (11)
H18B—C18—H18C	109.5	N1—Pd1—Cl2	179.19 (11)
C14—C19—H19A	109.5	Cl1—Pd1—Cl2	93.09 (4)
C14—C19—H19B	109.5	N1—Pd1—Cl3	96.02 (10)
H19A—C19—H19B	109.5	Cl1—Pd1—Cl3	177.71 (4)
C14—C19—H19C	109.5	Cl2—Pd1—Cl3	84.78 (4)
H19A—C19—H19C	109.5	N2—Pd2—Cl4	87.33 (10)
H19B—C19—H19C	109.5	N2—Pd2—Cl3	176.73 (9)
C10—C20—H20A	109.5	Cl4—Pd2—Cl3	91.69 (4)
C10—C20—H20B	109.5	N2—Pd2—Cl2	96.64 (10)
H20A—C20—H20B	109.5	Cl4—Pd2—Cl2	176.02 (4)
C10—C20—H20C	109.5	Cl3—Pd2—Cl2	84.35 (4)
N1—C1—C2—C3	−70.0 (4)	C12—C13—C14—C19	−173.8 (4)
N1—C1—C2—C7	112.9 (4)	C15—C13—C14—C19	3.2 (6)
C7—C2—C3—C4	−2.4 (6)	C10—C9—C14—C13	−3.8 (6)
C1—C2—C3—C4	−179.5 (4)	C8—C9—C14—C13	−179.5 (4)
C7—C2—C3—C16	177.0 (4)	C10—C9—C14—C19	173.9 (4)
C1—C2—C3—C16	−0.1 (6)	C8—C9—C14—C19	−1.9 (6)
C2—C3—C4—C5	−2.0 (6)	C12—C13—C15—N2	−65.6 (4)
C16—C3—C4—C5	178.6 (4)	C14—C13—C15—N2	117.3 (4)
C3—C4—C5—C6	2.3 (6)	C2—C1—N1—C22	163.9 (3)
C3—C4—C5—C17	179.7 (4)	C2—C1—N1—Pd1	−59.3 (4)
C4—C5—C6—C7	1.9 (6)	C23—C22—N1—C1	49.3 (5)
C17—C5—C6—C7	−175.4 (4)	C24—C22—N1—C1	170.1 (4)
C4—C5—C6—C8	177.8 (4)	C25—C22—N1—C1	−72.3 (5)
C17—C5—C6—C8	0.5 (6)	C23—C22—N1—Pd1	−85.4 (4)
C5—C6—C7—C2	−6.2 (6)	C24—C22—N1—Pd1	35.3 (4)
C8—C6—C7—C2	178.0 (4)	C25—C22—N1—Pd1	153.0 (3)
C5—C6—C7—C18	171.1 (4)	C13—C15—N2—C26	162.7 (3)
C8—C6—C7—C18	−4.6 (6)	C13—C15—N2—Pd2	−60.0 (4)

C3—C2—C7—C6	6.5 (6)	C29—C26—N2—C15	70.3 (5)
C1—C2—C7—C6	−176.5 (4)	C28—C26—N2—C15	−168.9 (3)
C3—C2—C7—C18	−170.8 (4)	C27—C26—N2—C15	−51.7 (5)
C1—C2—C7—C18	6.2 (6)	C29—C26—N2—Pd2	−63.0 (4)
C7—C6—C8—C9	−44.5 (6)	C28—C26—N2—Pd2	57.8 (4)
C5—C6—C8—C9	139.7 (4)	C27—C26—N2—Pd2	175.0 (3)
C6—C8—C9—C10	136.6 (5)	C1—N1—Pd1—Cl1	117.2 (3)
C6—C8—C9—C14	−47.6 (7)	C22—N1—Pd1—Cl1	−106.5 (3)
C14—C9—C10—C11	2.1 (6)	C1—N1—Pd1—Cl3	−63.7 (3)
C8—C9—C10—C11	178.0 (4)	C22—N1—Pd1—Cl3	72.6 (3)
C14—C9—C10—C20	−174.5 (4)	Pd2—Cl2—Pd1—Cl1	−161.48 (4)
C8—C9—C10—C20	1.4 (6)	Pd2—Cl2—Pd1—Cl3	19.38 (4)
C9—C10—C11—C12	−0.5 (6)	Pd2—Cl3—Pd1—N1	160.38 (10)
C20—C10—C11—C12	176.4 (4)	Pd2—Cl3—Pd1—Cl2	−19.48 (4)
C10—C11—C12—C13	0.4 (6)	C15—N2—Pd2—Cl4	117.0 (2)
C10—C11—C12—C21	−178.0 (4)	C26—N2—Pd2—Cl4	−106.7 (3)
C11—C12—C13—C14	−2.1 (6)	C15—N2—Pd2—Cl2	−63.1 (2)
C21—C12—C13—C14	176.3 (4)	C26—N2—Pd2—Cl2	73.1 (3)
C11—C12—C13—C15	−179.3 (3)	Pd1—Cl3—Pd2—Cl4	−161.03 (4)
C21—C12—C13—C15	−0.9 (6)	Pd1—Cl3—Pd2—Cl2	19.34 (4)
C12—C13—C14—C9	3.8 (6)	Pd1—Cl2—Pd2—N2	157.49 (10)
C15—C13—C14—C9	−179.2 (4)	Pd1—Cl2—Pd2—Cl3	−19.38 (4)

Fig. 1


C17
C20
C8
C5
C9
C10
C4
C6
C11
C3
C14
C7
C18
C2
C12
C16
C19
C13
C21
C1
Cl4
N1
C15
Cl3
N2
C25
C22
C23
Pd1
Pd2
C26
Cl1
Cl2
C27
C24
C28
C29