fondamentalement de celui observé dans le composé $[Cu^{II}(\text{D-pds})]_2.9H_2O$ où les unités de $[Cu^{II}(\text{D-pds})]_2$ constituent des dimères cyclisés.

La cohésion entre les différentes couches est assurée par des liaisons hydrogène mettant en jeu les molécules d'eau de coordination $H_2(OW1)$ et les atomes d'oxygène des groupements carboxylates du ligand, liés entre eux par l'intermédiaire des molécules d'eau de solvatation $H_2(OW2)$ et $H_2(OW3)$ (Fig. 2).

La cohésion cristalline fait également intervenir de nombreuses liaisons de van der Waals.

En conclusion, ce travail a permis la mise en évidence, pour le composé cité en titre, d'une structure polymère en couches assez peu fréquente et l'existence pour le ligand *L* de dix sites de coordination, ce qui paraît également assez exceptionnel. Par ailleurs, les distances Cu—Cu [4,632 (2) Å] sont beaucoup plus courtes que dans $[Cu^{II}(\text{D-pds})]_2.9H_2O$ [6,399 (5) Å], ce qui permet d'envisager la possibilité d'une interaction magnétique indirecte entre les atomes métalliques par l'intermédiaire du pont disulfure.

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Acta Cryst. (1985). C**41**, 1742–1745

Di-μ-chloro-bis[(benzophenone phenylhydrazonido-*N*,*C*)palladium(II)]

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(*Received* 20 *February* 1985; *accepted* 4 *July* 1985)

Abstract. $C_{38}H_{30}Cl_2N_4Pd_2$, $M_r = 826{\cdot}4$, triclinic, $P\bar{1}$, $a = 14{\cdot}068\ (6)$, $b = 12{\cdot}075\ (5)$, $c = 5{\cdot}581\ (4)$ Å, $\alpha = 80{\cdot}73\ (4)$, $\beta = 80{\cdot}46\ (5)$, $\gamma = 60{\cdot}21\ (3)°$, $V = 808{\cdot}0\ (7)$ Å^3, $Z = 1$, $D_m = 1{\cdot}67$, $D_x = 1{\cdot}70\ (1)$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 1{\cdot}29$ mm^{-1}, $F(000) = 412$, $T = 298$ K, $R = 0{\cdot}030$ for 2475 unique observed reflections. The complex molecule is a centrosymmetric di-chloro-bridged dimer with square-planar stereochemistry about each palladium. The Pd—C(σ) and Pd—N bonds are 1·967 (3) and 2·027 (4) Å respectively while the Pd—Cl bridges are asymmetric, 2·460 (1) Å (*trans* to C) and 2·330 (1) Å (*trans* to N) giving a Pd–Pd separation of 3·575 (1) Å.

Introduction. Cyclometalation reactions involving Pt^{II} or Pd^{II} and *N*,*N*-dimethylbenzylamine and certain substituted *N*,*N*-dimethylbenzylamines to form complexes with metal—C(σ) bonds were first described by Cope & Friedrich (1968). The crystal structure of the dimeric complex di-μ-chloro-bis[(azobenzenido-*N*,*C*)-platinum(II)] (1) (Elder, Cruea & Morrison, 1976) and those of the isomeric ring-substituted methoxy analogues of palladium(II) (2),(3),(4) (Barr, Dyke, Smith, Kennard & McKee, 1985) confirmed a *trans* relationship in the benzylamine moieties. Furthermore, with the Pd^{II} isomers, the position of the methoxy substituent in the ring did not result in any structural differences within the Pd_2Cl_2 rhomboid, nor did it

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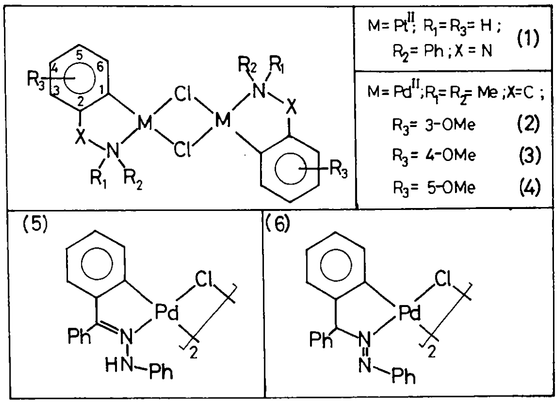
influence the lengths of the Pd—Cl bridge bonds. An analogous system involving the ligand benzophenone phenylhydrazone may undergo cyclopalladation to give either the isomer with the double bond within the chelate ring (*endo*) (5) or *exo* (6) (Cockburn, Howe, Keating, Johnson & Lewis, 1973).



To resolve the ambiguity of this reaction route, the structure of the complex prepared by refluxing benzophenone phenylhydrazone (5·0 mmol) and lithium tetrachloropalladate (5·0 mmol) in methanol was determined. For this compound, $\nu_{\rm NH} = 3250\ {\rm cm}^{-1}$ and $\delta_{\rm NH} = 9{\cdot}95$.

Experimental. Crystals were obtained as large red-brown aggregates from a mixture of methylene chloride and methanol. Although soluble, density was measured by flotation in $CHCl_3/CHBr_3$ mixture. Cleaved fragment (0·26 × 0·26 × 0·22 mm) used to collect intensity data on a Syntex $P\bar{1}$ four-circle diffractometer (graphite-monochromatized radiation), 15 reflections used for lattice-parameter determination; reduced cell: $a = 5{\cdot}581\ (4)$, $b = 12{\cdot}075\ (5)$, $c = 13{\cdot}226\ (6)$ Å, $\alpha = 112{\cdot}61\ (5)$, $\beta = 91{\cdot}67\ (4)$, $\gamma = 99{\cdot}27\ (4)$°; transformation matrix: $00\bar{1}$, 010, $1\bar{1}0$; $2\theta_{\rm max} = 50$°, h, $\pm k$, $\pm l$; standard reflections: I_{300} 1·24 (3) × 10^5, I_{040} 1·31 (8) × 10^5, I_{004} 1·08 (2) × 10^4; 2793 unique reflections collected (79 unobserved) with 2481 having $I > 2{\cdot}5\sigma(I)$ used in structure analysis; no corrections for absorption; reflections $\bar{1}01$, $\bar{2}20$ affected by extinction and removed. Pd atom located by direct methods with *SHELX* (Sheldrick, 1976) and verified in Patterson synthesis, remaining atoms found by difference-Fourier methods. Hydrogens located towards end of refinement and set at fixed positions with $U = 0{\cdot}05$ Å^2. Full-matrix least-squares refinement based on F gave final $R = 0{\cdot}030$ and $wR = 0{\cdot}032$ with $w = 1{\cdot}99/[\sigma^2(F_o) + 2{\cdot}4 \times 10^{-4}(F_o)^2]$; max. and av. Δ/σ 1·9 (scale factor) and 0·71. Final difference electron density max. 0·20, min. −0·16 e Å^{-3}. Scattering factors: for non-hydrogens from Cromer & Mann (1968); for hydrogens from Stewart, Davidson & Simpson (1965). Anomalous-dispersion corrections from Cromer & Liberman (1970). Computer: DEC-10. Atomic coordinates are listed in Table 1, bond distances and angles in Table 2.*

Table 1. *Atomic coordinates* (×10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3; *for* Pd, Cl Å^2 × 10^4)

$U_{\rm eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	$U_{\rm eq}$
Pd	1001·9 (2)	4092·9 (3)	2125·6 (5)	378 (2)
Cl	70 (1)	3681 (1)	−394 (2)	533 (6)
N(12)	1943 (2)	4253 (3)	4289 (6)	39 (2)
N(22)	1804 (3)	5409 (3)	4967 (6)	42 (2)
C(12)	2700 (3)	3202 (3)	5282 (7)	37 (2)
C(1*A*)	1872 (3)	2284 (4)	3335 (7)	38 (2)
C(2*A*)	2699 (3)	2049 (3)	4787 (7)	39 (2)
C(3*A*)	3459 (3)	795 (4)	5526 (8)	48 (2)
C(4*A*)	3390 (4)	−221 (4)	4906 (9)	54 (3)
C(5*A*)	2573 (4)	8 (4)	3546 (10)	61 (3)
C(6*A*)	1819 (3)	1244 (4)	2761 (8)	53 (3)
C(1*B*)	3542 (3)	3137 (4)	6683 (7)	37 (2)
C(2*B*)	4175 (3)	3728 (4)	5709 (7)	45 (2)
C(3*B*)	5014 (4)	3578 (4)	6944 (9)	55 (3)
C(4*B*)	5228 (4)	2867 (5)	9124 (9)	58 (3)
C(5*B*)	4603 (4)	2275 (4)	10127 (8)	52 (3)
C(6*B*)	3772 (3)	2409 (4)	8916 (7)	44 (2)
C(1*C*)	1761 (3)	6346 (4)	3100 (7)	43 (2)
C(2*C*)	2389 (3)	6025 (4)	884 (8)	47 (2)
C(3*C*)	2347 (4)	6989 (5)	−885 (8)	65 (3)
C(4*C*)	1696 (5)	8256 (5)	−478 (11)	74 (3)
C(5*C*)	1085 (4)	8570 (4)	1734 (11)	67 (3)
C(6*C*)	1106 (4)	7640 (4)	3511 (8)	53 (3)

Discussion. The structure determination confirms the chemical reaction route that incorporates the double bond [C(12)=N(12)] in the chelate ring (5) rather than that giving the *exo* isomer (6). Bond distances C(12)=N(12) [1·295 (4) Å] and =N(12)—N(22) [1·416 (6) Å] are comparable with 1·317 (9) and 1·416 (8) Å respectively found in the analogous monomeric complex (acetophenone phenylhydrazonido-*N*,*C*)bromochloropalladium(II) (Dehand, Fischer, Pfeffer, Mitschler & Zinsius, 1976). The complex consists of a centrosymmetric di-chloro-bridged dimer (Fig. 1). The stereochemistry about each Pd is distorted square planar with the C—Pd—N 'bite' angle within the chelate ring contracted to 80·1 (2)°. The Pd—C and Pd—N distances show little variation among dimeric palladium complexes with comparable bonding systems. This point is emphasized by the series of values found for the isomeric mono methoxy substituted di-μ-chloro-bis-[(*N*,*N*-dimethylbenzylamine-*N*,*C*)palladium(II)] complexes (2)–(4) (Barr *et al.*, 1985). The Pd—C, Pd—N and Pd—Cl bond lengths are 1·976 (5), 2·075 (4),

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* Lists of H-atom coordinates, structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42423 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

2·341 (1), 2·471 (1) Å for (2); 1·986 (3), 2·069 (3), 2·334 (2), 2·488 (2) Å for (3); 1·987 (6), 1·967 (6); 2·068 (5), 2·072 (5); 2·337 (2), 2·338 (2); 2·478 (2), 2·466 (2) Å for (4), two values for each. Furthermore, the structure of the analogous Pt^{II} complex (1) (Elder *et al.*, 1976), in which the Pt—C, Pt—N and Pt—Cl bond distances are 1·94, 1·98, 2·33 and 2·46 Å respectively, reflects the similarities between the Pt^{II} and Pd^{II} systems.

Table 2. *Bond distances* (Å) *and angles* (°)

Primed atoms are generated by the inversion operation.

Pd—Cl	2·330 (1)	Pd—C(1*A*)	1·967 (3)
Pd—Cl′	2·460 (1)	Pd—N(12)	2·027 (4)
C(2*A*)—C(12)	1·463 (7)	N(12)—N(22)	1·416 (6)
C(12)—N(12)	1·295 (4)	N(22)—C(1*C*)	1·394 (5)
C(12)—C(1*B*)	1·488 (7)	Pd—Pd′	3·575 (1)

	Ring *A*	Ring *B*	Ring *C*
C(1)—C(2)	1·415 (6)	1·394 (7)	1·383 (6)
C(2)—C(3)	1·394 (6)	1·385 (8)	1·383 (7)
C(3)—C(4)	1·378 (8)	1·355 (7)	1·372 (7)
C(4)—C(5)	1·371 (8)	1·389 (9)	1·372 (7)
C(5)—C(6)	1·384 (5)	1·374 (8)	1·365 (7)
C(6)—C(1)	1·384 (8)	1·389 (7)	1·400 (6)

Cl—Pd—C(1*A*)	94·2 (1)	C(1*A*)—Pd—N(12)	80·1 (2)
Cl—Pd—N(12)	173·8 (1)	C(1A)—Pd—Cl′	176·9 (1)
Cl—Pd—Cl′	83·5 (1)	N(12)—Pd—Cl′	102·1 (1)
C(2*A*)—C(1*A*)—Pd	114·1 (3)	C(12)—N(12)—Pd	117·3 (3)
C(6*A*)—C(1*A*)—Pd	127·4 (3)	N(22)—N(12)—Pd	126·2 (2)
Pd—Cl—Pd′	96·5 (1)		
C(2*A*)—C(1*A*)—C(6*A*)	118·2 (3)	C(2*B*)—C(3*B*)—C(4*B*)	120·8 (5)
C(1*A*)—C(2*A*)—C(3*A*)	120·1 (4)	C(3*B*)—C(4*B*)—C(5*B*)	119·7 (5)
C(1*A*)—C(2*A*)—C(12)	114·5 (3)	C(4*B*)—C(5*B*)—C(6*B*)	120·2 (5)
C(3*A*)—C(2*A*)—C(12)	125·4 (4)	C(5*B*)—C(6*B*)—C(1*B*)	120·8 (5)
C(2*A*)—C(3*A*)—C(4*A*)	120·2 (5)	C(12)—N(12)—N(22)	116·3 (4)
C(3*A*)—C(4*A*)—C(5*A*)	119·6 (4)	N(12)—N(22)—C(1*C*)	117·4 (3)
C(4*A*)—C(5*A*)—C(6*A*)	121·2 (5)	N(22)—C(1*C*)—C(2*C*)	121·4 (3)
C(5*A*)—C(6*A*)—C(1*A*)	120·6 (5)	N(22)—C(1*C*)—C(6*C*)	119·4 (3)
C(2*A*)—C(12)—N(12)	113·6 (4)	C(2*C*)—C(1*C*)—C(6*C*)	119·2 (4)
C(2*A*)—C(12)—C(1*B*)	122·0 (3)	C(1*C*)—C(2*C*)—C(3*C*)	119·3 (4)
C(1*B*)—C(12)—N(12)	124·3 (4)	C(2*C*)—C(3*C*)—C(4*C*)	121·2 (4)
C(12)—C(1*B*)—C(2*B*)	120·9 (3)	C(3*C*)—C(4*C*)—C(5*C*)	119·3 (5)
C(12)—C(1*B*)—C(6*B*)	120·8 (4)	C(4*C*)—C(5*C*)—C(6*C*)	120·9 (4)
C(2*B*)—C(1*B*)—C(6*B*)	118·2 (4)	C(5*C*)—C(6*C*)—C(1*C*)	120·2 (4)
C(1*B*)—C(2*B*)—C(3*B*)	120·4 (4)		

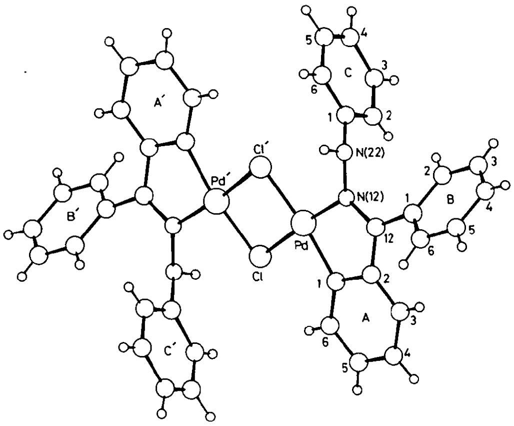

Fig. 1. Molecular configuration and atom numbering scheme. Primed atoms are generated by an inversion operation.

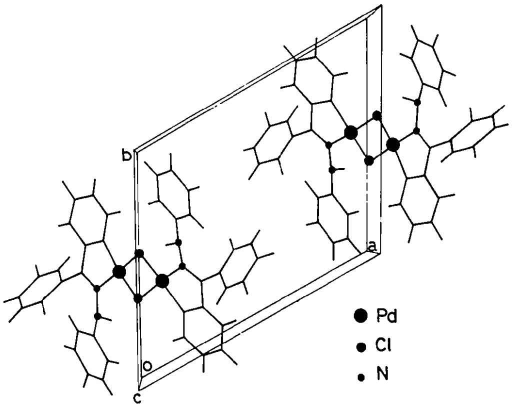

Fig. 2. Packing in the unit cell viewed down the *c* axis.

There is evidence of the *trans* effect in all of these examples where the Pd—Cl bond *trans* to Pd—C is substantially elongated relative to the one *trans* to the Pd—N bond. This is consistent with the greater *trans* influence of the Pd—C *cf.* Pd—N bond (Appleton, Clark & Manzer, 1973). In the monomeric benzylamine complex (*N*)benzylidenebenzylaminido-*N*,C)(2,4-pentanedionato)palladium(II) (Clark, Dyke, Smith & Kennard, 1985), the Pd—C and Pd—N bond distances [1·955 (7), 2·008 (5) Å respectively] are also comparable with those for the dimer (5), indicating that the presence of the double bond within the chelate results in only a slight strengthening of the Pd—N bond. The five-membered chelate ring (ring 1), the phenyl ring *A* (ring 2), the bridge chlorines and the atoms C(1*B*), N(22) and C(1*C*) of the substituent phenyl and benzyl groups are essentially planar, maximum deviation from the least-squares plane being 0·22 Å [N(22)]. The torsion angle between ring 1 and ring 2 is 4·5 (1)°. The packing of the complex in the unit cell (Fig. 2) involves discrete dimers with no significant intermolecular associations.

The authors thank the Queensland Institute of Technology and the Universities of Queensland and Western Australia for support. The Johnson Matthey Research Centre is thanked for providing the sample of palladium chloride.

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Acta Cryst. (1985). C**41**, 1745–1748

Structure of a Red Macrocyclic Ligand Complex*

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(*Received* 11 *March* 1985; *accepted* 20 *August* 1985)

Abstract. (1*RS*,4*RS*,5*SR*,7*RS*,8*SR*,11*SR*,12*RS*,14*SR*)-5,7,12,14-Tetraethyl-7,14-dimethyl-1,4,8,11-tetraazacyclotetradecane)copper(II) diperchlorate, $[\mathrm{Cu(C_{20}H_{44}N_4)}](\mathrm{ClO_4})_2$, $M_r = 603{\cdot}00$, orthorhombic, *Pbca*, $a = 14{\cdot}516$ (6), $b = 11{\cdot}674$ (7), $c = 16{\cdot}225$ (9) Å, $V = 2749{\cdot}5$ (3) Å^3, $Z = 4$, $D_m = 1{\cdot}47$ (3) (by flotation in $\mathrm{CCl_4}$/hexane mixture), $D_x = 1{\cdot}457$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 1{\cdot}070$ mm^{-1}, $F(000) = 1278$, $T = 296$ (4) K, $R(F) = 0{\cdot}069$ for 1516 observed reflections. The coordination about Cu$^{\mathrm{II}}$ is a tetragonally distorted centrosymmetric octahedron, with the macrocyclic ligand equatorial and the perchlorate ions axial. This complex has the 1*RS*, 4*RS*, 8*SR*, 11*SR* configuration at the chiral nitrogen centers; the six-membered chelate rings exhibit chair forms and the five-membered rings take *gauche* forms.

Introduction. The macrocyclic ligand (5*SR*,7*RS*,12*RS*,14*SR*)-5,7,12,14-tetraethyl-7,14-dimethyl-1,4,8,11-tetraazacyclotetradecane, $\mathrm{Et_4Me_2}$[14]aneN$_4$, takes a variety of isomeric forms with transition-metal ions that exhibit a number of features that are of particular stereochemical interest. In a previous paper we have reported the crystal structure of a nickel(II) complex of this ligand (Lee, Lu, Liang, Chung & Lee, 1981). In this study, the title compound, $[\mathrm{Cu(Et_4Me_2}[14]\mathrm{aneN_4})](\mathrm{ClO_4})_2$ has been synthesized and the three-dimensional structure determination by X-ray diffraction has been completed.

Experimental. *C-meso*-5,7,12,14-Tetraethyl-7,14-dimethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene dihydroperchlorate prepared with procedure described by Curtis (1974). 50 g of this compound added to 500 ml methanol and stirred until completely dissolved, then 10 g sodium borohydride added slowly. Solution stirred continuously for 2 h until no more bubbles occurred. 500 ml water added to solution and stirred again until room temperature reached. Solution cooled overnight to precipitate white product, $\mathrm{Et_4Me_2}$[14]aneN$_4$, which was filtered, washed with water, and then recrystallized from methanol–water mixture. Copper(II) perchlorate (2·0 g) and $\mathrm{Et_4Me_2}$[14]aneN$_4$ (2·0 g) mixed in 200 ml 50% (by weight) methanol–water mixture. Solution of sodium hydroxide (10 ml of 1·0 *M*) added. After 4 h, sodium perchlorate monohydrate added. Red crystals of $[\mathrm{Cu(Et_4Me_2}[14]\mathrm{aneN_4})](\mathrm{ClO_4})_2$ filtered, washed with water, recrystallized from methanol–water mixture (50% by weight), and dried in vacuum oven at 323 K (Juang, 1984).

Experimental data and structure solution parameters together with the standard refinement procedures are listed in Table 1. In the last stage of least-squares refinement with coordinates and anisotropic temperature factors for non-hydrogen atoms, $R(F) = 0{\cdot}096$. The four perchlorate O atoms were disordered and each O atom is located at two positions with populations $P_{\mathrm{O(1)}} = P_{\mathrm{O(2)}} = P_{\mathrm{O(3)}} = P_{\mathrm{O(4)}} = 0{\cdot}81$ and $P_{\mathrm{O(1}A)} = P_{\mathrm{O(2}A)} = P_{\mathrm{O(3}A)} = P_{\mathrm{O(4}A)} = 0{\cdot}19$ respectively. With positions and isotropic temperature factors of these four additional oxygens included in the subsequent calculation, $R(F)$ reduced to 0·084. All 22 H atoms located in difference Fourier map. Temperature factors of H atoms assigned according to $B_{\mathrm{H}} = B_n + 1$, where n is atom to which H is bonded (Fawcett, Rudich, Toby, Lalancette, Potenza & Schugar, 1980). With these isotropic temperature factors and coordinates of H atoms refined in last cycle of least-squares calculation, $R(F)$ reduced to 0·069.

Discussion. The atomic coordinates and temperature factors are listed in Table 2.† A perspective view of the molecule with the numbering scheme and the deviations of the atoms from the plane through Cu, N(1) and N(2) are shown in Fig. 1. The bond distances and angles are listed in Table 3.

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* Work supported by the National Science Council Grant NSC73-0208-M007-23, Taiwan.

† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42442 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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